Lecture 14: Calibrating a RSM Sub-Regional Model Using PEST

This lecture introduces the Parameter Estimation (PEST) Software.

NOTE:

A copy of the PEST User Manual can be found in the $RSM/labs/lab13_PEST directory.
The automated Parameter Estimation approach was adopted because of the complexity of calibrating the RSM with a large number of model parameters that should be calibrated and the large number (>300) of observed time series that could be used for calibration. To simplify the parameter calibration, the parameters were lumped into spatial “zones” which received the same calibrated parameter value. This is consistent with the uncertainty associated with available parameter estimations. An objective function was created that summed the bias and root mean square error (RMSE) at each flow and stage calibration location.

The files used in this lecture can be found in the Palm Beach directory ($RSM/data/palmbeach). These files are included for browsing because it is likely that the student will need to review these files during the lecture. The PEST manual is also a useful document.
The surface water management practices in Palm Beach County are complex, with both primary and secondary canals and Water Control Districts (WCDs) with maintained water levels. The primary and secondary systems provide both drainage and water supply to the areas they serve. The “maintained” systems are subject to water level fluctuations depending on the flood control or water supply functions they are providing at any given time.

The primary canals in the model area include Hillsboro canal along the southern boundary, the L-40 and L-8 canals on the western boundary, the C-51, C-16 and C-15 canals. The only primary canal where flow is routed or “floated” is the C-51 canal with an upstream reach. There, historical flows were specified at the tailwater of the S5A structure (site name S5AE in DSS file), stages specified at the headwater of the G124 structure, as with a downstream reach where flows were specified at the tailwater of the G124 structure and a stage boundary condition at the headwater of the S155 structure. For all other primary canals, historical stages were fixed for all segments.

The secondary canal system in Palm Beach County is a dense network of canals maintained by local WCDs, which include Lake Worth Drainage District, the Acme Improvement District, the Loxahatchee Groves WCD, the Indian Trail Improvement District, the Northern Palm Beach Improvement District and the Seminole Water Control District.

The secondary canals and structures are modeled in RSM indirectly using WCD waterbodies and watermovers. The WCD waterbodies use a lumped equivalent storage term for all secondary canals within a WCD, which is maintained at a control elevation. The WCD watermovers interact with the groundwater system through seepage watermovers, which can be calibrated to match the observed water levels in secondary canals within the WCD waterbody. The WCD watermovers also interact with the primary canal system using water control structure watermovers which are typically genxweirs, to maintain the water level at the control elevation desired within the WCD.
Several parameter zones were selected for calibration. Nine hydraulic conductivity zones were derived from mesh conductivity values.

Two tidal general head boundary condition zones were established based on tidal data available at the Palm Beach and Delray tidal stations.

Three levee seepage zones were created based on two zones for the L40 canal and a zone for the L8 canal.
The surficial aquifer in Palm Beach County is an aggregation of the unconfined sand/shell aquifer and the Biscayne aquifer. The system’s most productive zone is a northern extension of the Biscayne aquifer, and is comprised primarily of highly solutioned limestone. The aquifer extends from the Palm Beach – Broward county line to north of the M canal and pinches to the west around WCA-1. For the purposes of regional simulation in RSM, the aquifer has been aggregated to a single layer and given vertically averaged aquifer properties based on a number of pump tests available in the DBHYDRO-WILMA database.
The parameters to be estimated during calibration include canal leakance to the aquifer, Manning’s roughness for the canals and conductance of the WCD waterbodies that represent the secondary canals. Parameter values were estimated for all features within selected zones. The zones for canals and WCD waterbodies are shown here. In total, 29 parameters were estimated. However, two were found to be significantly correlated and thus the values were tied together by a proportionality constant. 

- 8 Canal leakance zones
- 2 canal zones for Manning’s n
- 4 WCD canal conductance zones
- 28 total PEST parameters for model calibration, of which 2 were tied
The PEST calibration is conducted by using various linear techniques to minimize the objective function. In the case of RSM, the objective function is based on the historical and simulated daily stage values for canals and groundwater wells.
Running PEST requires three sets of files;

**Instruction file (*.ins):**

The instruction file provides the information for the location of the output values that are compared to measured data for model optimization. For the Palm Beach County Model this is the residuals.ins file.

**Template file (*.tpl):**

The template files are the same as the model input files that contain the parameters that are going to be optimized, except the template files have the variable names substituted for the parameter values in the template files. There are several template files because the parameters are located in several XML files. The files are listed at the bottom of the control file `palm_24.pst`.

**Control file (*.pst):**

The control file (`palm_24.pst`) contains all of the parameter values used to control the operation of the PEST model run.
Pest control file (.pst) used by the “pestgen” utility the very first time.

Npar- Number of parameters including adjustable, fixed and tied. 39 = 26(adj)+2(tied)+11(fixed).

Npargp – Number of similar parameters grouped together.

There are 8 parameter groups including hydraulic conductivity, storage, Manning’s n, canal k/del, levee-seepage coefficient, the vegetation ET coefficients (kturf), lumped canal conductance for WCDs, and the GHB value for tidal boundary condition.

For parameter groups, ‘relative’ means the increment used for calculation of forward differences will be 0.01 times the current value.

The value for the lower increment, here set to “0.0”, is the smallest value by which the parameter can be changed for calculating derivatives.

Switch means PEST can choose between forward and central differences for derivative calculations.

2.0 is the increment for the central difference over the forward difference.

Parabolic means a parabola is fitted through the three points used to calculate the central difference and the derivative of the parabola is computed.

For each parameter, enter the current value, lower limit, upper limit and the group name.
The information in the “parameter data” section controls the parameter estimation process in PEST. A few of the key attributes of this file are as follows:

Enter ‘fixed’ for a parameter which does not change during PEST runs.

Enter ‘log’ for parameters which change in orders of magnitude like hydraulic conductivity.

The tied or correlated parameters should be entered after all the other parameters have been listed in this section.

Observation groups include both bias and root mean square error (RMSE) statistics for:

- groundwater stage or cell head (ch)
- canal stage or segment head (sh)
- Water Control District Stage (wh)
- canal flow or segment flow (sf)
For calibration, 176 “observations” are used which include cell heads (CH), segment heads (SH), segment flows (SF) and WCD heads (WH) including both bias and RMSE. Both bias and RMSE have the same weight for stage data. Zero values for weights tell PEST not to use this observation in the objective function. This is useful when configuring different PEST calibration runs.
The flow monitoring sites were weighted with lower values to account for the magnitude of flow values. Again, due to the uncertainty of the flow data reported as pump logs for secondary WCDs, the weights were much less in magnitude as compared to the weights for primary canals where flow is computed based on the breakpoint data. The choice of weights for PEST calibration took into consideration the quality of the data. It was a trial and error procedure involving many initial PEST runs.

The flow values are much higher than stage values and thus the weights for the flow observations are high in order that the flows and stages are similarly valued in the objective function.
Template files are used to define the input files whose parameters get updated by PEST. The run_it.sh shell script runs the HSE along with Python scripts used in calculation of residuals. The last part of the control file lists the command lines to run the RSM. A template file is used for each of the parameter input files along with data files when the XML file has parameters which change with every PEST run. In this run there are six template files.

| SF_DEMAND_SEP_r | 0.00000 | 0.00000010 | sf_rms |
| SF_DEMAND_OCT_r | 0.00000 | 0.00000010 | sf_rms |
| SF_DEMAND_NOV_r | 0.00000 | 0.00000010 | sf_rms |
| SF_DEMAND_DEC_r | 0.00000 | 0.00000010 | sf_rms |

* model command line
  ./run_it.sh
* model input/output
  run_calib_pb_9kzones_9canalindex.xml.tpl run_calib_pb_wcd_wm_weirs.xml
  pb_levee-seepage.xml.tpl pb_levee-seepage.xml
  wcd_waterbodies.xml.tpl wcd_waterbodies.xml
  et_kc_quarterly.dat.tpl et_kc_quarterly.dat
  tide_wallghb_011506.xml.tpl tide_wallghb_011506.xml
  evap_prop_10_04_05.xml.tpl.tpl evap_prop_10_04_05.xml.tpl
  residuals.ins residuals.out
  * prior information
The template file is used to define placeholders for the conductivity values for the 9 hydraulic conductivity zones where the values are enclosed in double quotes. In this case before PEST runs, the PEST program will replace the strings “#pb_k1#”, “#pb_k2#”.... “#pb_k9#” with the current values of the parameters.
PEST creates the input files for the RSM model. The script run_it.sh runs the RSM and post-processes the results to create the file containing the bias and RMSE values. PEST uses those values to estimate the parameter values for the next iteration.

Obtaining the optimal set of parameter values from PEST will require many iterations using the parameter upgrade vector. Each iteration will require “n” runs. To complete a calibration exercise, PEST is run in parallel on a Linux processor cluster with multiple CPUs and common RAM and storage. A temporary directory is set up for each processor. The directory includes the input and template files and run_it.sh script. This script runs the RSM implementation and creates the necessary statistics (bias and RMSE) for the objective function.
The residuals or the difference between observed and model computed is calculated using a script which reads the DSS file of the observed data and the path of the DSS file is specified in the `fetch_calib.ctl` file.

While PEST is running, the objective function, matrix condition number, parameter sensitivities and Jacobian matrix can be viewed. The covariance/correlation matrix and eigenvalues/eigenvectors can be viewed only after the PEST run is complete.
Check the Phi values in the PEST run record file by using the “grep” command.

For Palm Beach County Run 14, the biggest reduction in Phi was from iteration 6 to 7.

PEST Optimization is terminated when the objective function values are within 0.01 for the last 3 iterations.
Jacobian matrix is the derivative matrix and is the rate of change of the computed value at the observation point with respect to the parameter. Derivatives are calculated only for adjustable parameters and not for fixed or tied parameters. The simplest way to calculate a derivative is to use the forward difference method. This is done by adding an increment to the current value, unless the current value is at its upper bound, in which case the value is subtracted. Central difference gives more accurate derivative values than forward difference, but requires two model runs, and is required when the objective function minimum is approached. The most time-consuming part of PEST is by far the calculation of the derivatives.

The Jacobian matrix is used to calculate the model response to changes in the parameters and the parameter upgrade vectors.

\[ J_{i,j} = \frac{\partial o_i}{\partial b_j} \]

J is an mxn matrix, \( J'J \) is an nxn matrix which can be inverted. \( \text{Inv}(J'J)' \) is an nxm matrix. \( \mathbf{b} \) is the parameter vector of n values and \( \mathbf{c} \) is the vector of m model calculated observations. \( \mathbf{Q} \) is the diagonal matrix of weights.

\[ \mathbf{c} = \mathbf{c}_o + J(\mathbf{b} - \mathbf{b}_o) \]

\[ \mathbf{u} = (J^T\mathbf{Q}J)^{-1}J^T\mathbf{Q}(\mathbf{c} - \mathbf{c}_o) \]
After converting the binary `palm_24.jco` file to text, use the text editor to view it.
The Jacobian/correlation matrix can be saved as a graphic output using the RSM GUI toolbar. Start the RSM GUI and from Tools->Misc Tools->Pest Visualization->import Pest Jacobian/Correlation->File-Save as PNG.
The Jacobian values can be viewed graphically using the RSM GUI utility. This is used to identify parameters and observations that are highly correlated and thus do not help obtain an optimal solution.
Diagonal elements of the matrix are the variances of the calculated results at the observation points. Diagonal elements with the largest variances are the ones with the highest uncertainty. The parameters pb_k7 and pb_k6 have the highest variances.

The Manning’s n roughness values for the two canal groups are not correlated.
There is a high covariance between some of the canal-aquifer interaction terms (k/del).

Correlated parameters are parameters that can be varied in groups with little effect on model output and therefore little effect on the objective function. If PEST is having difficulty in reducing the objective function in one of your models, check the degree of parameter correlation. If you find that parameters are strongly correlated, PEST is providing valuable feedback on your observation data that might not have been noticed otherwise. Specifically, you’ve learned that additional observations are required to resolve the parameters. In many circumstances, heads by themselves are inadequate for resolving model non-uniqueness. You will have better luck in calibrating transport models if you also have observations of flow and/or concentration.
The graphic display of the correlation coefficients created by the Rsmtoolbar (corrln.png) shows the parameters that are highly correlated, both positively and negatively. The dark colored off diagonal elements show very high correlations.

Open the PEST record file (palm_24.rec) to look at the correlation coefficients for parameters. The parameters pb_k1 and pb_ghb2 are highly correlated as well as pb_k3 and pb_ghb1. This is likely because pb_k1 is the groundwater conductivity associated with the general head boundary condition used in pb_ghb2, and similarly for pb_k3 and pb_ghb2.
Once correlated parameters are identified they should be tied together so they don’t degrade the parameter upgrade vector.

Only tie parameters that have correlations with $r > 0.9$. Remember that tying parameters together takes them out of the picture.
The eigenvectors and eigenvalues provide useful information about which parameters are important and which parameters are causing problems in the calibrations.

The highest eigenvalue is the direction in the parameter space where the estimation is the weakest. The eigenvector components of largest eigenvalue are dominated by a single component. Normally the highest eigenvalue is the most important because this is the direction in parameter space in which parameters are most poorly estimated, i.e. the probability ellipsoid is longest in this direction. Looking to the eigenvector corresponding to the highest eigenvalue, we can often see at a glance what may be causing problems in parameter estimation. If the model is insensitive to a single parameter, the eigenvector corresponding to the largest eigenvalue will be dominated by a single component, this pertaining to the insensitive parameter.
Shown are the eigenvectors and eigenvalues for the Palm Beach County Model. The columns are the eigenvectors. Vectors1, Vector2 ... Vector26. The largest eigenvalue is 41.64 and the eigenvector corresponding to this has 4 components shown in color. These groups of parameters are somewhat insensitive. A similar pattern is seen for the next highest eigenvalue corresponding to 24.62.
Condition numbers indicate how well-posed the calibration problem is. Large condition numbers indicate the matrix is ill-conditioned.

If the condition number of a matrix is around 1, it is well-conditioned.

If the condition number of a matrix is $10^5$, it is ill-conditioned.

PEST has to work hard when a condition number is large to find a solution.
It is important to review the parameter sensitivities to identify those parameters that are insensitive and thus inhibit the effectiveness of PEST to obtain a good solution.

The higher the number, the more sensitive the parameter is. Exclude parameters at the upper and lower bounds. The upper and lower bounds were defined in the control file.
A plot of sensitivities with PEST iterations shows that the parameters are the most sensitive within the first iteration and sensitivity changes with subsequent iterations.
All quantities are only approximate because their calculation is based on linearity assumption which is often not true. Regardless of the approximate nature of this analysis, much can be learned about the model, its parameterization and its appropriateness for a specific application. Depending on the use of the model, parameter uncertainty due to high correlations between parameters may not be a defect. High correlations between parameters are easily recognized from the correlation matrix and the eigenvector eigenvalue analysis. The test is to use the model for predictive analysis. If the predictions made by the model are of the same type as the measurements used in the calibration process, and if the “stress condition” imposed is no different from that which the model went through during calibration, the effect of parameter correlation on model predictions will not be very large.

Parameter uncertainty caused by parameter insensitivity is often more of a challenge than correlation.

Confidence values provide a useful means of comparing the certainty with which different parameter values are estimated by PEST. Parameters with tight confidence limits are generally not correlated with other parameters. For the Palm Beach County Model the parameters pb_k7, pb_canal_n2, pb_canal_kd5, pb_canal_kd7, pb_canal_kd8 and the levee seepage parameters have large margins of uncertainty.
These are the results for the calibration statistics; bias and root mean-squared error, for the selected wells for the Palm Beach County RSM implementation and the SFWMM. The RSM produced results that are comparable to the SFWMM.
PEST results for secondary canal stage monitoring locations within the WCDs for the time period 1984-1995. The RSM was able to produce results for canals that are not available in the SFWMM.

There is only one primary canal in this model, the C51 canal. The stage and canal flow were within acceptable ranges. The negative bias indicates that the calibrated model does not predict the peak flows well. The flow in the secondary system is calibrated against the water supply demands of the WCD. The high bias may be caused by the limited model formulation for the WCD and the poor quality data available for calibration.
The automated parameter estimation software PEST was used for the Palm Beach model calibration given the complexities of the model and the large number of model parameters and observation data involved. PEST analysis was conducted by creating parameter zones for aquifer conductivity, the canal network leakance and Manning’s n, the lumped leakance for WCD canals, the levee seepage coefficients and the conductance for the tidal boundaries. Objective was to minimize the weighted sum of squares of the bias and RMSE calculated at each observation point.
KNOWLEDGE ASSESSMENT
(pre- and post-lecture quiz to assess efficacy of training materials)

1. What are the two common components of objective functions used for calibrating RSM?
2. How are spatially distributed parameters implemented in RSM?
3. Which parameters are implemented in zones?
4. What are three primary files need to run PEST?
5. Within the PEST control file, what values are provided with each model parameter?
6. What values are provided with each observation?
7. What information is provided in the template files?
8. What processes are implemented in the run_it.sh script?
9. What information is in the fetch_calib.ctl file?
10. How do we view phi values and what do they tell us about the PEST run?
11. Why do we want to review the parameter correlation coefficients?
12. What do the eigenvectors tell us about the model parameters?
13. What does the condition number tell us?
14. Which are parameter sensitivities important to review?
Answers

1. Bias and root mean squared error (RMSE).

2. The spatially distributed parameters are lumped together into “zones” of equal value.

3. Hydraulic conductivity, canal leakance, manning’s n, canal conductance, levee seepage and tidal general head boundary conditions.


5. The current value, lower limit and upper limit for parameter adjustment are provide for each parameter.

6. The initial value and weight for including in the objective function.

7. The template files contain placeholders for parameters adjusted during calibration.

8. The run_it.sh script creates the et_kc template file, runs the RSM model and then runs a script that calculates the bias and RMSE values for selected stations used by PEST.

9. The fetch_calib.ctl file identifies the times series DSS files and records that are used by the calcStats.py program to calculate bias and RMSE.

10. The phi values can be extracted from the .rec file using the “grep” command. Phi should decrease with each iteration or the PEST process is not improving the parameter values.

11. The parameter correlation coefficients tell us which parameters are highly correlated and side-tracking the PEST solution.

12. High values for parameters within the eigenvectors identify insensitive parameters.

13. The condition number tells how well posed the calibration problem is. If the value is greater than $10^7$ PEST may not be able to solve the problem.

14. Insensitive parameters inhibit the PEST process.
Lab 14: RSM Calibration using PEST

Time Estimate: 2.5 hours

Training Objective: To investigate the use of PEST for calibrating the RSM.

The Regional Simulation Model (RSM) can be calibrated using Parameter Estimation (PEST) on a simple laptop or desktop Linux computer. However, typically the calibration is conducted on an 80-node Linux cluster using the parallel PEST (PPEST) methods.

This lab reviews the results of a complete PEST calibration and implements a PEST calibration on the Biscayne Bay Coastal Wetlands (BBCW) RSM with five variables.

This is a simple exercise so that the student becomes familiar with the PEST implementation. For more details, see the PEST Manual located in the labs/lab13_PEST directory.
NOTE:

For ease of navigation, you may wish to set an environment variable to the directory where you install the RSM code using the syntax:

```sh
setenv RSM <path>
```

For SFWMD modelers, the path you should use for the NAS is:

```sh
/nw/oomdata_ws/nw/oom/sfrsm/workdirs/<username>/trunk
```

Once you have set the RSM environment variable to your trunk path, you can use `$RSM` in any path statement, such as:

```sh
cd $RSM/benchmarks
```

Training files are currently located in the following directories:

```
INTERNAL_TRAINING
   |__data
   |   |__geographic
   |   |   |__C111
   |   |__rain+et
   |   |__glades_lecsa
   |   |__losa_eaa
   |   |__BBCW
   |__trunk
   |   |__benchmarks
   |   |__hpmbud
   |__labs
```

Files for this lab are located in the labs/lab14_RSM_PEST directory. Additional materials in the directory include:

PEST User Manual ([pestman.pdf](#))

BBCW7.ppt

BBCW_13_Run_Report_021407.doc

PEST_addendum_11.pdf
Activity 14.1 Reviewing PEST Results for Biscayne Bay Coastal Wetlands RSM

Overview

Activity 14.1 includes two exercises:

- Exercise 14.1.1. Review results of BBCW PEST run
- Exercise 14.1.2. Create statistics for BBCW PEST run

This activity is designed to review the files associated with a PEST run. Several PEST runs were conducted for the Biscayne Bay Coastal Wetlands (BBCW) and examining the directory content is useful to determine how the PEST runs were set up and to analyze the outcomes.

Exercise 14.1.1 Reviews results of BBCW PEST run.

1. Go to the BBCW RSM PEST model directory to investigate the results of the PEST calibration: 
   \$RSM/data/BBCW/Final_Results_BBW16_sens1

2. Find the PEST files and information to answer the following questions:
   - How many parameters are being estimated?
   - How many parameter groups are used?
   - What are the groups?
   - In what input files are the parameters located?
   - How many observations are used for calibration?
   - What kinds of data are used for calibration?
     - How many of each?

   **HINT**
   The parameters being calibrated are in the template files (*.tpl)

3. Plot the change in the objective function Phi.
   - How many model runs were made?
   - How many iterations were conducted?
   - How many parameters were highly correlated?

   **HINT**
   grep the values of “phi” from the *.rec file.
   (grep -n phi bbw16.rec)
4. Plot the correlation coefficients using the RSM Graphical User Interface (RSM GUI) tools.

**HINT**

See Lecture 6 for use of RSM GUI.

5. Which observations are important to the calibration?
   - Run "Identpar" utility for PEST where 8 is the number of singular values to use:
     ```
     identpar bbw_16.pst 8 outbase outfile.dat identfile.dat
     ```
   - Import `identfile.dat` into Excel, transpose the values and plot a stacked bar chart of the observation with the eigenvectors.
Exercise 14.1.2 Create statistics for the PEST model run.

Look at the results from the PEST run. After obtaining the results from PEST, the model was rerun with standard output: flowgages, global monitors and water budgets. These data are useful for developing an understanding of the hydrology of the system.

Although the performance measures are constructed from model metrics, these cannot be run with PEST because the resulting netCDF file is too large and the model would take too long to run.

The post-processing from the RSM calibration runs produces goodness-of-fit statistics between simulated values and observed data (canal and groundwater stages, and canal flows) and results from the South Florida Water Management Model (SFWMM). We can also compare the calibration statistics of the SFWMM simulations with the historical data.

The statistics can be created using the command line jython (Java/Python) script or through the RSM GUI. There are two commands for calculating the statistics: calcStats.py that calculates the bias and Root Mean-Squared Error (RMSE) for stage and flow time series, and makePlots.py that creates the time series plots for comparing runs.

1. Go to the $RSM/data/BBCW/Final_Results_BBW16_sens1 directory.
2. Run calcStats.py. (The file bbcw_fetch_94-00.ctl (Fig. 14.1) contains the identification of the files and the time series to be used in the comparison.)
3. Create time series plots for the RSM PEST run.

Time series plots can be created using a command line script or through the RSM GUI. Plots can be made of the RSM simulated heads plotted against historical data and the SFWMM simulated data for the same time period.

Run makePlots_94-00.py in the ./BBCW/Final_Results_BBW16_sens1/plots94-00 directory.

4. Observe the results in this subdirectory.
   - At which sites did the RSM produce better results than the SFWMM for this set of parameter values?
Figure 14.1 Contents of bbw_fetch_calibqh.crl control file

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<thead>
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<th>Run</th>
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<th>SFWMM Path</th>
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Figure 14.2 Contents of bbw_fetch_wtk_qc3.crl control file

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<th>SFWMM Path</th>
</tr>
</thead>
<tbody>
<tr>
<td>mon SF_S176</td>
<td>/SFRSM/S176/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S176/FLOW//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>mon SF_S177</td>
<td>/SFRSM/S177/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S177/FLOW//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>mon SF_S178</td>
<td>/SFRSM/S178/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S178/FLOW//1DAY/DBHYDRO/</td>
</tr>
<tr>
<td>mon SF_S194</td>
<td>/SFRSM/S194/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S194/FLOW//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>mon SF_S196</td>
<td>/SFRSM/S196/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S196/FLOW//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>mon SF_S165</td>
<td>/SFRSM/S165/FLOW//1DAY/COMPUTED/</td>
<td>/SFWMM/S165/FLOW//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>run SH_S118_T</td>
<td>/SFRSM/S118_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S118_T/STAGE//1DAY/HISTORICAL/</td>
</tr>
<tr>
<td>run SH_S119_T</td>
<td>/SFRSM/S119_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S119_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run SH_S121_T</td>
<td>/SFRSM/S121_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S121_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run SH_S140_T</td>
<td>/SFRSM/S140_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S140_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run SH_S165_T</td>
<td>/SFRSM/S165_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S165_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run SH_S166_T</td>
<td>/SFRSM/S166_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S166_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run SH_S167_T</td>
<td>/SFRSM/S167_T/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/S167_T/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_EPSW</td>
<td>/SFRSM/EPSW/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/EPSW/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_EVER1</td>
<td>/SFRSM/EVER1/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/EVER1/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_EVER2B</td>
<td>/SFRSM/EVER2B/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/EVER2B/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_EVER4</td>
<td>/SFRSM/EVER4/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/EVER4/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_F358</td>
<td>/SFRSM/F358/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/F358/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G1183</td>
<td>/SFRSM/G1183/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G1183/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G1362</td>
<td>/SFRSM/G1362/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G1362/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G1363</td>
<td>/SFRSM/G1363/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G1363/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G1486</td>
<td>/SFRSM/G1486/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G1486/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G3354</td>
<td>/SFRSM/G3354/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G3354/STAGE//1DAY/HIST_MOD1/</td>
</tr>
<tr>
<td>run CH_G3355</td>
<td>/SFRSM/G3355/STAGE//1DAY/COMPUTED/</td>
<td>/SFWMM/G3355/STAGE//1DAY/OBSERVED/</td>
</tr>
</tbody>
</table>
In Figure 14.1, each line of the control file identifies a RSM model output dataset, the corresponding historical data and the corresponding simulation results from the SFWMM. The calcStats.py script will calculate the bias and RMSE between the RSM simulated results and historical data, as well as between the SFWMM simulated results and historical data. The following chart identifies prefixes used in the code:

<table>
<thead>
<tr>
<th>Prefix</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>SF</td>
<td>Segment Flow</td>
</tr>
<tr>
<td>SH</td>
<td>Segment Head</td>
</tr>
<tr>
<td>CH</td>
<td>Cell Head</td>
</tr>
</tbody>
</table>

Figure 14.2 Typical time series graph of computed stage, observed historical stage and SFWMM simulated stage created using the makePlots.py jython script.
Activity 14.2 Constructing a Simple BBCW RSM PEST run

Overview

Activity 14.2 includes one exercise:

- Exercise 14.2.1. Run BBCW PEST using a laptop or a desktop computer

In the next exercise, you will construct a simple PEST run for the Biscayne Bay Coastal Wetlands (BBCW). There are two approaches for completing the PEST run:

- Using a laptop or desktop computer
- Using the South Florida Water Management District (SFWMD) Linux cluster: `dclust2`

The PEST runs are typically run in parallel on the Linux cluster. However, as a training exercise, the Linux cluster is not available.

Exercise 14.2.1 Run BBCW PEST using a laptop or desktop computer

5. Create a new `pest` subdirectory in the `lab14_RSM_PEST/BBCW1` directory:
   
   ```bash
   mkdir $RSM/labs/lab14_RSM_PEST/BBCW1/pest
   ```

6. Copy the following files from the `$RSM/data/BBCW/pest/` sub-directory into the `BBCW1` directory:

<table>
<thead>
<tr>
<th>Template file</th>
<th>run_calib_bbcw.xml.tpl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input files</td>
<td>run_calib_bbcw.xml</td>
</tr>
<tr>
<td></td>
<td>canal_indexed_attr_122706.xml</td>
</tr>
<tr>
<td></td>
<td>lvspg_BBCW_12212006.xml</td>
</tr>
<tr>
<td></td>
<td>tide_wallghb.xml</td>
</tr>
<tr>
<td>hse103 files*</td>
<td>hse103</td>
</tr>
<tr>
<td></td>
<td>hse103.dtd</td>
</tr>
<tr>
<td>Instruction file</td>
<td>residuals.ins</td>
</tr>
<tr>
<td>PEST control file</td>
<td>bbcw_qh.pst</td>
</tr>
<tr>
<td>output</td>
<td>residuals.out</td>
</tr>
<tr>
<td>Batch file</td>
<td>run_it_ef.sh (copy this file from BBCW1 directory into the <code>pest</code> subdirectory for running PEST and post-processing statistics for objective function)</td>
</tr>
</tbody>
</table>
7. Edit `run_it_ef.sh` and change the reference location of `hse103`.

8. Edit the `run_calib_bbcw.xml` and `run_calib_bbcw.xml.tpl` files and change the reference location for the `hse103.dtd`, `rainfall` and `refET` files.

9. Copy `/bin` directory to the Lab 14 directory:
   
   ```
   cp –r $RSM/data/BBCW/pest/bin $RSM/labs/lab14_RSM_PEST/BBCW1
   ```

10. Copy `/input` directory:
    
    ```
    cp –r $RSM/data/BBCW/pest/input $RSM/labs/lab14_RSM_PEST/BBCW1
    ```

11. Make an output directory. Which parameters will be calibrated in this run?
    
    ```
    mkdir output
    ```

12. In the `$RSM/labs/lab14_RSM_PEST/BBCW1/bin` directory, check/edit the file `bbcw_fetch_calibqh.ch` to make sure that the references to the input files on the first line are correct.

13. Run the PEST check utility to ensure that the necessary files are okay.
    
    ```
    pestchek bbcw_qh.pst
    ```

14. Run PEST from the batch file
    
    ```
    pest bbcw_qh.pst
    ```

**NOTE:**

This PEST run will take approximately 2.5 hours to run on a Dell Latitude D810 laptop with 2MB DDRR memory.

If there is insufficient time to complete the model run, the results can be reviewed by copying the `$RSM/data/BBCW/pest/bbcw_ef*` files and looking at the results.

- `bbcw_ef.rec` – model run, correlation coefficients, objective function, etc.
- `bbcw ef.par` – final best fit parameter values

15. Evaluate the PEST results.

   - Plot the Phi values and look at the convergence of the PEST calibration.
   - Evaluate the **eigenvectors**: Is the ratio between the highest and lowest less than $10^6$?

**HINT**

Look at the eigenvalues at the bottom of the `bbcw_ef.rec` file.
• Are the parameters correlated?

**HINT**

Look at the `bbcw_ef.rec` or `bbcw_ef.mtt` files.

• How much has the final parameter values changed from the initial values?
• What are the confidence intervals for the parameters?
Answers for Lab 14.

Exercise 14.1.1

2. PEST answers:
   - 95 parameters
   - 5 groups
   - Parameter groups:
     - hydraulic conductivity
     - levee seepage
     - canal leakage coefficient
     - wcd leakage coefficient
     - general head boundary condition conductivity
   - input files for parameters:
     - run_PEST_calib_bbw.xml.tpl
     - BBW_canal_indexed_attr.xml.tpl
     - BBW_levee_seepage.xml.tpl
     - BBW_tide_bc_wall_ghb.xml.tpl
     - BBW_Northern_BC_Cell_ghb.xml.tpl, BBW_Western_BC_Wall_ghb.xml.tpl, bbw_wcd.xml.tpl
   - 1042 observations
   - CH – cell head (256); SH – segment head (66); SF – monthly segment flow (720)

3. See the plot in the PhiPlot.xls file in the Lab14_RSM_PEST directory.
   - 1840 model runs
   - 16 iterations
   - about 23 parameter pairs. Dark blue and dark red in Correlation matrix.

4. Correlation matrix:

![Correlation Matrix](image)

5. Important Observations:
Exercise 14.1.2

4. Several sites including E146, E158, EPSW, EVER1, EVER2, F358, FROGP, G551, G553.
Exercise 14.2.1

7. Calibrated parameters:
   - Kmult_1
   - Kmult_3
   - Kmult_4
   - Kmult_8
   - Kmult_10
   - Kmult_200
   - Transmissivity

11. Simple BBCW RSM PEST calibration

Phi Plot

Eigenvalues ----->
5.9048E-03  8.2884E-03  1.0089E-02  2.8936E-02  0.1428  0.4133
Ratio: 70 very well conditioned for this example.

Parameter correlation coefficient matrix ----->
None of the parameters are highly correlated.

<table>
<thead>
<tr>
<th></th>
<th>kmult_1</th>
<th>kmult_3</th>
<th>kmult_4</th>
<th>kmult_8</th>
<th>kmult_10</th>
<th>kmult_200</th>
</tr>
</thead>
<tbody>
<tr>
<td>kmult_1</td>
<td>1.000</td>
<td>-0.1860</td>
<td>-0.1565</td>
<td>0.2750</td>
<td>0.0615</td>
<td>0.02722</td>
</tr>
<tr>
<td>kmult_3</td>
<td>-0.1860</td>
<td>1.000</td>
<td>0.0106</td>
<td>-0.0905</td>
<td>0.4792</td>
<td>-0.2036</td>
</tr>
<tr>
<td>kmult_4</td>
<td>-0.1565</td>
<td>0.0106</td>
<td>1.000</td>
<td>-0.4591</td>
<td>0.3207</td>
<td>-0.1277</td>
</tr>
<tr>
<td>kmult_8</td>
<td>0.2750</td>
<td>-0.0905</td>
<td>-0.4591</td>
<td>1.000</td>
<td>-0.2770</td>
<td>0.1036</td>
</tr>
<tr>
<td>kmult_10</td>
<td>-0.0601</td>
<td>0.4792</td>
<td>0.3207</td>
<td>-0.2770</td>
<td>1.000</td>
<td>-0.4209</td>
</tr>
<tr>
<td>kmult_200</td>
<td>0.0272</td>
<td>-0.2036</td>
<td>-0.1277</td>
<td>0.1036</td>
<td>-0.4209</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Initial versus Final values:

<table>
<thead>
<tr>
<th>Initial value</th>
<th>Final Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Hydrologic and Environmental Systems Modeling
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Estimated</th>
<th>95% percent confidence limits</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Value</td>
<td>lower limit</td>
</tr>
<tr>
<td>kmult_1</td>
<td>2.000000E-04</td>
<td>4.4061738E-05</td>
</tr>
<tr>
<td>kmult_3</td>
<td>7.000000E-04</td>
<td>3.4940013E-05</td>
</tr>
<tr>
<td>kmult_4</td>
<td>5.000000E-04</td>
<td>4.9057131E-04</td>
</tr>
<tr>
<td>kmult_8</td>
<td>2.000000E-05</td>
<td>1.8639147E-05</td>
</tr>
<tr>
<td>kmult_10</td>
<td>6.000000E-05</td>
<td>1.3315163E-05</td>
</tr>
<tr>
<td>kmult_200</td>
<td>2.000000E-06</td>
<td>2.3148000E-04</td>
</tr>
</tbody>
</table>
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