GENMOD1.0 README

June 1, 2018

1 Introduction

This file describes software of the General Groundwater-Model (General Models) Construction System Version 1.0 (Genmod1.0; Starn and others, 2018). This readme file briefly describes the required input, dependencies, output, and order of processing, from Jupyter Notebooks (JN) for the creation of MODFLOW groundwater flow models created using Genmod1.0, which then can be used in a separate series of JN to create and process groundwater residence time distributions (GRTD). A user guide, software, and data supporting this work is available through the Science Base catalog of the U.S. Geological Survey at https://doi.org/10.5066/F72V2FDC (Starn and others, 2018).

A user is encouraged to read the user guide report available at: https://doi.org/10.5066/F72V2FDC before attempting to run the JN of Genmod1.0.

More information is available in the user guide report for Genmod1.0 available at: https://doi.org/10.5066/F72V2FDC and jupyter notebooks [JN] and supporting files are available at https://github.com/usgs/gw-general-models.git. The user guide for Genmod1.0 documents subsequent revisions and improvements to the JN of Genmod0.1 (Starn and Carlson, 2018) that were used to generate 30 general models from which GRTD were determined in the work of Starn and Belitz (2018).

As described below, the JN of Genmod1.0 function with input datasets that cover the Glacial Aquifer System within the conterminous United States. The extent is that covered by the Glacial Environments and Surficial Sediments dataset also described below. Some input data sets do not include features in Canada. With some modification, input datasets covering an area of interest outside of the Glacial Aquifer System can be used by Genmod1.0.

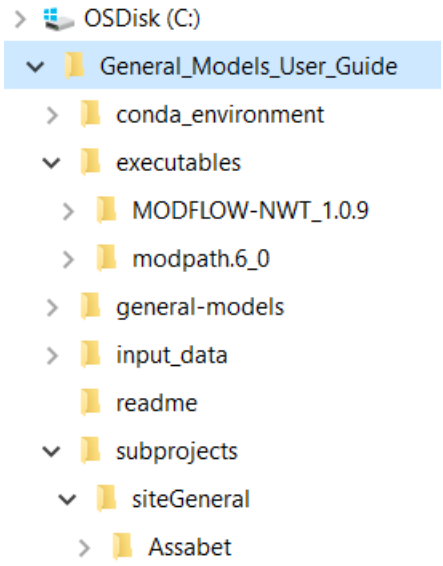
Once downloaded, zipped files denoted by the extension ".7z" can be unzipped using right-click and selecting "7-Zip" and "extract here" on each ".7z" file.

1.1 Disclaimer

This software is subject to revision. It is being provided to meet the need for timely best science. No warranty, expressed or implied, is made by the USGS or the U.S. Government as to the functionality of the software and related material nor shall the fact of release constitute any such warranty. The software is provided on the condition that neither the USGS nor the U.S. Government shall be held liable for any damages resulting from the authorized or unauthorized use of the software.

1.2 Folder structure

The following folder structure is used to organize JN and supporting files and is used for pathnames specified in MS (see below). "Assabet" is used as an example model.



1.3 Input

1.3.1 Provided in/input_data; see links for downloading datasets below and in file **MS** described further below. Also see compressed file `input_data.7z` that serves as a template with empty folders of the folder structure and folder names for the user to populate with the required input data. Folder path and names of datasets used as input to JN are listed below.

- **/Geology –** A geodatabase of the Glacial Environments and Surficial Sediments (GESS) data that includes a polygon file with multiple attributes which describe the lithology, geomorphology, and related depositional environment of Quaternary-age surfical sediments in the glaciated conterminous United States. Where geologic units were mapped to either fine (`CrseStratSed = 0`) or coarse (`CrseStratSed = 1`) sediments. https://doi.org/10.5066/F71R6PQG

  `/Geology/GESS_poly.gdb`

- **/NHDPlusV2Data** -- National Hydrography Dataset (NHD), the National Elevation Dataset (NED), and the Watershed Boundary Dataset (WBD); includes `NHDflowline.shp` and `NHDWaterbody.shp`; contains Hydrologic Unit Codes (HUC); and available at http://www.horizon-systems.com/NHDPlus/index.php (overall description) and http://www.horizon-systems.com/NHDPlus/NHDPlusV2_01.php (specific vector processing unit [VPU] for the example model). `NHDPlusNE/NHDPlus01` are specific to the location of the Assabet example model. The location for another model may differ.

  `/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NEDSnapshot/Ned01a/elev_cm`

  `/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDPlusCatchment/cat`

  `/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDSnapshot/Hydrography/NHDFlowline.shp`

/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDSnapshot/Hydrography/NHDWaterbody.shp

/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDPlusAttributes/PlusFlowlineVAA.dbf

/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDSnapshot/NHDFCode.dbf

/NHDPlusV2Data/NHDPlusNE/NHDPlus01/NHDPlusAttributes/ElevSlope.dbf

/NHDPlusV2Data/NHDPlusNE/NHDPlus01/WBDSnapshot/WBD/WBD_Subwatershed.shp

- **/NLCD/nlcd_2011_landcover_2011_edition_2014_10_10** -- land cover written to **MGCSV0** (see below) in JN1 and used in GRTD; available at https://www.mrlc.gov/nlcd11_data.php

  /NLCD/nlcd_2011_landcover_2011_edition_2014_10_10/nlcd_2011_landcover_2011_edition_2014_10_10.img

- **/recharge_Reitz/2013** -- used for recharge; available at https://www.sciencebase.gov/catalog/item/55d383a9e4b0518e35468e58

  /recharge_Reitz/2013/RC_eff_2013.tif

- **/recharge_Wolock** -- alternative source for recharge; available at https://water.usgs.gov/lookup/getspatial?rech48grd

  /recharge_Wolock/rech48grd

- **/Soller/sim3392_spatialdata/sim3392_sheet1** -- thickness of surficial sediments; available at https://doi.org/10.3133/sim3392

  /Soller/sim3392_spatialdata/sim3392_sheet1/sim3392_sheet1_driftthickness.img

- **/Soller/sim3392_spatialdata/sim3392_sheet2** -- bedrock surface elevation; available at https://doi.org/10.3133/sim3392

  /Soller/sim3392_spatialdata/sim3392_sheet2/sim3392_sheet2_bedrocktopo.img

1.4 Dependencies

1.4.1 Provided in /conda_environment; see compressed file conda_environment.7z

- **I** -- Instructions+for+installing+Python.html file containing instructions for installation of python and creation of Conda environment using E
- **E** -- explicit-spec-file.txt specification file used to create Conda environment and enable use of Jupyter to run JN

1.4.2 Provided in /executables; see compressed file executables.zip

- **MF** -- /MODFLOW-NWT_1.0.9 folder of executable version of MODFLOW used in JN
- **MP** -- /modpath.6_0 folder of executable version of MODPATH used in JN

1.4.3 Provided in /general-models; see compressed file general-models.zip

- **MFG** -- /MFGrid folder with python grid feature used in JN1
- **GMD** -- gen_mod_dict.py supporting file used by JN; contains default as well as scenario and model specific values for input variables. Most values require no change, except "scen =" which defines the scenario. Default is "scen =3" which defines a model with 3 surficial

layers underlain by a bedrock layer. See included comments for explanation

- **MS** -- model_specs.py supporting file used by JN; contains pathnames for data sources and executable files used by JN
- **JN0** -- UserGuide_General_Model_0_Create_Domain_Shapefile0.ipynb JN used to create W and LM (see below)
- **JN1** -- UserGuide_General_Model_1_Geospatial_processing_v2.0_GESS.ipynb JN that use W to determine the extent and orientation of a model grid and then process the many input datasets to each model cell in that grid; the individual attributes are then summarized and saved in tabular file **MGCSV0** -- model_grid.csv (see below) used in later JN
- **JN2** -- UserGuide_General_Model_2_Generate_Observations_GESS.ipynb an optional JN used to make observation files; it is not necessary to run JN2 for this series of JN; observations added as new columns to MGCSV0;
- **JN3** -- UserGuide_General_Model_3_Create_the_Model--Multi_layer_GESS.ipynb JN that creates a preliminary MODFLOW model
- **JN4** -- UserGuide_General_Model_4_Calibrate_Model-Kv-PP.ipynb JN that creates a calibrated MODFLOW model from the result of JN3. Run-time for JN4 could be quite long depending on model complexity. See the user guide for more information

1.5 Output

1.5.1 Created in /subprojects/siteGeneral; see compressed file subprojects.7z

- **SG** -- /{} where curly braces {} represent a folder named from the model name (for example 'Assabet'); folder that contains each MODFLOW model created from running JN0 through JN4

1.5.2 Created in JN0 and written to SG

- **W** -- {}_domain.shp polygon shapefile of the model domain (watershed) boundary that contains a field named "ibound" with a value of one; shapefile of watershed boundary used to create a General Model; where {} is the name of the surface water feature used to select HUC watersheds where the overall outline of those selected will become the model domain boundary
- **LM** -- {}.html Leaflet map in html format of the model domain; where {} is identical to that in W; an optional feature

1.5.3 Created in JN1 and written to SG

- **MGCSV0** -- model_grid.csv tabular file where individual attributes of the model grid are summarized and saved
- {}.tif -- tif image files of all attribute fields found in MGCSV0 where {} represents each field name
- **DOM** -- domain_outline.shp shape file of the model domain (watershed) boundary; same as W but with a general filename
- **CBOX** -- clip_box.shp shape file of the bounding box that contains the model domain extent; used to clip larger datasets
- **LKS** -- lakes.shp shape file of all lake polygons in the model domain clipped from NHDWaterbody.shp for the model area
- **NHDC** -- NHD_clip.shp shape file of all stream segments in the model domain clipped from NHDflowline.shp for the model area

- **GS** -- grid_spec.txt file of resulting attributes of the model grid

1.5.4 Optional tif images created in JN2 and written to SG

- **CRSG** -- coarse_grp.tif
- **HQ** -- hypo_quant.tif
- **PCRS** -- pct_coarse.tif
- **SO** -- stream_obs.tif
- **TQ** -- top_quant.tif

1.5.5 Created in JN3 and written to SG/layers

- **LAY** -- SG/layers folder for the layers scenario as specified in GMD where MODFLOW input files created by JN3 for this preliminary General Model are written
- **PH** -- pre-heads.tif tif image of pre-calibration head values
- **MGCSV1** -- model_grid.csv tabular file MGCSV0 updated with head and hydraulic conductivity model grid attributes from the upper-most layer for the preliminary General Model
- **ZA** -- zone_array.npz zone array for hydraulic conductivity values to be used in the calibration process JN4
- **ERM** -- {}_layers_error_map.png image file for map of model errors for the preliminary General Model; where {} is the model name found in SG
- **XS** -- {}_layers_xs.png image file of model cross section showing model layering and hydraulic conductivity values along a particular row for the calibrated General Model; where {} is the model name found in SG
- **AR** -- LAY/arrays folder of data arrays made by JN3 for input to the General Model such as bottom elevation, hydraulic conductivity, ibound, starting head, and vertical anisotropy values by layer; also distance along rows and columns, top of model surface, recharge, drain, and river arrays

1.5.6 Created in JN4 and written to SG/layers_cal_wt_1.00

- **LAYCAL**-- SG/layers_cal_wt_1.00 folder for contents of LAY copied here by JN4; MODFLOW input files are updated and reflect the calibrated General Model; certain other copied files remain unaltered
- **PARCSV** -- par.csv summary tabular file of parameter combinations of both broad order-of-magnitude estimates and refined estimates from the calibration process; the "best" parameter set is indicated by "low_diff" on the corresponding line in the "Best" column; due to non-uniqueness in parameter sets there may be alternative parameters sets that are as good as the "best" set; check par.csv to investigate these alternatives
- **ERMC** -- {}_layers_error_map_cal.png image file for map of model errors for the calibrated General Model; where {} is the model name found in SG
- **XSC** -- {}_layers_xs_cal.png image file of model cross section showing model layering and hydraulic conductivity values along a particular row for the calibrated General Model; where {} is the model name found in SG
- **MB** -- mf.bat batch file for repeated running of MODFLOW during the calibration process
- **ARC** -- LAY/arrays folder of data arrays updated from AR by JN4 for input to the final calibrated General Model

2 Conda environment

A conda environment is a self-contained folder located on a local computer system that consists of a version of Python and specific versions of any number of different Python packages and their dependencies. It is therefore possible that many such environments, each for a different purpose, could be maintained and run on a local computer system without interference with one another. An environment is identified by the name given to it. The JN of the General Groundwater-Model Construction System Version 1.0 use specific versions of various Python packages.

Refer to instruction file I and specification file E in section 1.4.1 to create a conda environment with the specified Python packages and install the jupyter notebook. Specification file E contains links to versions of the packages that work with the notebooks; more recent versions will probably work.

2.1 Input

- **I**
- **E**

3 Genmod JNs

To begin the General Groundwater-Model Construction System Version 1.0 (Genmod1.0), start the conda environment with the following procedure. Open a command window at `C:\General_Models_User_Guide\general-models`. Type "activate myenvironment", where "myenvironment" is the name given to the conda environment. Then type "jupyter notebook" to start the jupyter notebook. A "Home" folder will open which lists the notebooks in the `general-models` folder. By clicking on the name of each JN, each will open in a separate jupyter notebook window.

3.1 Run sequence of JN for a new model (when W does not exist)

- **JN0**
- **JN1**
- **JN2; optional**
- **JN3**
- **JN4**

3.2 Run sequence of JN for an existing model (when W exists or when changes are to be made to a model)

- **JN1**
- **JN2; optional**

- **JN3**
- **JN4**

4 Running JN0

JN0 is intended to be run one cell at a time when creating a new groundwater model because of the interactive selection procedure for the Hydrologic Unit Codes.

The user may have to change the pathname for the variable "nhd_dir =" in the second code cell to reflect the location of the `General_Models_User_Guide` folder in the users system (for example, `C:/General_Models_User_Guide/input_data/NHDPlusV2Data`). While "nhd_basin_dir =" reflects folder names of datasets that correspond to the geographic location of the example model domain (the example model named `Assabet` is located in the `NHDPlusNE/NHDPlus01` area, and the river name `Concord` is used to find the relevant HUC number[s]), these may be customized to reflect datasets for another area. Example input values for "bname = `'Concord'` " (name[s] of the river[s] of interest within the intended model domain) and "WS = ['01070005']" (the HUC number[s] for the basin[s] of interest whose overall boundary will form the model domain) are specified, but must be changed to reflect those for a new model domain of interest.

Use the following information to create a new model (the example model `Assabet` is used to illustrate the procedure). After JN0 has run, make a new folder in `C:\General_Models_User_Guide\subprojects\siteGeneral` and name it `Assabet`. Then move the html file (`Concord.html`) and all of the files associated with the newly created domain shapefile `Concord_domain.shp` from `C:\General_Models_User_Guide\general-models` into the new `C:\General_Models_User_Guide\subprojects\siteGeneral\Assabet` folder. This will position the files for use in the following JN. A new dictionary entry will have to be made in GMD to reflect this new model. See the example for "`model_dict['Assabet']`" in GMD.

4.1 Output

- See section 1.5

5 Running JN1 through JN4

JN1 through JN4 are run one cell at a time (keyboard shortcut, "shift"-"enter") until a dropdown list of model names appears after code cell three is run. This list results from the model-specific dictionaries found in GMD. A name is then selected by the user and after clicking in the next cell below, the remainder of the JN can be run with the "Run All Below" command.

5.1 Output

- See section 1.5

6 References

- Starn, J.J. and Belitz, K., 2018, Regionalization of groundwater residence time using metamodeling. Water Resources Research. Accepted Author Manuscript. doi:10.1029/2017WR021531. [Also available at: https://doi.org/10.1029/2017WR021531]

- Starn, J.J. and Carlson, C.S., 2018, Supporting Datasets Used in the General Groundwater-Model Construction System Version 0.1: U.S. Geological Survey preliminary software release, https://doi.org/10.5066/F7FQ9VTD

- Starn, J.J., Carlson, C.S., and Kauffman, L.J., 2018, Genmod1.0—User Guide for the General Groundwater-Model (General Models) Construction System Version 1.0: U.S. Geological Survey software release, https://doi.org/10.5066/F72V2FDC