“Hands On” Exercise
Calibration of the PSRP SWPF model
ERDC FIRO Project Meeting WPB

Purpose

The purpose of this exercise is to introduce the calibration process in the HPC system for a given GSSHA H&H model. In this exercise, a five parameter calibration for the Picayune Strand South West Protection Features (PSRP-SWPF) long term model will be used. The following step-by-step instructions describe the process of generating PEST related input files and PBS scripts for a model calibration in TOPAZ.

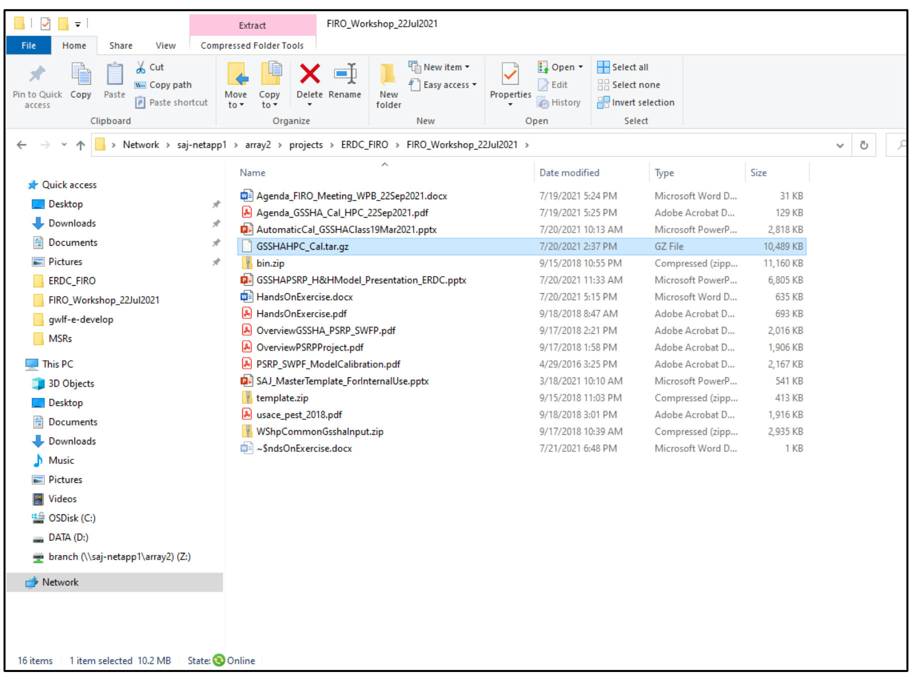
(Note: PEST and GSSHA V7.142 were compiled on ONYX for this workshop.)

1. System Log-on

- Log-in to the ONYX HPC system via Kerberos (CAC Card or YUB KEY).

2. File Uploading and unzipping

- Using the psftp application under “C:\Program Files (x86)\HPCMP Kerberos\psftp.exe” upload the file to your ONYX “workspace” (/p/work/”username”)
    - GSSHAHPC_Cal.tar.gz



- “unzip” and “untar” the uploaded file with:
    - tar -xzvf GSSHAHPC_Cal.tar.gz
- This creates all the sub-directories and necessary files for the PSRP GSSHA model, including the project file. The “template” directory contains the PEST files to be used for the PEST process and the “CommonGSSHAInput” directory contains all the GSSHA input files. The “bin” directory contains all the necessary executable and script files.

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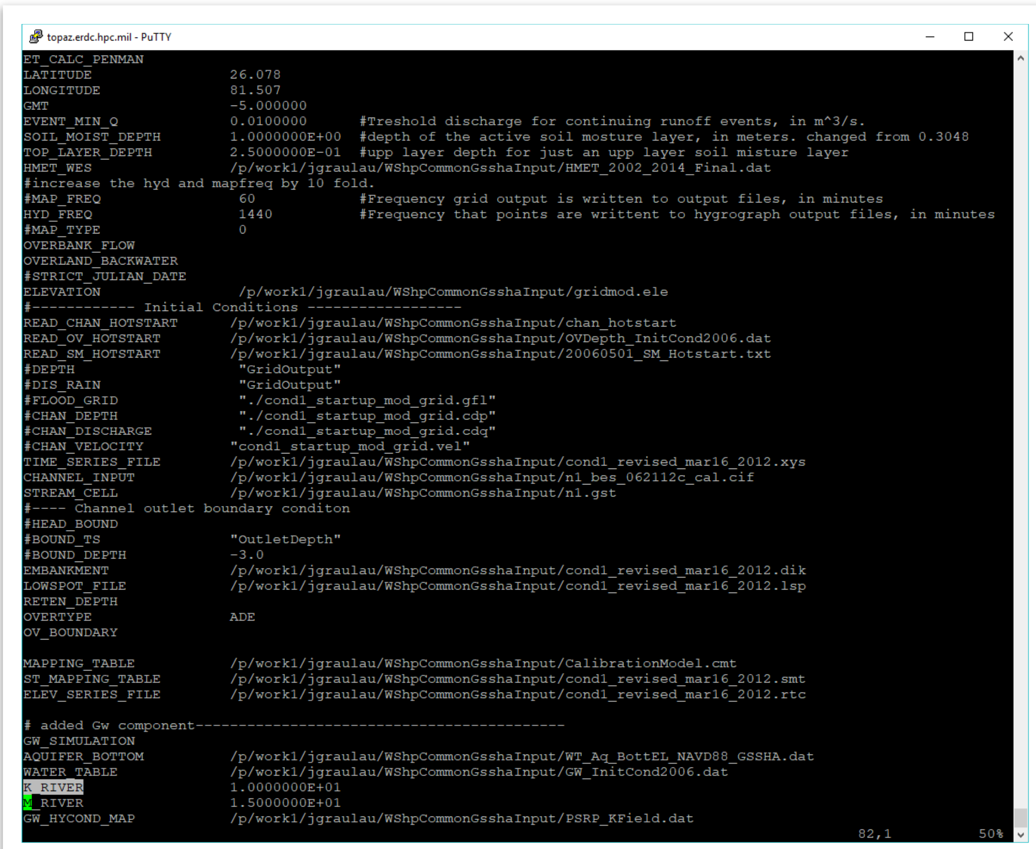
3. PEST GSSHA model template file

- Navigate to the “template” directory and create a sub-directory named “template_files”
- From the directory “CommonGSSHAInput” copy the file “CalibrationModel.prj” into the “template_files” sub-directory
- Five parameters in this file will be used as calibration parameters
  - SINGLE_UNSAT_SAT
  - SOIL_MOIST_DEPTH
  - TOP_LAYER_DEPTH
  - K_RIVER
  - M_RIVER



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```
ET_CALC_PENMAN
LATITUDE                26.078
LONGITUDE               81.507
GMT                     -5.000000
EVENT_MIN_Q             0.0100000      #Treshold discharge for continuing runoff events, in m^3/s.
SOIL_MOIST_DEPTH        1.0000000E+00  #depth of the active soil mosture layer, in meters. changed from 0.3048
TOP_LAYER_DEPTH         2.5000000E-01  #upp layer depth for just an upp layer soil misture layer
HMET_WES                /p/work1/jgraulau/WShpCommonGsshaInput/HMET_2002_2014_Final.dat
#increase the hyd and mapfreq by 10 fold.
#MAP_FREQ                60            #Frequency grid output is written to output files, in minutes
HYD_FREQ                 1440          #Frequency that points are writtent to hygrograph output files, in minutes
#MAP_TYPE                0
OVERBANK_FLOW
OVERLAND_BACKWATER
#STRICT_JULIAN_DATE
ELEVATION                /p/work1/jgraulau/WShpCommonGsshaInput/gridmod.ele
#------------ Initial Conditions ------------------
READ_CHAN_HOTSTART      /p/work1/jgraulau/WShpCommonGsshaInput/chan_hotstart
READ_OV_HOTSTART        /p/work1/jgraulau/WShpCommonGsshaInput/OVDepth_InitCond2006.dat
READ_SM_HOTSTART        /p/work1/jgraulau/WShpCommonGsshaInput/20060501_SM_Hotstart.txt
#DEPTH                   "GridOutput"
#DIS_RAIN                "GridOutput"
#FLOOD_GRID              "./cond1_startup_mod_grid.gfl"
#CHAN_DEPTH              "./cond1_startup_mod_grid.cdp"
#CHAN_DISCHARGE          "./cond1_startup_mod_grid.cdq"
#CHAN_VELOCITY          "cond1_startup_mod_grid.vel"
TIME_SERIES_FILE        /p/work1/jgraulau/WShpCommonGsshaInput/cond1_revised_mar16_2012.xys
CHANNEL_INPUT           /p/work1/jgraulau/WShpCommonGsshaInput/n1_bes_062112c_cal.cif
STREAM_CELL             /p/work1/jgraulau/WShpCommonGsshaInput/n1.gst
#---- Channel outlet boundary conditon
#HEAD_BOUND
#BOUND_TS               "OutletDepth"
#BOUND_DEPTH            -3.0
EMBANKMENT              /p/work1/jgraulau/WShpCommonGsshaInput/cond1_revised_mar16_2012.dik
LOWSPOT_FILE            /p/work1/jgraulau/WShpCommonGsshaInput/cond1_revised_mar16_2012.lsp
RETEN_DEPTH
OVERTYPE                ADE
OV_BOUNDARY

MAPPING_TABLE           /p/work1/jgraulau/WShpCommonGsshaInput/CalibrationModel.cmt
ST_MAPPING_TABLE        /p/work1/jgraulau/WShpCommonGsshaInput/cond1_revised_mar16_2012.smt
ELEV_SERIES_FILE        /p/work1/jgraulau/WShpCommonGsshaInput/cond1_revised_mar16_2012.rtc

# added Gw component-------------------------------------------
GW_SIMULATION
AQUIFER_BOTTOM          /p/work1/jgraulau/WShpCommonGsshaInput/WT_Aq_BottEL_NAVD88_GSSHA.dat
WATER_TABLE             /p/work1/jgraulau/WShpCommonGsshaInput/GW_InitCond2006.dat
K_RIVER                 1.0000000E+01
M_RIVER                 1.5000000E+01
GW_HYCOND_MAP           /p/work1/jgraulau/WShpCommonGsshaInput/PSRP_KField.dat
                                                                            82,1          50%
```

- Edit the “CalibrationModel.prj” file using and editor such as EMACS, or Vim and insert a line at the top of the file and type “ptf @”. This instructs PEST that this file is a pest template file.
- Locate the following fields in the “CalibrationModel.prj file and replace the parameter values as below:
  - SINGLE_UNSAT_SAT @SGL_UNS_SAT@
  - SOIL_MOISTURE_DEPTH @S_MOIST_DEP@
  - TOP_LAYER_DEPTH @T_LAYER_DEP@
  - K_RIVER @ K_RIVER @

  - M_RIVER @ M_RIVER @

- Replace all reference links in this file pointing to “jgraulau” to your ONYX username.
- Save this file as “CalibrationModel.prj.tpl” in the “template_files” sub-directory

4. PEST Control and Instructions File

- In the “template” directory, the “PESTControlFile.pst” is the PEST control file that will be modified in this exercise.
- Open this file in a text editor (e.g., EMACS, Vim)

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```
pcf
* control data
restart  estimation
            5      132    2    0     27
            1      1 single point   1    0    0
          20.0    -2.0    0.3   0.03   5 999 LAMFORGIVE DERFORGIVE
          5.0    5.0 0.001   0
          0.1
           10   0.005      3      3   0.01      3
            1      1      1      1
* singular value decomposition
        2
        5 1.0e-7
        1
* parameter groups
ParGroup1  relative     0.05  0  switch  2  parabolic
ParGroup2  relative     0.05  0  switch  2  parabolic
...
...
...
ParGroupN  relative     0.05  0  switch  2  parabolic
* parameter data
param1   log factor   0.500000    0.001   1.0000    ParGroup1   1.0   0    1
param2   log factor   1.000000    0.001   2.0000    ParGroup2   1.0   0    1
...
...
...
paramN   log factor   0.250000    0.001   0.5000    ParGroupN   1.0   0    1
* observation groups
ObsGp1
ObsGp2
...
...
...
ObsGpN
* observation data
obs1     1.0560       0.50    ObsGp1
obs2     1.0468       0.50    ObsGp2
...
...
...
obsN     1.0468       0.50    ObsGpN
* model command line
./run_my_model.sh
* model input/output
./template_files/GSSHA_template.tpl GSSHAInput/GSSHA.prj
Instructions.ins PostProcessing.out
* prior information
++ AUTO_NORM(4)
~
                                                        1,1           All
```

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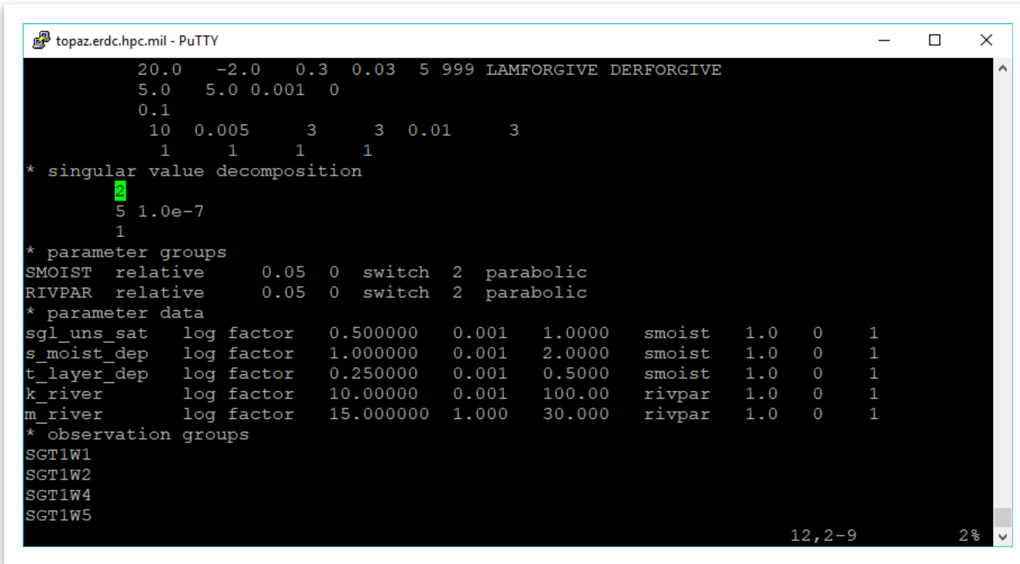
Lines that start with “*” represent sections that instruct and control the PEST parameter estimation, sensitivity, optimization, and other user selected processes.

- “* control data” and “* singular value decomposition”: In this exercise, these sections will be used as-is. Only one parameter in the “control data” section will be modified.
- “*parameter groups” and “*parameter data”: Edit these sections as shown in the screenshot below. Ensure the name of the parameters in the “*parameter data” section match the name of the parameters in the “CalibrationModel.prj.tpl” file created previously.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```
          20.0   -2.0   0.3  0.03  5 999 LAMFORGIVE DERFORGIVE
          5.0   5.0 0.001  0
          0.1
           10  0.005     3     3  0.01     3
            1     1     1     1
* singular value decomposition
        2
        5 1.0e-7
        1
* parameter groups
SMOIST  relative     0.05  0  switch  2  parabolic
RIVPAR  relative     0.05  0  switch  2  parabolic
* parameter data
sgl_uns_sat   log factor  0.500000   0.001   1.0000   smoist   1.0   0    1
s_moist_dep   log factor  1.000000   0.001   2.0000   smoist   1.0   0    1
t_layer_dep   log factor  0.250000   0.001   0.5000   smoist   1.0   0    1
k_river       log factor  10.00000   0.001   100.00   rivpar   1.0   0    1
m_river       log factor  15.000000  1.000   30.000   rivpar   1.0   0    1
* observation groups
SGT1W1
SGT1W2
SGT1W4
SGT1W5
                                                                 12,2-9         2%
```

- “* observation groups”: Edit this section to include the following labels:
  SGT1W1
  SGT1W2
  SGT1W4
  SGT1W5
  SGT2W1
  SGT2W2
  SGT2W3
  SGT2W4
  SGT2W5
  SGT2W6
  SGT3W1
  SGT3W2
  SGT3W3
  SGT3W4
  SGT3W5
  SGT3W6
  SGT3W7
  SGT4W1
  SGT4W2

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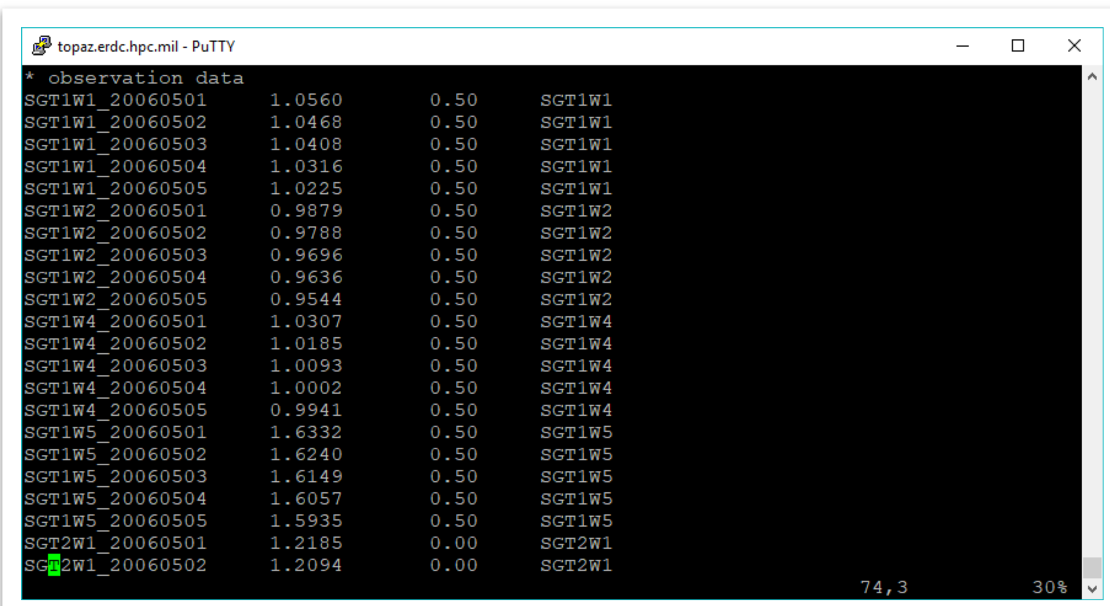
SGT4W3
SGT4W4
SGT4W5
SGT4W6
SGT5W1
SGT5W2
SGT5W3
MASS

These labels represent the way in which the historical groundwater level data will be grouped for the purpose of the PEST estimation process.

- “* observation data”: This section includes the historical observations PEST will use to compare GSSHA generated outcomes during the estimation process. In the PSRP-SWPF model, there are a total of 26 observation wells with daily stage data collected over the last 10+ years. For the purpose of this exercise, groundwater level data collected for the 5-day period between May 1, 2006 and May 5, 2006 will be used. The file “ObsData.dat” has been created and already includes the historical observation data to be included in the PEST control file. Copy the contents of the “ObsData.dat” into the PEST control file “*observation data” section. This section shall look as shown in the screenshot below.



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```
* observation data
SGT1W1_20060501     1.0560      0.50     SGT1W1
SGT1W1_20060502     1.0468      0.50     SGT1W1
SGT1W1_20060503     1.0408      0.50     SGT1W1
SGT1W1_20060504     1.0316      0.50     SGT1W1
SGT1W1_20060505     1.0225      0.50     SGT1W1
SGT1W2_20060501     0.9879      0.50     SGT1W2
SGT1W2_20060502     0.9788      0.50     SGT1W2
SGT1W2_20060503     0.9696      0.50     SGT1W2
SGT1W2_20060504     0.9636      0.50     SGT1W2
SGT1W2_20060505     0.9544      0.50     SGT1W2
SGT1W4_20060501     1.0307      0.50     SGT1W4
SGT1W4_20060502     1.0185      0.50     SGT1W4
SGT1W4_20060503     1.0093      0.50     SGT1W4
SGT1W4_20060504     1.0002      0.50     SGT1W4
SGT1W4_20060505     0.9941      0.50     SGT1W4
SGT1W5_20060501     1.6332      0.50     SGT1W5
SGT1W5_20060502     1.6240      0.50     SGT1W5
SGT1W5_20060503     1.6149      0.50     SGT1W5
SGT1W5_20060504     1.6057      0.50     SGT1W5
SGT1W5_20060505     1.5935      0.50     SGT1W5
SGT2W1_20060501     1.2185      0.00     SGT2W1
SGT2W1_20060502     1.2094      0.00     SGT2W1
                                                   74,3          30%
```

- “* model command line”: This section specifies the model PEST will use during the parameter estimation process. Note this is NOT the GSSHA model. GSSHA executable is part of the script used to generate the simulated or “measured” data PEST needs.

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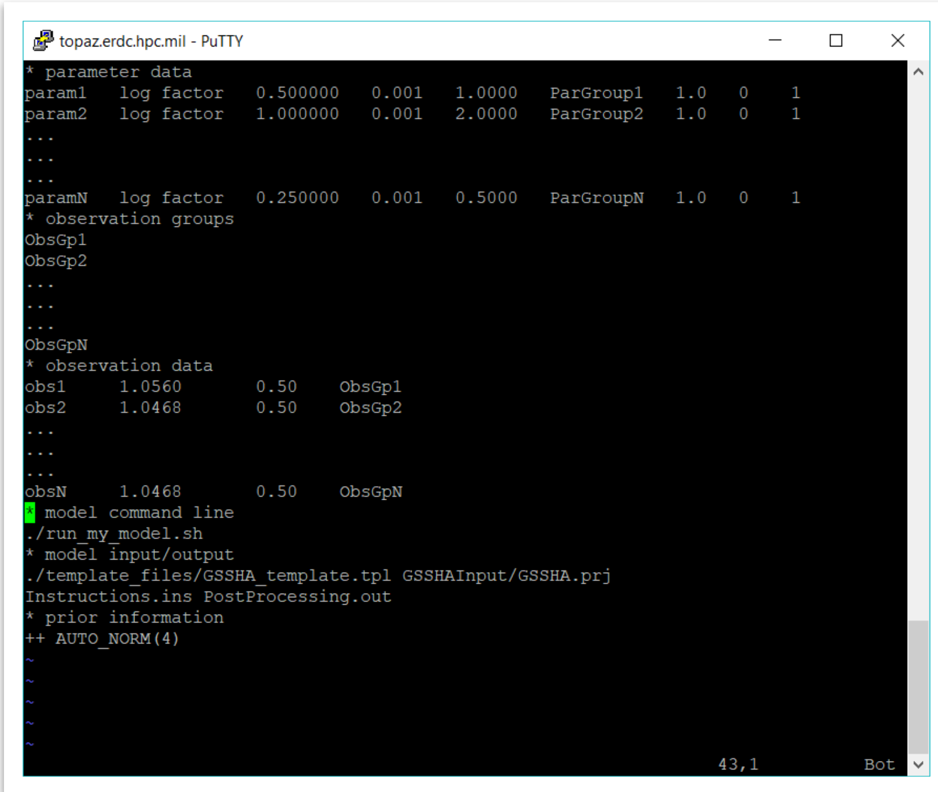
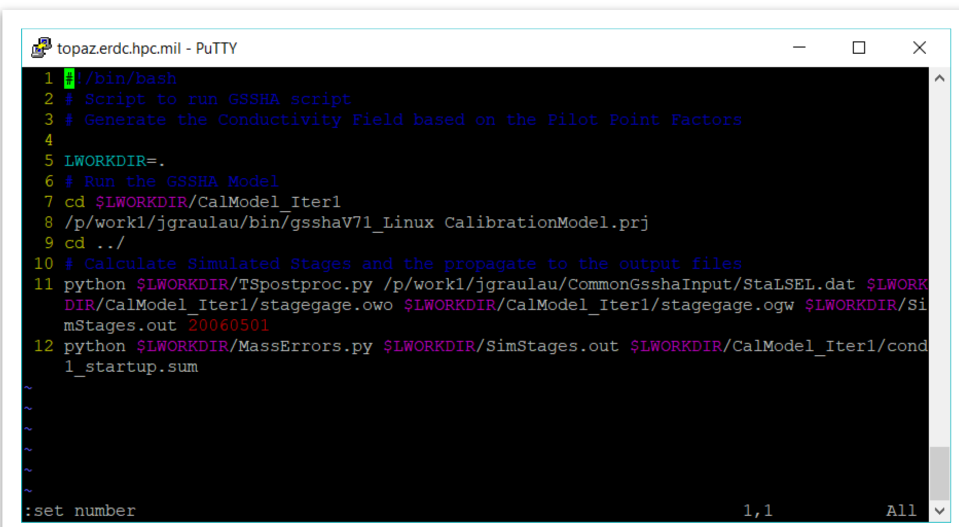


```
topaz.erdc.hpc.mil - PuTTY
* parameter data
param1   log factor   0.500000   0.001   1.0000   ParGroup1   1.0   0   1
param2   log factor   1.000000   0.001   2.0000   ParGroup2   1.0   0   1
...
...
...
paramN   log factor   0.250000   0.001   0.5000   ParGroupN   1.0   0   1
* observation groups
ObsGp1
ObsGp2
...
...
...
ObsGpN
* observation data
obs1     1.0560      0.50    ObsGp1
obs2     1.0468      0.50    ObsGp2
...
...
...
obsN     1.0468      0.50    ObsGpN
* model command line
./run_my_model.sh
* model input/output
./template_files/GSSHA_template.tpl GSSHAInput/GSSHA.prj
Instructions.ins PostProcessing.out
* prior information
++ AUTO_NORM(4)
~
~
~
~
~
                                                  43,1          Bot
```

- In the “template” directory, the script “run_my_model.sh” is the model PEST will execute during the estimation process. Open and inspect this script. It shall look similar to the screenshot below.



```
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  1 #!/bin/bash
  2 # Script to run GSSHA script
  3 # Generate the Conductivity Field based on the Pilot Point Factors
  4
  5 LWORKDIR=.
  6 # Run the GSSHA Model
  7 cd $LWORKDIR/CalModel_Iter1
  8 /p/work1/jgraulau/bin/gsshaV71_Linux CalibrationModel.prj
  9 cd ../
 10 # Calculate Simulated Stages and the propagate to the output files
 11 python $LWORKDIR/TSpostproc.py /p/work1/jgraulau/CommonGsshaInput/StaLSEL.dat $LWORK
    DIR/CalModel_Iter1/stagegage.owo $LWORKDIR/CalModel_Iter1/stagegage.ogw $LWORKDIR/Si
    mStages.out 20060501
 12 python $LWORKDIR/MassErrors.py $LWORKDIR/SimStages.out $LWORKDIR/CalModel_Iter1/cond
    1_startup.sum
~
~
~
~
~
:set number                                              1,1           All
```
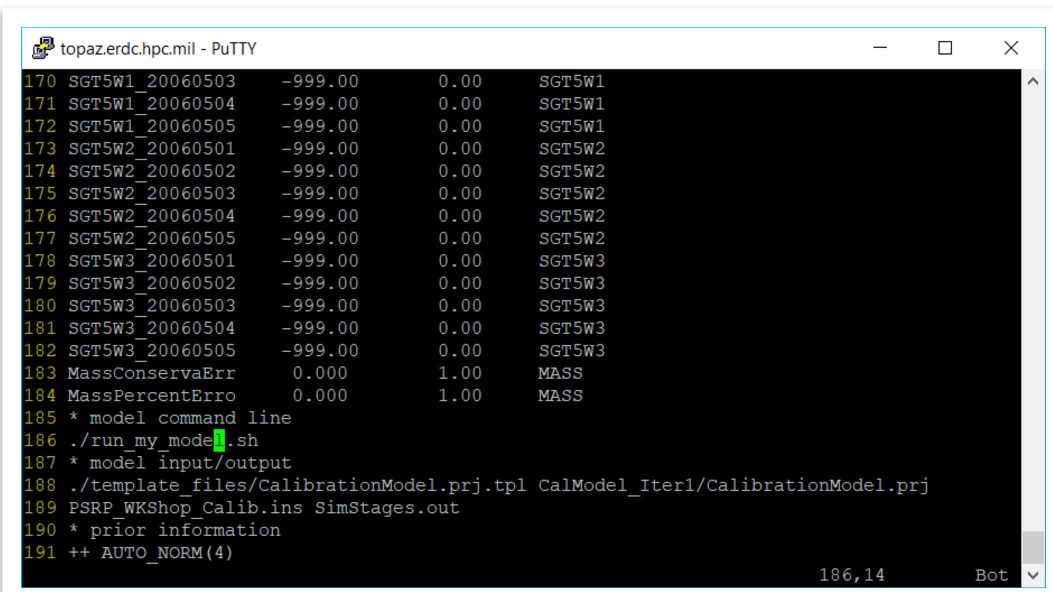

Line 8 in the “run_my_model.sh” script executes the “gssha-7.142” executable with the “CalibrationModel.prj” argument. Other lines are used to extract and post-process the GSSHA output in a format compatible with PEST. Edit this file accordingly to ensure the directories point to the right location associated with your ONYX work directory. For example, in line 8 replace the /p/work/jgraulau/… with /p/work/”yourUserName”/. Save and close the script after editing.

- “* model input/output”: This section specifies the model input/output for the PEST process. In this case, the model input is the GSSHA template file created previously. PEST will modify this file during each single model run by replacing the calibration parameters with values estimated by the PEST process. The output is the GSSHA *.prj file. Replace the filename in this line with the name of the PEST template file crated previously (i.e., “CalibrationModel.prj.tpl”)
- Replace the second argument in this line with “CalibModelIter1/CalibrationModel.prj”. This is the directory where the PEST generated GSSHA project file and GSSHA generated output files will reside.
- The next line in the control file specifies the PEST instruction file. Open the file PESTIntructFile.ins and inspect its contents. This file specifies how PEST reads the simulated model data that is compared against the observed data specified in the “* observation data”. There shall be a 1 to 1 correspondence between the entries in the instruction file and the contents of the observation data section in the PEST control file. For the purpose of this exercise an instruction file has been previously created:
    - Rename the file “InstructionFile.dat” to “PSRP_WKShop_Calib.ins”.
    - Open the PEST control file (“PESTControlFile.pst”) and change the line near the bottom that starts with “Instruction.ins” with the instruction file just created.
    - Change the 2nd field on this line with “SimStages.out”. This is the “output” of “run_my_model.sh” script that contains the GSSHA simulated stages for each model run. The file should look like the screenshot below.



- This completes the PEST control file. Close and Save the control file.

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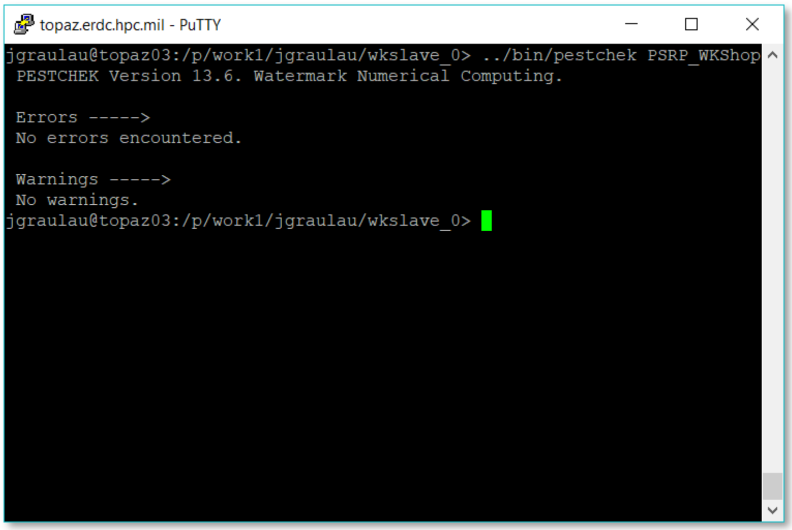
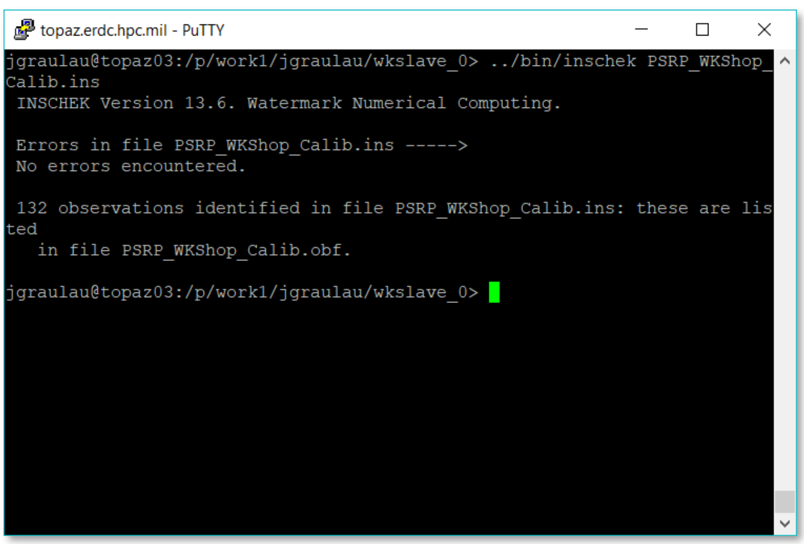
5. PEST utilities: *pestchek*, *inschek*, and *tempchek*

- The utilities pestchek, inschek, and tempchek in the bin directory are provided with the PEST distribution to check and debug the contents of the control, instruction, and template files.
- Execute pestchek with the “PESTControlFile.pst” as argument and inspect the screen output (screenshot below). If errors are found, edit the file as needed.



- Execute inschek with the “PEST_WKShop_Calib.ins” file as argument and inspect the screen output (screenshot below). This screen output should indicate the number of observations in the instruction file. If errors are found, edit the file as needed.



- Execute tempchek with the “CalibrationModel.prj.tpl” file as argument and inspect the screen output (screenshot below). The screen output states the number of adjustable parameters found in the model template file. If errors are found, edit the file as needed.

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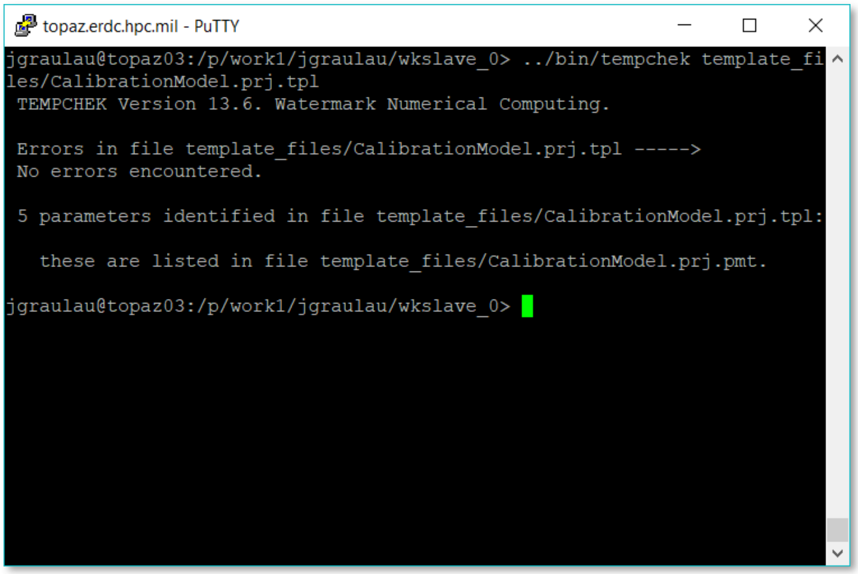

6. **“agent” directories:**
   With all the edits in the previous steps, the *template* directory should contain all necessary PEST files for the parameter estimation process in the HPC system. The template directory should be copied to a directory which, will be the “manager” for the PEST execution process.
   - Copy the *template* directory to a directory named “manager”
     cp –r template/ manager
   - Generate “agents” by executing the python script “make_dirs.py” included in the *bin* directory
     python ./bin/make_dirs.py
     This should generate 10 additional directories named agent_1, agent_2, …, agent_10
7. **Testing PEST with a single model run:**
   - Navigate to the *manager directory*
   - Edit the PEST control file by changing the first field on line from “2” to “0”. This instructs PEST to execute one single forward model run with the initial parameter values.
   - At the command prompt type “../bin/pest PESTControlFile.pst”. The model should start execution.
8. **Creating a pbs script for the PEST estimation process**
   - In the manager directory, open a text editor window and type the following PBS instructions:

     #!/bin/bash

     #PBS -V
     #PBS -N PSRP_WKShop_Calib
     #PBS -q debug
     #PBS -A ERDCV00898ENQ

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#PBS -l select=2:ncpus=44:mpiprocs=4
#PBS -l walltime=01:00:00
#PBS -j oe
#PBS -m be
#PBS -M “youremail@your.server.com”

export MPICH_ENV_DISPLAY=1

cd $PBS_O_WORKDIR

 # turn on debugging output
set -x

aprun -n 10 /p/work/”YourUserName”/bin/beopest ${PBS_O_WORKDIR}/PESTControlFile /M /p/work1/jgraulau/agent_ /p1

- This is the script that will be used to submit the PEST parameter estimation job to the HPC system. Replace the work directory with your username in the system.
- Save this file as “GSSHACalib.pbs” inside the “manager” directory

9. Submitting the job to the computational nodes.

- At the command prompt type the following command:
  qsub MyPBSScript.pbs

  This submits the job to the computational nodes in the HPC system. You should get a response from the system with the “Job ID”.

- Inspect the status of the job submitted by typing the following at the command prompt:
  qstat –u “username”

  This shall generate information about the status of the submitted job.

10. Reviewing the results of the PEST estimation process.

Once the job finishes execution:

- Open the PESTControlFile.rec and inspect its contents.
- Other PEST generated files from the estimation process included in the “manager” directory.
- Open the PESTControlFile.res and inspect its contents. This file summarizes the residuals for the PEST estimation process. The “Measured” and “Simulated” columns can be extracted and imported to excel for further post-processing.