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A Practical Guide to Calibration of a GSSHA Hydrologic Model Using ERDC Automated Model Calibration Software – Efficient Local Search

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Brian E. Skahill and Charles W. Downer

Coastal and Hydraulics Laboratory
U.S. Army Engineer Research and Development Center
3909 Halls Ferry Rod
Vicksburg,MSL 39180

Jeffrey S. Baggett

University of Wisconsin at La Crosse
1725 State Street
La Crosse, WI 54601

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Washington, DC 20314-1000

Abstract

The objective of this technical note is to demonstrate, by way of example(s), how to use the Engineer Research and Development Center (ERDC) implementation of the Levenberg-Marquardt (LM) and Secant LM (SLM) method for model independent parameter estimation to calibrate a Gridded Surface Subsurface Hydrologic Analysis (GSSHA) hydrologic model. The purpose is not to present or focus on the theory which underlies the parameter estimation method(s), but rather to carefully describe how to use the ERDC software implementation of the secant LM method that accommodates the PEST model independent interface to calibrate a GSSHA hydrologic model. We will consider variations of our Secant LM (SLM) implementation in attempts to provide the interested reader with an intuitive sense of how the method works. We will also demonstrate how our LM/SLM implementation compares with its counterparts as implemented in the popular PEST software.

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Preface

This report describes, by way of multiple examples, how to use model independent software to calibrate the physics based, distributed parameter, hydrologic model Gridded Surface Subsurface Hydrologic Analysis (GSSHA).

Research presented in this technical report was developed under the U.S. Army Corps of Engineers Flood and Coastal Storm Damage Reduction Research and Development Program. Dr. William Curtis, Coastal and Hydraulics Laboratory (CHL), is the director.

The work was performed by Drs. Brian E. Skahill and Charles W. Downer of the Hydrologic Systems Branch (HF-H) of the Flood and Storm Protection Division (HF), U.S. Army Engineer Research and Development Center – Coastal and Hydraulics Laboratory (ERDC-CHL), and Dr. Jeffrey S. Baggett of the University of Wisconsin – La Crosse. At the time of publication, Earl V. Edris was Chief, CEERD-HF-H; Bruce A. Ebersole was Chief, CEERD-HF. The Deputy Director of ERDC-CHL was Jose E. Sanchez and the Director was Dr. William D. Martin.

COL Kevin J. Wilson was the Commander and Executive Director of ERDC, and Dr. Jeffery P. Holland was the Director.

1 Introduction

Recent research at the U.S. Army Engineer Research and Development Center (ERDC) has focused on the development of methodologies, or improvement of the efficiency of native algorithms, for the computer-based calibration of hydrologic and environmental models (wherein by efficiency we mean the number of forward model calls necessary for the calibration algorithm to converge on a solution). These include, among others, an accelerated derivative-based local search algorithm, a stochastic global optimization algorithm for intelligently sifting through local minima to find a global minimum, and most recently a state-of-the-art evolutionary strategy for global parameter identification of difficult problems with noise or other features that make derivatives estimation difficult. Minimizing the number of required model runs is one of the primary factors driving the research and development activities, such that the resulting optimization tool(s) are more compatible with the computationally expensive physics-based models that are becoming more commonly used within the practice community.

Background

The context for this technical note is the previously mentioned derivative-based local search algorithm, in particular, the Levenberg-Marquardt (LM) method of computer-based parameter estimation (Levenberg, 1944; Marquardt, 1963). The LM method has several features that make it attractive for model calibration. One, is its ability to readily report estimates of parameter uncertainty, correlation, and (in)sensitivity as a by-product of its use both during and after the parameter estimation process. The LM method is also easily adapted by the inclusion of various regularization devices to maintain numerical stability and robustness in the face of potential numerical problems (that adversely affect all parameter estimation methodologies) caused by parameter insensitivity and/or parameter correlation (Menke, 1984; de Groot-Hedlin and Constable, 1990; Doherty and Skahill, 2006). Skahill et al. (2010) and Skahill and Doherty (2006) both provide lengthy summaries of the LM method.

The model independent LM method based parameter estimation software PEST (Doherty, 2004, 2007a, b), which quantifies model to measurement misfit in the weighted least squares sense, is now widely used to support hydrologic and environmental model calibration. In addition to its traditional groundwater model calibration application setting (Zyvoloskia et al. 2003; Tonkin and Doherty, 2005; Moore and Doherty, 2005; Gallagher and Doherty, 2007a), it is now employed to calibrate ecological models (Rose et al. 2007), land surface models (Santanello Jr. et al. 2007) and models in other application areas including nonpoint source pollution (Baginska et al. 2003; Haydon and Deletic, 2007), surface hydrology (Doherty and Johnston, 2003; Gutiérrez-Magness and McCuen, 2005; Kunstmann et al. 2006; Skahill and Doherty, 2006; Doherty and Skahill, 2006; Gallagher and Doherty, 2007b; Goegebeur and Pauwels, 2007; Iskra and Droste, 2007; Kim et al. 2007; Maneta et al. 2007), and surface water quality (Rode et al. 2007).

A drawback associated with LM-based model independent parameter estimation as implemented in PEST is that it requires the derivatives of the objective function with respect to the model parameters. Model independent LM implementations can become computationally expensive when elements of the Jacobian matrix must be computed using finite differences based on model runs with incrementally varied parameter values. While using multiple processors can decrease the time required to construct the Jacobian matrix, **X**, it would be better, as Skahill et al. (2010) demonstrated, to not populate the entire Jacobian matrix unless really necessary.

With a conventional model independent implementation of the LM method, only outputs of the model are available and elements of the matrix **X** are often obtained by numerical differentiation. The LM method implemented in PEST (Doherty, 2004) requires anywhere between m and $2m$ (m is the dimension of adjustable model parameter space) forward model calls (dependent upon whether forward or central finite differences are employed) to populate the column space of the matrix **X** at each optimization iteration. It has been suggested that this is a general requirement for model independent derivate-based methods, such as LM, that employ perturbation sensitivities to populate the matrix **X** at each optimization iteration (Doherty, 2004; Tonkin and Doherty, 2005). To the contrary, there are well established methods (Broyden, 1965) available that allow for better efficiency with respect to updating the matrix **X** at each optimization iteration.

Incorporating Broyden's rank one (secant) update into the LM implementation eliminates the requirement to conduct any additional forward model calls to populate an update to the Jacobian matrix, $\mathbf{X}_{new}$, at each optimization iteration. To mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations, $\mathbf{X}_{new}$ can occasionally be fully updated in the usual manner using finite differences. Furthermore, this occasional full updating can also be supplemented through cyclic updating, using finite differences, at each optimization iteration, of anywhere between one and m individual columns of $\mathbf{X}$ (Madsen et al. 2004).

Our independent LM implementation accommodates the model independent PEST interface (Doherty, 2004) and includes the following additional abilities with respect to updating the matrix $\mathbf{X}$ (Skahill and Baggett, 2006) which in all cases is initially approximated by a full update using forward and/or central finite differences:

1. A full update, at each optimization iteration, using forward and/or central finite differences;
2. Use of the Broyden rank one update;
3. Use of the Broyden rank one update, with a recomputation, i.e., a full update of $\mathbf{X}$ whenever the ratio of the new and old objective function values is greater than a specified input value;
4. Use of the Broyden rank one update, with a recomputation, i.e., a full update of $\mathbf{X}$ whenever the ratio of the new and old objective function values is greater than a specified input value, and also cyclic updating, using finite differences, at each optimization iteration, of anywhere between one and m (a specified input) individual columns of $\mathbf{X}$.

Our secant LM (SLM) method may be used as an alternative to PEST (Doherty, 2004, 2007a, b) for more efficient model independent LM-based parameter estimation. Only slight modifications to the PEST control file are required to utilize the Broyden update functionalities noted above. Our software also provides linear based information on parameter uncertainty, correlation, and sensitivity. Doherty (2007a, b) reportedly did implement the Broyden rank one update, but evidently still computes a full update to the Jacobian matrix at each optimization iteration. This approach does not fully realize the potential efficiency gains of a secant version of the LM method and in some cases, as was shown in Skahill et al. (2010), significantly increases the number of model runs required to find a local minimum.

Skahill et al. (2010) demonstrated efficiency gains that can be achieved from a properly implemented secant version of the LM method relative to conventional LM application by examining the reduction in the total number of model calls for single local searches. The efficiency gains from their independent LM implementation were also compared against efficiencies associated with the model independent LM based PEST software (Doherty, 2004, 2007a, b), using an eight parameter Hydrological Simulation Program-FORTRAN (HSPF) (Bicknell et al. 2001) hydrologic model, a ten parameter Fast All-season Soil Strength (FASST) state-of-the-ground model (Frankenstein and Koenig, 2004), and a sixteen parameter GSSHA (Downer and Ogden, 2003a, b) hydrologic model as case study examples.

The three previously mentioned environmental model structures were employed to examine efficiencies associated with variations of our SLM implementation relative to a conventional model independent LM application wherein the column space of the model Jacobian/sensitivity matrix is fully updated at each optimization iteration. For each of the three model structures, using our software, we performed thirty LM inversions and thirty SLM inversions for each variation considered, and in each case started from the same initial points. Each individual trial; however, used a different initial guess. Moreover, we used PEST (Doherty, 2004, 2007a, b), since it reportedly supports a variation of secant LM, to repeat the same runs using the same input control files and initial points.

Based on their thirty trials with each of the three model structures, Skahill et al. (2010) found that they could find local minima using their SLM implementation with 36 percent to 84 percent fewer model runs than a conventional model independent LM application, and with only modest reductions in objective function improvement. In addition, they discovered that while PEST (Doherty, 2004, 2007a, b) reportedly does include the ability to utilize Broyden updates, that implementation does not realize the complete efficiency gains that are possible with a secant version of the LM method. For example, with the FASST and GSSHA model structures, the SLM implementation of PEST (Doherty, 2004, 2007a, b) required additional model calls. The results also suggested that additional efficiency gains could possibly be achieved with a future SLM implementation by adaptively activating cyclic updating during an inverse model run.

Methodology

The steps necessary to use our implementation of the LM/SLM method will now be demonstrated and documented while applying it to calibrate a GSSHA hydrologic model for the Goodwin Creek Experimental Watershed (GCEW) (Senarath et al. 2000; Downer and Ogden, 2003b). The general approach involves the following steps:

1. Develop or obtain a functional forward model to calibrate (e.g., in this case, a GSSHA hydrologic model for the GCEW);
2. Initially determine the forward model parameters that will be selected as adjustable;
3. Create PEST template files for the model input files that contain the selected adjustable model parameters;
4. Identify the observation data, and their related model simulated counterparts, that will be used to calibrate the forward model;
5. Use the Time Series Processor (TSPROC) (Doherty, 2007c) to formulate the objective function that will be used to characterize model to measurement misfit and be minimized during model calibration;
6. Create a batch file that includes the following elements: for a given parameter set, modified forward model input file(s), forward model execution, and subsequent objective function evaluation;
7. Use TSPROC to generate an initial working PEST input control file;
8. Prior to performing an inverse model run, possibly modify the initial working PEST input control file (e.g., among others, fix, tie, or log transform the adjustable model parameters, specify initial values for the adjustable model parameters, set lower and upper bounds for the adjustable model parameters, and modify weights assignments to the observation data groups);
9. Verify that the modified PEST input control file is functional using the PEST executable PESTCHEK;
10. Set the PEST input control file control data parameter NOPTMAX to -1 and examine which adjustable forward model parameters, if any, are effectively/completely insensitive before performing a potentially costly inverse model run;
11. Slightly modify the PEST input control file to interface with the ERDC LM/SLM software implementation;

12. Perform an inverse model run to estimate the selected adjustable model parameters using the PEST and/or ERDC model calibration software.

As previously mentioned, our software was written to accommodate the popular PEST model independent and input control file protocol; hence, the interested reader is directed to Doherty (2004, 2007a, b, c) for additional details regarding the PEST model independent interface.

2 Examples

The method is best explained by example. For the benefit of the reader, we present numerous examples to illustrate the methods and their related features.

Example 1

In this first example, we will document the steps necessary to perform a LM local search to calibrate a GSSHA hydrologic model for the GCEW using the PEST and ERDC model calibration software.

Step 01 – Obtain forward model. Obtain a GSSHA model for the GCEW. The interested reader is referred to the GSSHA Wiki Knowledge Hub (https://knowledge.usace.army.mil/) for detailed information regarding the GSSHA model in general, including, among others, software download, the user's manual, tutorials, and example applications. The GSSHA model that was obtained for the GCEW consists of the following files:

1. goodwin_cal_1982.prj,
2. goodwin_opt.cmt,
3. goodwin_opt.cif,
4. id_map_1.idx,
5. id_map_2.idx,
6. id_map_3.idx,
7. id_map_4.idx,
8. goodwin.ele,
9. goodwin.gst,
10. goodwin.msk,
11. newhydlocs.inp,
12. extend82.gag,
13. extend82.met, and
14. gssha.exe,

As mentioned, the interested reader is directed to the GSSHA user's manual for a detailed description of GSSHA model features and related input requirements. However, briefly, the GSSHA file with the extension "prj" could be interpreted by the general user as the principal GSSHA project model input file. Upon examination of the project file, one can see references to many of the remaining GCEW GSSHA model input files listed above. Moreover, GSSHA model execution requires its specification at the command prompt. In particular, to execute the GCEW GSSHA hydrologic model, one would type the following at the command prompt and press enter:

gssha.exe goodwin_cal_1982.prj

In so doing, one would see that successful GSSHA GCEW hydrologic model execution commences on 22 May 1982 and ends on 02 July 1982, which is the period that was selected for model calibration (Senarath et al. 2000). It is always helpful, of course, to ensure that the forward model, to calibrate successfully, runs for the designated calibration (and verification) period(s) prior to interfacing it with computer-based model calibration software.

Step 02 – Select adjustable model parameters. Given the structure of the GSSHA GCEW hydrologic model that was obtained in Step 01, for simplicity, model parameters selected for adjustment were chosen to be consistent with those selected for adjustment in the study performed by Senarath et al. (2000). The sixteen GSSHA GCEW model parameters that were selected for adjustment are listed in Table 1.

Step 03 – Prepare templates for forward model input files. For this particular example, the GSSHA model input files with extensions “cmt” (for mapping table file) and “cif” (for channel input file) contain the input parameter values that are designated as adjustable. To support the interface of the GSSHA GCEW model with the independent PEST and ERDC LM implementations, PEST template files are prepared for these two GSSHA GCEW model input files. The files, named goodwin_opt.cmt.tpl and goodwin_opt.cif.tpl, are shown in Appendix 1 and Appendix 2, respectively (Please note that all of the appendices associated with this technical report are available in a separate document made publicly available on the GSSHA USACE Knowledge Hub at https://knowledge.usace.army.mil/). Upon examination of the template files, and also a perusal of the documentation related to template files itself, one can see that the template for the channel input file provides the basis for adjustment of the channel Manning’s n value during a given inverse model run; while the template for the GSSHA input mapping table file provides the basis for adjustment of the remaining selected adjustable model parameters. Two additional files; viz., par2par.dat and

Table 1. Name and meaning of GSSHA adjustable model parameters.

Name	Meaning	Bounds imposed during calibration process
ro_pine	Overland Flow Roughness Coefficient – Forest	0.075-0.45
ro_cottn	Overland Flow Roughness Coefficient – Cotton/Soy Fields	0.075-0.45
ro_pastr	Overland Flow Roughness Coefficient – Pasture	0.075-0.45
ro_gully	Overland Flow Roughness Coefficient – Gullied Land	0.075-0.45
re_pine	Overland Flow Retention Depth – Forest	0.1-2.00 mm
re_cottn	Overland Flow Retention Depth – Cotton/Soy Fields	0.1-2.00 mm
re_pastr	Overland Flow Retention Depth – Pasture	0.1-2.00 mm
re_gully	Overland Flow Retention Depth – Gullied Land	0.1-2.00 mm
hcnd_GSL	Soil Saturated Hydraulic Conductivity – Gullied Land / Silt Loam	0.17-1.3 cm h^{-1}
hcnd_PCL	Soil Saturated Hydraulic Conductivity – Pasture / Clay Loam	0.025-0.41 cm h^{-1}
hcnd_CCL	Soil Saturated Hydraulic Conductivity – Cotton / Clay Loam	0.025-0.41 cm h^{-1}
hcd_PnCL	Soil Saturated Hydraulic Conductivity – Pine / Clay Loam	0.025-0.60 cm h^{-1}
hcd_PnSL	Soil Saturated Hydraulic Conductivity – Pine / Silt Loam	0.025-0.2 cm h^{-1}
hcnd_CSL	Soil Saturated Hydraulic Conductivity – Cotton / Silt Loam	0.07-1.5 cm h^{-1}
hcnd_PSL	Soil Saturated Hydraulic Conductivity – Pasture / Silt Loam	0.08-1.3 cm h^{-1}
ch_rough	Channel Roughness Coefficient	0.0275-0.0375

par2par.tpl, are also prepared, as shown in Appendix 3 and Appendix 4, respectively, to support the interface process. A call of the executable PAR2PAR (Doherty, 2004) will result in an update of the GSSHA model input files with extensions “cmt” and “cif” with the adjustable model parameter values currently specified in the file par2par.dat. In particular, to execute PAR2PAR with the prepared template and input files, one would type the following at the command prompt and press enter:

par2par.exe par2par.dat

In so doing, one would see the display shown in Figure 1 at the command prompt (if one used the files as prepared and shown in Appendices 1 – 4):

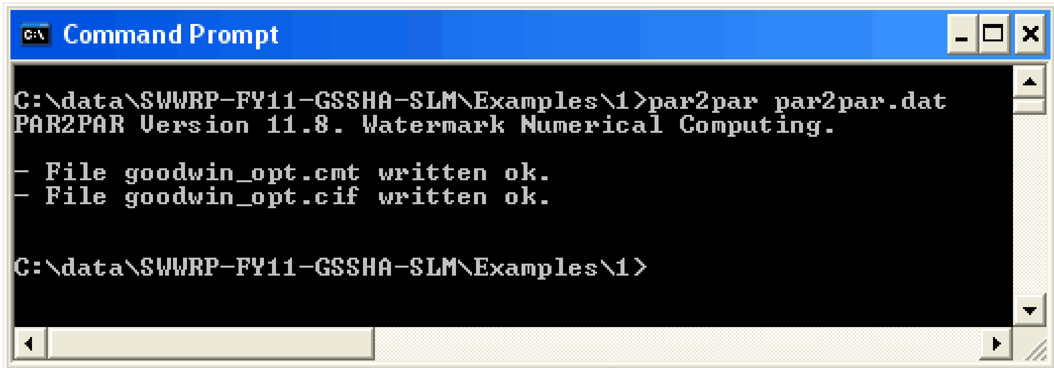

Figure 1. Terminal display for PAR2PAR execution.

Step 04 – Collect and process observed and modeled data. Stream discharge data, in cubic meters per second (cms), measured at the outlet of Goodwin Creek for the period 22 May 1982 – 02 July 1982 will be used to calibrate the GSSHA GCEW continuous simulation hydrologic model. Although available, no data from interior stream flow gauges will be used to calibrate the model. The observed flow data used for model calibration, prepared in site sample file format for eventual use with TSPROC, is presented in Appendix 5. Appendix 6 lists the C source code that was written to process the GCEW GSSHA output file *goodwin_cal_1982.otl* into site sample file format. The GCEW GSSHA output file *goodwin_cal_1982.otl* contains the model simulated flow values, in cms, at the GCEW outlet. An additional file was also prepared as part of the process, named *dates_for_sim_outlet_hydrograph.txt*, and its contents are listed in Appendix 7. The executable file associated with the noted C source code for processing the model simulated flow values into site sample file format is named *mf2ssf.exe* (for modeled flows to site sample file format), and its execution yields a file named *sim_flows_ssf.txt*. To execute *mf2ssf.exe* with the required input files *goodwin_cal_1982.otl* and *dates_for_sim_outlet_hydrograph.txt*, one would type the following at the command prompt and press enter:

```
mf2ssf.exe
```

Step 05 – Prepare TSPROC input file. The objective function will be composed of a single observation group defined as the sum of weighted squared differences between 233 modeled and observed transformed flow values, with all weights assigned a value of 1.0. To reduce heteroscedascity, the Box-Cox transformation,

$$T(Q)_{\lambda} = \left((Q+1)^{\lambda} - 1\right)/ \qquad (1)$$

with λ = 0.3 (Box and Jenkins, 1976; Misirli et al. 2003), will be employed to transform the observed and modeled flows. A TSPROC input file was prepared as part of the interface process and its contents are listed in Appendix 8. To execute TSPROC with the input file tsproc.dat, one would type the following at the command prompt and press enter:

tsproc tsproc.dat

In so doing, one would see the TSPROC execution record at the command prompt, as shown in Figure 2:

Summarizing the record displayed above, execution of TSPROC with the input file tsproc.dat involves the following:

1. Reading the model simulated flows (the series is named mf);
2. Reading the observed flows (the series is named of);
3. Reducing the observed flow data set to a specific date and time window (the reduced series is named of1);
4. Interpolating the modeled flows to the reduced observed flow data set (the interpolated modeled flow series is named imf);
5. Transforming the interpolated modeled flows (the transformed modeled flows, interpolated to the reduced observed data set, is named tmf);
6. Transforming the reduced observed flows (the transformed observed flows, reduced, is named omf);
7. Writing the transformed modeled flows to the output file tsproc_gc1.out, as specified in the file tsproc.dat.

Step 06 – Prepare batch file for model execution. A batch file named model.bat was prepared and its contents are listed in Appendix 9. Its contents sequentially include the following elements for a given parameter set:

1. par2par par2par.dat > nul – modify the forward model input file(s) goodwin_opt.cmt and goodwin_opt.cif (via PAR2PAR).
2. gssha.exe goodwin_cal_1982.prj > nul – forward model execution (i.e., the GSSHA GCEW hydrologic model).
3. mf2ssf > nul – put the forward model simulated flow values into site sample file format.
4. tsproc < tsproc.in > nul – create an interpretable output file (in this case, tsproc_gc1.out), via execution of TSPROC, that includes all of the specified calculated values for quantifying the objective function.

```
Command Prompt

C:\data\SWWRP-FY11-GSSHA-SLM\Examples\1>tsproc

 Program TSPROC is a general time-series processor. It can also be used for
   PEST input file preparation where time series data, or processed time
   series data, comprises at least part of the observation dataset.

 Enter name of TSPROC input file: tsproc.dat
 Enter name for TSPROC run record file: tsproc.rec

 Processing information contained in TSPROC input file tsproc.dat....

 Processing SETTINGS block....
    DATE_FORMAT mm/dd/yyyy
    CONTEXT model_run
    Processing of SETTINGS block complete.

 Processing GET_SERIES_SSF block....
    CONTEXT all
    FILE sim_flows_ssf.txt
    SITE sim_flows
    NEW_SERIES_NAME mf
    DATE_1 05/22/1982
    TIME_1 01:00:00
    DATE_2 07/02/1982
    TIME_2 08:40:00
    Reading site sample file sim_flows_ssf.txt....
    Series "mf" successfully imported from file sim_flows_ssf.txt

 Processing GET_SERIES_SSF block....
    CONTEXT all
    FILE OBS_OUTLET_Q_VALUES_1.txt
    SITE obs_flows
    NEW_SERIES_NAME of
    DATE_1 05/22/1982
    TIME_1 00:00:00
    DATE_2 07/02/1982
    TIME_2 13:58:00
    Reading site sample file OBS_OUTLET_Q_VALUES_1.txt....
    Series "of" successfully imported from file OBS_OUTLET_Q_VALUES_1.txt

 Processing REDUCE_TIME_SPAN block....
    CONTEXT all
    SERIES_NAME of
    NEW_SERIES_NAME of1
    DATE_1 05/22/1982
    TIME_1 01:00:00
    DATE_2 07/02/1982
    TIME_2 08:40:00
    Series "of1" successfully calculated.

 Processing NEW_TIME_BASE block....
    CONTEXT all
    SERIES_NAME mf
    TB_SERIES_NAME of1
    NEW_SERIES_NAME imf
    New series "imf" successfully calculated.

 Processing SERIES_EQUATION block....
    CONTEXT all
    NEW_SERIES_NAME tmf
    EQUATION "3.33333333333333*( (imf+1.0)^0.3 - 1.0 )"
    Series "tmf" successfully calculated using series equation.

 Processing SERIES_EQUATION block....
    CONTEXT all
    NEW_SERIES_NAME tof
    EQUATION "3.33333333333333*( (of1+1.0)^0.3 - 1.0 )"
    Series "tof" successfully calculated using series equation.

 Processing LIST_OUTPUT block....
    CONTEXT all
    FILE tsproc_gc1.out
    SERIES_NAME tmf
    SERIES_FORMAT long
    Writing output file tsproc_gc1.out....
    File tsproc_gc1.out written ok.

 Processing WRITE_PEST_FILES block....
    CONTEXT pest_prep
    Requested actions not undertaken because no CONTEXT option in the
     block coincides with the current run context.

 End of TSPROC input file tsproc.dat - no more blocks to process.
```

Figure 2. Terminal display for TSPROC execution.

Step 07 – Prepare preliminary control file. We are now ready to generate an input control file, the main input file for execution of the LM method not only associated with the PEST, but also our own independent LM implementation. It is a relatively straightforward process using the TSPROC input file, tsproc.dat, that has already been prepared. Simply modify the SETTINGS section at the top of the file as shown directly below

```
####################################################
##########################
### The settings block
####################################################
##########################


START SETTINGS
 DATE_FORMAT mm/dd/yyyy
# CONTEXT compare
# CONTEXT model_run
CONTEXT pest_prep
END SETTINGS
```

After that minor change is made, save the file and execute TSPROC with the input file by typing the following at the command prompt and pressing enter:

```
tsproc tsproc.dat
```

In so doing, one would see the record of TSPROC execution at the command prompt, as shown in Figure 3:

By changing the CONTEXT to "pest_prep" in the SETTINGS block of the TSPROC input file, *tsproc.dat*, the WRITE_PEST_FILES block is now activated; whereas, before it was not. Now, the files *gc_1.pst* and *gc_1.ins* are created during TSPROC execution. The ".pst" file is the noted control file while the ".ins" file is the instruction file for reading the forward model output file(s), in this case the single file *tsproc_gc1.out* (the interested reader is referred to the PEST documentation for explanations related to control and instruction files). The contents of the control/instruction file *gc_1.pst/gc_1.ins* are listed in Appendix 10/Appendix 11. Before proceeding to step 08, change the CONTEXT back to "model_run" in the SETTINGS block of the TSPROC input file, *tsproc.dat*.

```
Command Prompt
C:\data\SWWRP-FY11-GSSHA-SLM\Examples\1>tsproc < tsproc.in

 Program TSPROC is a general time-series processor. It can also be used for
   PEST input file preparation where time series data, or processed time
   series data, comprises at least part of the observation dataset.

 Enter name of TSPROC input file:  Enter name for TSPROC run record file:
 Processing information contained in TSPROC input file tsproc.dat....

 Processing SETTINGS block....
    DATE_FORMAT mm/dd/yyyy
    CONTEXT pest_prep
    Processing of SETTINGS block complete.

 Processing GET_SERIES_SSF block....
    CONTEXT all
    FILE sim_flows_ssf.txt
    SITE sim_flows
    NEW_SERIES_NAME mf
    DATE_1 05/22/1982
    TIME_1 01:00:00
    DATE_2 07/02/1982
    TIME_2 08:40:00
    Reading site sample file sim_flows_ssf.txt....
    Series "mf" successfully imported from file sim_flows_ssf.txt

 Processing GET_SERIES_SSF block....
    CONTEXT all
    FILE OBS_OUTLET_Q_VALUES_1.txt
    SITE obs_flows
    NEW_SERIES_NAME of
    DATE_1 05/22/1982
    TIME_1 00:00:00
    DATE_2 07/02/1982
    TIME_2 13:58:00
    Reading site sample file OBS_OUTLET_Q_VALUES_1.txt....
    Series "of" successfully imported from file OBS_OUTLET_Q_VALUES_1.txt

 Processing REDUCE_TIME_SPAN block....
    CONTEXT all
    SERIES_NAME of
    NEW_SERIES_NAME of1
    DATE_1 05/22/1982
    TIME_1 01:00:00
    DATE_2 07/02/1982
    TIME_2 08:40:00
    Series "of1" successfully calculated.

 Processing NEW_TIME_BASE block....
    CONTEXT all
    SERIES_NAME mf
    TB_SERIES_NAME of1
    NEW_SERIES_NAME imf
    New series "imf" successfully calculated.

 Processing SERIES_EQUATION block....
    CONTEXT all
    NEW_SERIES_NAME tmf
    EQUATION "3.33333333333333*( (imf+1.0)^0.3 - 1.0 )"
    Series "tmf" successfully calculated using series equation.

 Processing SERIES_EQUATION block....
    CONTEXT all
    NEW_SERIES_NAME tof
    EQUATION "3.33333333333333*( (of1+1.0)^0.3 - 1.0 )"
    Series "tof" successfully calculated using series equation.

 Processing LIST_OUTPUT block....
    CONTEXT all
    FILE tsproc_gc1.out
    SERIES_NAME tmf
    SERIES_FORMAT long
    Writing output file tsproc_gc1.out....
    File tsproc_gc1.out written ok.

 Processing WRITE_PEST_FILES block....
    CONTEXT pest_prep
    NEW_PEST_CONTROL_FILE gc_1.pst
    TEMPLATE_FILE par2par.tpl
    MODEL_INPUT_FILE par2par.dat
    NEW_INSTRUCTION_FILE gc_1.ins
    MODEL_COMMAND_LINE model.bat
    OBSERVATION_SERIES_NAME tof
    MODEL_SERIES_NAME tmf
    SERIES_WEIGHTS_EQUATION "1.0"
    SERIES_WEIGHTS_MIN_MAX .10000E-9    1000.0000
    Reading template file par2par.tpl ....
    - 16 parameter names read from file par2par.tpl
    Writing instruction file gc_1.ins ....
    - file gc_1.ins written ok.
    Writing PEST control file gc_1.pst ....
    - file gc_1.pst written ok.

 End of TSPROC input file tsproc.dat - no more blocks to process.

C:\data\SWWRP-FY11-GSSHA-SLM\Examples\1>
```

Figure 3. Terminal display for TSPROC execution.

Step 08 – Modify control file. The parameter data section of the input control file was subsequently manually modified. In particular, initial values, and lower and upper bounds were specified for each of the adjustable model parameters. Its new contents are listed in Appendix 12. The lower and upper bound for each adjustable model parameter was specified based on the available guidance presented in the GSSHA user's manual, and their values are specified in the 5^{th} and 6^{th} columns, respectively, of the parameter data section listed in Appendix 12. For this particular example, the initial value for each adjustable model parameter, specified in the 4^{th} column of the parameter data section listed in Appendix 12, was randomly generated based on a uniform random sample from feasible parameter space defined by the user-supplied lower and upper bounds. To better accommodate scaling issues resulting from the use of different units for different parameters, and in an attempt to decrease the degree of nonlinearity of the parameter estimation problem, the logs of the adjustable model parameters were estimated instead of their native values (as indicated by the presence of "log" uniformly in the second column of the parameter data section of the control file – see Appendix 10 and Appendix 12); past experience has demonstrated that greater efficiency and stability of the parameter estimation process can often be achieved through this means (Skahill and Doherty, 2006). If one did not want to estimate the log of an adjustable model parameter, but rather its native value, then one would replace "log" with "none" in the second entry on the row for that paramter in the parameter data section of the input control file.

Step 09 – Verify control file is functional. One can check to see if there are any errors with the input control file as now prepared by typing the following at the command prompt and pressing enter:

PESTCHEK gc_1

In so doing, one would see the following record of PESTCHEK execution at the command prompt, as shown in Figure 4:

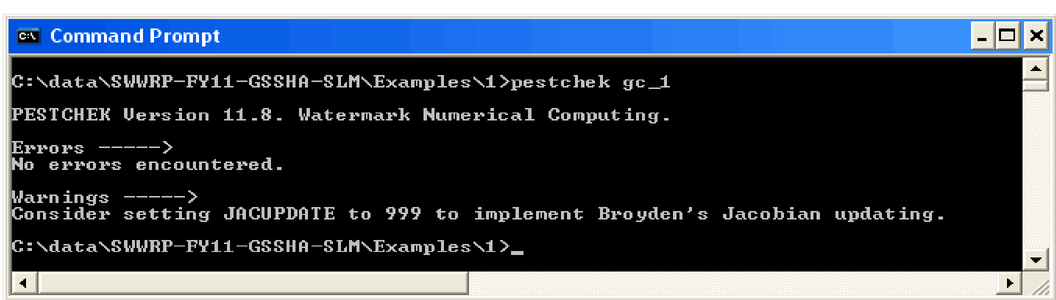

Figure 4. Terminal display for PESTCHEK execution.

Step 10 – Modify control file for use with independent ERDC LM method implementation. To employ our independent ERDC LM implementation, two additional rows of input data are appended to the end of the control data section of the control file *gc_1.pst*, as shown in Appendix 13, and a new file was saved named *gc_1_bu1.pst*. The first of the two added rows has four entries to be specified while the second row that is added contains a single entry. The first of the noted four entries whose values are to be specified on the first row that is appended to the end of the control data section of the input control file signifies whether the LM or SLM method will be employed. If its value is 0, then the LM method will be employed and the remaining three values to be specified are effectively disregarded; whereas, if its value is 1, the SLM method will be employed and the next three values will impact how the SLM method proceeds during a given local search. The second of the noted four entries is also specified to be 0 or 1, and, as just mentioned, is only potentially active if the first entry is specified a value of 1. If its value is set to 1, then there will be a full update of **X**, the model Jacobian matrix, whenever the ratio of the new and old objective function values is greater than a specified input value; viz., the next (the third) entry. The fourth entry is an integer value that can be anywhere between 0 and *m*, inclusive, where *m* is the dimensionality of adjustable model parameter space. It dictates the use of cyclic updating, using finite differences, at each optimization iteration, of anywhere between 0 and *m* individual columns of **X**. The single entry on the second row appended to the end of the control data section of the input control file is associated with a separate functionality that utilizes our independent ERDC SLM implementation, but that is not the focus of this report and hence is not discussed.

Step 11 – Calibrate GSSHA GCEW hydrologic model using PEST LM method implementation. A model independent LM method local search was employed to calibrate the GSSHA GCEW continuous simulation hydrological model using the prepared input control file *gc_1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

pest gc_1

Step 12 – Calibrate GSSHA GCEW hydrologic model using ERDC LM method implementation. Our own independent implementation of the LM method was also employed to calibrate the GSSHA GCEW continuous simulation hydrological model, also in a model independent manner, using the prepared input control file *gc_1_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_1_bu1

Step 13 – Summarize LM local searches. The files *gc_1.rec/gc_1_bu1.rec* summarize the PEST/ERDC software supervised LM-based local searches for the GCEW GSSHA continuous simulation hydrologic model. For the ERDC LM method implementation, the contents of the record file *gc_1_bu1.rec* include:

1. A summary of the inverse model run, including;
   a. The initial parameter values and the initial objective function value;
   b. For each optimization iteration,
      (1) at the beginning,
         (a) The iteration number,
         (b) The number of forward model calls executed so far, and
         (c) The starting objective function value;
      (2) Upon completion of populating the model Jacobian (in this example by way of a full update), a summary of the alternate Marquardt lambda values considered and the related objective function values, and
      (3) At the end of a given iteration, the beginning and ending parameter values;
   c. The reason for the termination of the LM-based local search, and
   d. The total model calls
2. A summary of the optimized parameter values;
3. A linear-based estimate of model (i.e., the final estimated parameter values) uncertainty;
4. A listing of the measured values, the calculated values (associated with the final estimated model), the residuals, the weights associated with each observation, and the name of the observation group associated with each observation;
5. The objective function value associated with the estimated model; and
6. Estimates of the model covariance matrix, its normalized eigenvectors and related eigenvalues, and the parameter correlation coefficient matrix.

The contents of the record file *gc_1_bu1.rec* are listed in Appendix 14. For this particular example, using the independent ERDC LM implementation, the initial and final objective function values are 2.133993E+002/5.842522E+001, 286 total model calls were required to complete the LM local search, and the initial and final estimated parameter values are listed in Table 2.

Table 2. Final calibration parameters for GSSHA GCEW model.

Parameter name	Initial value	Final model
ro_pine	0.079168	0.252474
ro_cottn	0.374765	0.450000
ro_pastr	0.388070	0.450000
ro_gully	0.232765	0.450000
re_pine	1.469107	2.000000
re_cottn	0.700701	2.000000
re_pastr	1.104456	2.000000
re_gully	1.008325	2.000000
hcnd_gsl	1.127866	1.300000
hcnd_pcl	0.139293	0.025000
hcnd_ccl	0.105020	0.025000
hcd_pncl	0.464401	0.025000
hcd_pnsl	0.095130	0.167483
hcnd_csl	1.255712	1.454846
hcnd_psl	0.688709	0.080000
ch_rough	0.030411	0.035732

The file *gc_1_bu1.sen* contains the estimated values for composite parameter sensitivities (see Doherty, 2004 for a definition), which of course can be useful, possibly also in coordination with the information contained in the record file, to identify any adjustable model parameters that may be impairing the LM-based local search due to insensitivity (either individually or by way of correlation). The contents of the file *gc_1_bu1.sen* are listed in Appendix 15. The file *gc_1_bu1.par* contains the final estimated model, and its contents are listed in Appendix 16.

The interested reader is directed to the PEST documentation to interpret the PEST generated output files (e.g., .rec, .sen, .par, …). As with the independent ERDC LM implementation, the total model calls and final objective function value are both listed in the record file (".rec"). The PEST supervised LM method based local search required 305 total model calls to converge, using the same initial values and convergence criteria as the independent ERDC LM implementation.

Example 2

This example will demonstrate how to start, stop and restart an ERDC LM implementation LM method local search, using the GCEW GSSHA hydrologic model that was described in Example 1.

Step 01 – Start the LM local search. Start a LM method local search to calibrate the GCEW GSSHA hydrologic model that was described in Example 1, using the independent ERDC LM implementation, by typing the following at the command prompt and pressing enter:

slm_chl gc_2_bu1

For clarity, the control file *gc_2_bu1* is identical to the control file from Example 1, *gc_1_bu1*.

Step 02 – Prematurely stop the LM local search. Stop the LM local search that was started in the previous step, after at least one optimization iteration has completed, by opening a new command prompt window, changing the directory to the current working directory, and then typing the following at the command prompt and pressing enter:

pstop gc_2_bu1

Step 03 – Restart the LM local search. Restart the LM local search that was prematurely stopped in the previous step by typing the following at the command prompt and pressing enter:

slm_chl gc_2_bu1 /r

Step 04 – Examine and compare LM local search output files with those from Example 1.

Upon examination of the record, sensitivity, and final parameter output files (viz., *gc_2_bu1.rec, gc_2_bu1.sen*, and *gc_2_bu1.par*) and a comparison with the corresponding “rec”, “sen”, and “par” files obtained from Example 1, where the local search ran to completion without any interruption, one would see, as expected, that they are completely or effectively identical. The contents of the files *gc_2_bu1.rec*, *gc_2_bu1.sen*, and *gc_2_bu1.par* are presented in Appendix 17, Appendix 18, and Appendix 19, respectively.

Example 3

In this example, we will document the steps necessary to perform a SLM method based local search to calibrate the GSSHA hydrologic model for the GCEW that was described in Example 1 using the PEST and ERDC model calibration software.

Step 01 – Modify control file. Modify the control data section of the input control file *gc_1.pst* that was prepared in Example 1 as shown below:

```
* control data
restart estimation
 16 233 16 0 1
 1 1 single point 1 0 0
5.0 2.0 0.3 0.03 10 999
5.0 5.0 1.0e-3
0.1 noaui
30 .005 4 4 .005 4
1 1 1
```

The only change, relative to the control data section of the input control file gc_1, is the addition of the final entry of 999 on the 3rd row. This is the value recommended in the PEST manual for activation of the Broyden rank one (secant) update with the PEST implementation of the SLM method. After making the noted change to activate utilization of the Broyden rank one (secant) update, name the new PEST input control file *gc_1b.pst*.

Step 02 – Modify control file for use with independent ERDC SLM method implementation. Modify the control data section of the input control file *gc_1_bu1.pst* that was prepared in Example 1 as shown below:

```
* control data
restart estimation
 16 233 16 0 1
 1 1 single point 1 0 0
5.0 2.0 0.3 0.03 10
```

5.0 5.0 1.0e-3
0.1 noaui
30 .005 4 4 .005 4
1 1 1
1 0 1.0 0
0

The only change, relative to the control data section of the input control file *gc_1_bu1.pst*, is that the first entry on the next to the last row of the control data section is now 1 rather than 0. In consideration of the commentary provided earlier in this report, in particular, in Step 10 of Example 1, we're now employing the Broyden rank one update with no measures employed to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations. In particular, there will be no occasional full updating in the usual manner using finite differences nor any use of cyclic updating, using finite differences, at each optimization iteration, of anywhere between one and *m* individual columns of **X**. After making the noted change, name the new input control file *gc_1_bu2.pst*.

Step 03 – Calibrate GSSHA GCEW hydrologic model using PEST SLM method implementation. A model independent modified LM method local search was employed to calibrate the GSSHA GCEW continuous simulation hydrological model using the prepared input control file *gc_1b.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

pest gc_1b

Step 04 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was also employed to calibrate the GSSHA GCEW continuous simulation hydrological model, also in a model independent manner, using the prepared input control file *gc_1_bu2.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_1_bu2

Step 05 – Summarize LM local searches. The contents of the record files *gc_1b.rec* and *gc_1_bu2.rec* that are associated with the two local searches are provided in Appendix 20 and Appendix 21, respectively. The PEST supervised local search that employed its recommended use of the Broyden rank one update required 347 total model calls to converge. The ERDC SLM method implementation required 62 total model calls to converge. Both local searches used the same initial values and convergence criteria as the local searches performed, using the LM method, in Example 1.

Example 4

This example will demonstrate how to start, stop and restart an ERDC SLM method implementation local search, using the GCEW GSSHA hydrologic model that was described in Example 1.

Step 01 – Start the SLM local search. Start a SLM method local search to calibrate the GCEW GSSHA hydrologic model that was described in Example 1, using the independent ERDC SLM implementation, by typing the following at the command prompt and pressing enter:

slm_chl gc_4_bu2

For clarity, the control file *gc_4_bu2* is identical to the control file from Example 3, *gc_1_bu2*.

Step 02 – Prematurely stop the SLM local search. Stop the SLM local search that was started in the previous step, after at least one optimization iteration has completed, by opening a new command prompt window, changing the directory to the current working directory, and then typing the following at the command prompt and pressing enter:

pstop gc_4_bu2

Step 03 – Restart the SLM local search. Restart the SLM local search that was prematurely stopped in the previous step by typing the following at the command prompt and pressing enter:

slm_chl gc_4_bu2 /r

Step 04 – Examine and compare SLM local search output files with those from Example 3. Upon examination of the record, sensitivity, and final parameter output files (viz., *gc_4_bu2.rec*, *gc_4_bu2.sen*, and *gc_4_bu2.par*) and a comparison with the corresponding “rec”, “sen”, and “par” files obtained from Example 3, where the local search ran to completion without any interruption, one would see, as expected, that they are completely or effectively identical. The contents of the files *gc_4_bu2.rec*, *gc_4_bu2.sen*, and *gc_4_bu2.par* are presented in Appendix 22, Appendix 23, and Appendix 24, respectively.

Example 5

This example demonstrates a variation of the ERDC SLM implementation to calibrate the GCEW GSSHA continuous simulation hydrologic model, wherein cyclic updating is employed, employing one column at a time in this case, in an attempt to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the control data section of the input control file *gc_1_bu2.pst* that was prepared in Example 3 as shown below:

```
* control data
restart estimation
 16 233 16 0 1
 1 1 single point 1 0 0
5.0 2.0 0.3 0.03 10
5.0 5.0 1.0e-3
0.1 noaui
30 .005 4 4 .005 4
1 1 1
1 0 1.0 1
0
```

The only change, relative to the control data section of the input control file *gc_1_bu2*, is that the final entry on the next to the last row of the control data section is now 1 rather than 0. In consideration of the commentary provided earlier in this report, in particular, in Step 10 of Example 1, we’re now employing the Broyden rank one update, of course, but also with one measure employed to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations. In particular, there will be cyclic updating, using finite differences, at each optimization iteration, of one column of **X**. After making the noted change, name the new input control file *gc_5_bu1.pst*.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_5_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_5_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_5_bu1.rec, gc_5_bu1.sen*, and *gc_5_bu1.par* are presented in Appendix 25, Appendix 26, and Appendix 27, respectively. By employing one column cyclic updating, 79 total model calls were required for the SLM local search to converge.

Example 6

This example demonstrates a similar variation of the ERDC SLM implementation to that presented in Example 5, again with the intent of calibrating the GCEW GSSHA hydrologic model, but in this case cyclic updating is employed using three columns at a time, in an attempt to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the control data section of the input control file *gc_5_bu1.pst* that was prepared in Example 5 as shown below:

```
* control data
restart estimation
 16 233 16 0 1
 1 1 single point 1 0 0
5.0 2.0 0.3 0.03 10
5.0 5.0 1.0e-3
0.1 noaui
30 .005 4 4 .005 4
1 1 1
1 0 1.0 3
0
```

The only change, relative to the control data section of the input control file *gc_5_bu1*, is that the final entry on the next to the last row of the control data section is now 3 rather than 1. In consideration of the commentary provided earlier in this report, in particular, in Step 10 of Example 1, we're now employing the Broyden rank one (secant) update, of course, but also with one measure employed to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations. In particular, there will be cyclic updating, using finite differences, at each optimization iteration, of three columns of **X**. After making the noted change, name the new input control file *gc_6_bu1.pst*.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_6_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_6_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_6_bu1.rec, gc_6_bu1.sen*, and *gc_6_bu1.par* are presented in Appendix 28, Appendix 29, and Appendix 30, respectively. By employing three column cyclic updating, 154 total model calls were required for the SLM local search to converge.

Example 7

As with Example 6, this example also employs a variation of SLM using the ERDC SLM implementation to calibrate the GCEW GSSHA hydrologic model, wherein three column cyclic updating is employed to mitigate against the potential that $\mathbf{X}_{new}$ may eventually become a poor approximation to the true Jacobian after some optimization iterations. However, this example differs from Example 6 in that minor changes will be made to the input control file to indicate that only forward finite differences will be employed to approximate derivatives for the entire duration of the inverse model run.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the control data section of the input control file *gc_6_bu1.pst* that was prepared in Example 6 as shown below:

* parameter groups

ro_pine relative 1.0000E-02 0.000 always_2 2.000 parabolic

ro_cottn relative 1.0000E-02 0.000 always_2 2.000 parabolic

ro_pastr relative 1.0000E-02 0.000 always_2 2.000 parabolic

ro_gully relative 1.0000E-02 0.000 always_2 2.000 parabolic

re_pine relative 1.0000E-02 0.000 always_2 2.000 parabolic

re_cottn relative 1.0000E-02 0.000 always_2 2.000 parabolic

re_pastr relative 1.0000E-02 0.000 always_2 2.000 parabolic

re_gully relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcnd_gsl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcnd_pcl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcnd_ccl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcd_pncl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcd_pnsl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcnd_csl relative 1.0000E-02 0.000 always_2 2.000 parabolic

hcnd_psl relative 1.0000E-02 0.000 always_2 2.000 parabolic

ch_rough relative 1.0000E-02 0.000 always_2 2.000 parabolic

The fifth entry for each row (wherein each row is related to an adjustable model parameter) in the parameter groups section of the input control file was uniformly changed from “switch” to “always_2”. In so doing, derivatives calculations will be approximated using forward finite differences for the entire duration of the inverse model run; whereas, previously, derivative calculations initially started out using forward differences, but switched to central derivative calculations (better accuracy relative to forward differences, but at the cost of twice the number of forward model calls required to estimate the derivative) based on the value of a control data section control file input parameter value (the interested reader is referred to the PEST user’s manual for additional details). After making the noted change, name the new input control file *gc_7_bu1.pst*.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_7_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_7_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_7_bu1.rec, gc_7_bu1.sen*, and *gc_7_bu1.par* are presented in Appendix 31, Appendix 32, and Appendix 33, respectively. By employing three column cyclic updating together with forward differences for derivates calculation for the entire inverse model run, 112 total model calls were required for the SLM local search to converge.

Example 8

This example demonstrates the capacity to effectively reduce the number of adjustable model parameters for a given LM or SLM based local search. This is made possible by modifying the input control file in a manner such that the values for some of the parameters that were originally designated in a control file to be adjustable simply piggy-back off of the remaining parameters that in fact are treated as adjustable during a given LM or SLM based local search.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. In this example, we will modify the input control file so that now only the following five parameters will be treated as adjustable:

ro_pastr
re_pastr
hcd_pncl
hcnd_psl
ch_rough

The value of the remaining eleven GSSHA GCEW model parameters will be adjusted during a LM or SLM local search such that the ratio remains fixed with that of an actual adjustable model parameter that each individual parameter is tied to, as will be designated in the input control file. In particular, modify the parameter groups and parameter data sections of the input control file *gc_7_bu1.pst* that was prepared in Example 7 as shown below:

* parameter groups

ro_pine relative 1.0000E-02 0.000 switch 2.000 parabolic

ro_cottn relative 1.0000E-02 0.000 switch 2.000 parabolic

ro_pastr relative 1.0000E-02 0.000 switch 2.000 parabolic

ro_gully relative 1.0000E-02 0.000 switch 2.000 parabolic

re_pine relative 1.0000E-02 0.000 switch 2.000 parabolic

re_cottn relative 1.0000E-02 0.000 switch 2.000 parabolic

re_pastr relative 1.0000E-02 0.000 switch 2.000 parabolic

re_gully relative 1.0000E-02 0.000 switch 2.000 parabolic

hcnd_gsl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcnd_pcl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcnd_ccl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcd_pncl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcd_pnsl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcnd_csl relative 1.0000E-02 0.000 switch 2.000 parabolic

hcnd_psl relative 1.0000E-02 0.000 switch 2.000 parabolic

ch_rough relative 1.0000E-02 0.000 switch 2.000 parabolic

* parameter data

ro_pine tied factor 0.079168 0.075 0.45 ro_pine 1.000 0.000 1

ro_cottn tied factor 0.374765 0.075 0.45 ro_cottn 1.000 0.000 1

ro_pastr log factor 0.388070 0.075 0.45 ro_pastr 1.000 0.000 1

ro_gully tied factor 0.232765 0.075 0.45 ro_gully 1.000 0.000 1

re_pine tied factor 1.469107 0.1 2.00 re_pine 1.000 0.000 1

re_cottn tied factor 0.700701 0.1 2.00 re_cottn 1.000 0.000 1

re_pastr log factor 1.104456 0.1 2.00 re_pastr 1.000 0.000 1

re_gully tied factor 1.008325 0.1 2.00 re_gully 1.000 0.000 1 hcnd_gsl tied factor 1.127866 0.17 1.3 hcnd_gsl 1.000 0.000 1

hcnd_pcl tied factor 0.139293 0.025 0.41 hcnd_pcl 1.000 0.000 1

hcnd_ccl tied factor 0.105020 0.025 0.41 hcnd_ccl 1.000 0.000 1

hcd_pncl log factor 0.464401 0.025 0.60 hcd_pncl 1.000 0.000 1

hcd_pnsl tied factor 0.095130 0.025 0.2 hcd_pnsl 1.000 0.000 1

hcnd_csl tied factor 1.255712 0.07 1.5 hcnd_csl 1.000 0.000 1

hcnd_psl log factor 0.688709 0.08 1.3 hcnd_psl 1.000 0.000 1

ch_rough log factor 0.030411 0.0275 0.0375 ch_rough 1.000 0.000 1

ro_pine ro_pastr
ro_cottn ro_pastr
ro_gully ro_pastr
re_pine re_pastr
re_cottn re_pastr
re_gully re_pastr
hcnd_gsl hcnd_psl
hcnd_pcl hcd_pncl
hcnd_ccl hcd_pncl
hcd_pnsl hcnd_psl
hcnd_csl hcnd_psl

The modifications that are made in the parameter data section effect the change that we want to illustrate in this example. In the second column of the first sixteen rows of that section, one now sees five instances of “log”, indicating the five, rather than sixteen, adjustable parameters for the GSSHA GCEW model, and eleven instances of “tied”, which indicate the remaining parameters whose values now will simply piggy-back off of the adjustable model parameter values during the local search. At the end of the parameter data section, there are now eleven additional rows each containing two entries, the first entry being a parameter that is now designated as “tied”, and the second entry being a parameter that now remains as adjustable (indicated on the second entry of the first sixteen rows of the parameter data section, as in this case, by “log”, but an adjustable model parameter may also, as mentioned earlier, be specified at the same entry location with “none” to indicate estimation of the native value rather than its log transform) to which the first parameter is now tied. The noted ratio between a parameter that is designated as tied and the adjustable parameter that it is tied to is based on their initial values, which are also, as previously mentioned, specified in the input control file. For example, for the tied parameter ro_pine, which is tied to the adjustable model parameter ro_pastr, the ratio of their initial values is 0.204. The interested reader is referred to the PEST user's manual for additional details. By using tied parameters as specified above, with this example, the original GSSHA GCEW hydrologic model now has uniform values for the overland roughness value and retention depth, and only two hydraulic conductivity values, one for clay loam and one for silt loam rather than the original seven hydraulic conductivity values that were based on a cross product of soil type (clay loam or silt loam) and land cover type (gullied land, pasture, cotton, pine). Such manual parsimonizing, via the input control file, of the hydrologic and/or environmental forward model, may be prudent/necessary if, for example, insufficient observation data are available to effectively justify the level of model complexity originally incorporated into the forward model. After making the noted change, name the new input control file *gc_8_bu1.pst*.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_8_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_8_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_8_bu1.rec, gc_8_bu1.sen*, and *gc_8_bu1.par* are presented in Appendix 34, Appendix 35, and Appendix 36, respectively. By employing three column cyclic updating for the entire inverse model run with now what are five, rather than sixteen adjustable model parameters, 45 total model calls were required for the SLM local search to converge. Examining the final model as specified in either the ".rec" or ".par" file, we see that the ratios for the eleven tied parameters remain the same as they were at the beginning of the local search (see Table 3 directly below). With the information that is provided in the record file one could generate a table similar to that of Table 3 at the end of each optimization iteration, and if one did so one would see that the initial ratios remain fixed throughout the duration of the local search.

Table 3. Ratio of GSSHA GCEW tied parameters to their adjustable counterparts.

Tied Parameter			Adjustable Parameter Tied To				
Name	Initial Value	Final Value	Name	Initial Value	Final Value	Ratio at Initial Values	Ratio at Final Values
ro_pine	0.07917	0.09180	ro_pastr	0.38807	0.45	0.20400	0.20400
ro_cottn	0.37477	0.43457	ro_pastr	0.38807	0.45	0.96571	0.96572
ro_gully	0.23277	0.26991	ro_pastr	0.38807	0.45	0.59980	0.59980
re_pine	1.46911	2.66033	re_pastr	1.10446	2	1.33016	1.33016
re_cottn	0.70070	1.26886	re_pastr	1.10446	2	0.63443	0.63443
re_gully	1.00833	1.82592	re_pastr	1.10446	2	0.91296	0.91296
hcnd_gsl	1.12787	0.91026	hcnd_psl	0.68871	0.555833	1.63765	1.63765
hcnd_pcl	0.13929	0.00750	hcd_pncl	0.46440	0.025	0.29994	0.29996
hcnd_ccl	0.10502	0.00565	hcd_pncl	0.46440	0.025	0.22614	0.22616
hcd_pnsl	0.09513	0.07678	hcnd_psl	0.68871	0.555833	0.13813	0.13813
hcnd_csl	1.25571	1.01344	hcnd_psl	0.68871	0.555833	1.82328	1.82328

Example 9

This example is a follow-on to Example 8, and demonstrates an additional way to reduce the number of adjustable model parameters that will be estimated through modification of the input control file. In particular, one can fix what were originally designated to be adjustable model parameters at their initial values.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the parameter data section of the input control file *gc_8_bu1.pst* that was prepared in Example 8 as shown below:

```
* parameter data
ro_pine tied factor 0.079168 0.075 0.45 ro_pine 1.000 0.000 1
ro_cottn tied factor 0.374765 0.075 0.45 ro_cottn 1.000 0.000 1
ro_pastr log factor 0.388070 0.075 0.45 ro_pastr 1.000 0.000 1
ro_gully tied factor 0.232765 0.075 0.45 ro_gully 1.000 0.000 1
re_pine tied factor 1.469107 0.1 2.00 re_pine 1.000 0.000 1
re_cottn tied factor 0.700701 0.1 2.00 re_cottn 1.000 0.000 1
```

re_pastr log factor 1.104456 0.1 2.00 re_pastr 1.000 0.000 1

re_gully tied factor 1.008325 0.1 2.00 re_gully 1.000 0.000 1

hcnd_gsl tied factor 1.127866 0.17 1.3 hcnd_gsl 1.000 0.000 1

hcnd_pcl tied factor 0.139293 0.025 0.41 hcnd_pcl 1.000 0.000 1

hcnd_ccl tied factor 0.105020 0.025 0.41 hcnd_ccl 1.000 0.000 1

hcd_pncl log factor 0.464401 0.025 0.60 hcd_pncl 1.000 0.000 1

hcd_pnsl tied factor 0.095130 0.025 0.2 hcd_pnsl 1.000 0.000 1

hcnd_csl tied factor 1.255712 0.07 1.5 hcnd_csl 1.000 0.000 1

hcnd_psl log factor 0.688709 0.08 1.3 hcnd_psl 1.000 0.000 1

ch_rough fixed factor 0.037500 0.0275 0.0375 ch_rough 1.000 0.000 1

ro_pine ro_pastr
ro_cottn ro_pastr
ro_gully ro_pastr
re_pine re_pastr
re_cottn re_pastr
re_gully re_pastr
hcnd_gsl hcnd_psl
hcnd_pcl hcd_pncl
hcnd_ccl hcd_pncl
hcd_pnsl hcnd_psl
hcnd_csl hcnd_psl

The only modification is in the second entry of the sixteenth row of the section where before the entry contained “log” it now contains “fixed” to designate that the parameter named “ch_rough”, representing the channel roughness value that is uniformly used throughout the GSSHA GCEW model, is fixed at its initial value for the entire inverse model run. Hence, in combination with the 11 tied parameters from Example 8, there are now only four parameters that will be adjusted during the calibration process. After making the noted change, name the new input control file *gc_9_bu1.pst*.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_9_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_9_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_9_bu1.rec, gc_9_bu1.sen*, and *gc_9_bu1.par* are presented in Appendix 37, Appendix 38, and Appendix 39, respectively. Upon examination of the record file, one can see that the parameter "ch_rough" remained fixed at its intial value for the duration of the SLM local search.

Example 10

One can evaluate parameter (in)sensitivity and uncertainty; albeit local and linear, both during and upon completion of an LM or SLM based local search. With both the PEST and independent ERDC LM implementations, one can assess these quantities prior to performing what may potentially be a relatively expensive inverse model run. This example demonstrates how to estimate parameter (in)sensitivity and uncertainty at a given location in adjustable model parameter space without performing a local search.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the control data section of the control file from Example 1; viz., *gc_1_bu1.pst*, as shown below:

```
* control data
restart estimation
 16 233 16 0 1
 1 1 single point 1 0 0
5.0 2.0 0.3 0.03 10
5.0 5.0 1.0e-3
0.1 noaui
-1 .005 4 4 .005 4
1 1 1
0 0 1.0 0
0
```

and rename it *gc_10_bu1.pst*. The only modification is to the first entry on the 7^{th} row of the control data section. What was previously specified to be 30 has been changed to -1. The value of -1 indicates to both the PEST and independent ERDC LM implementations to perform either *m* or 2*m* forward model calls (dependent upon whether forward or central finite differences are employed) to populate the column space of the matrix **X**. Once the model sensitivity matrix **X** is estimated with a full update using either forward or central finite differences, approximations for model parameter sensitivity and uncertainty can then be determined, and as previously mentioned, that information is stored in the ".sen" and ".rec" files. This particular input control file control data section input parameter can take on integer values greater than or equal to -1. For specified values greater than or equal to 0, the input value specifies the maximum number of optimization iterations that are permitted for a given LM or SLM based local search. The interested reader is referred to the PEST user's manual for more information.

Step 02 – Run the GSSHA GCEW hydrologic model using ERDC SLM method implementation m times to estimate parameter (in)sensitivity and uncertainty. The independent ERDC implementation of the SLM method will be used to populate the model sensitivity matrix **X** in a model independent manner, using the prepared input control file gc_10_bu1.pst (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_10_bu1

Step 03 – Summarize LM. The contents of the files *gc_10_bu1.rec* and *gc_10_bu1.sen* are presented in Appendix 40 and Appendix 41, respectively.

Example 11

In this example we demonstrate how to include prior information into the LM/SLM parameter estimation process using our independent ERDC LM/SLM implementation. The interested reader is referred to the PEST user's manual for more information.

Step 01 – Modify control file for use with independent ERDC SLM method implementation. Modify the input control file to calibrate the GCEW GSSHA hydrologic model as shown in Appendix 42. The notable modifications are listed below:

1. The number of unique pieces of prior information, in this case four, are specified at the 4th entry of the 2nd row in the control data section of the input control file
2. The number of observation groups, in this case two, are specified at the 5th entry of the 2nd row in the control data section of the input control file
3. The observation groups section listed after the parameter data section in the input control file lists the names of the two observation groups; viz., "tmf" and "pinfo"
4. The prior information section listed after the model command line section in the input control file lists the four unique pieces of prior information; viz., specified preferred parameter values for the four adjustable model parameters. The weights for each of these four additional observations are uniformly assigned a value of 100 (determined by manually adjusting the uniformly assigned weights and performing a single model run (by setting NOPTMAX equal to zero) and observing the computed objective function values), so that the observation group name "pinfo" is of a similar magnitude to the observation named "tmf" at the start of the estimation process.

Save the file as *gc_11_bu1.pst*. This example is very similar to Example 9; however, here we are using prior information and one column cyclic updating; whereas, with Example 9 we used no prior information and three column cyclic updating.

Step 02 – Calibrate GSSHA GCEW hydrologic model using ERDC SLM method implementation. Our independent implementation of the SLM method was employed to calibrate the GSSHA GCEW continuous simulation hydrological model, in a model independent manner, using the prepared input control file *gc_11_bu1.pst* (and the related input files) by typing the following at the command prompt and pressing enter:

slm_chl gc_11_bu1

Step 03 – Summarize LM local search. The contents of the files *gc_11_bu1.rec*, *gc_11_bu1.sen*, and *gc_11_bu1.par* are presented in Appendix 43, Appendix 44, and Appendix 45, respectively. Examining the final estimated parameter set, we see that it is close to the preferred parameter state that we expressed in the prior information section of the input control file, and that the uncertainty associated with the final model is reduced when compared with the final model obtained in Example 9. With Example 9, all but one of the estimated parameters hit their bounds.

3 Results and Discussion

As was mentioned in the introduction, one of the objectives of this report was to provide the interested reader with an intuitive sense of how our implementation of the SLM method works, and to also demonstrate how our LM/SLM implementation compares with its counterparts as implemented in the popular PEST software. The third, and fifth through seventh examples addressed this objective, and Table 4 summarizes results obtained from Examples 1, 3, 5, and 6 using the independent ERDC LM/SLM implementations. Table 5 summarizes results obtained from Examples 1 and 3 using the PEST LM/SLM implementations.

Table 4. Summary of results (final objective function values and total model calls for local search to converge) associated with Examples 1, 3, 5, and 6 using the independent ERDC LM/SLM implementations.

		Broyden Update (SLM)		
		No full update		
	Full Update (LM)	no cyclic updating	1 column cyclic updating	3 column cyclic updating
Final Objective Function Value	58.43	59.56	60.07	60.76
Number of Total Model Calls	286	62	79	154

Table 5. Summary of results (final objective function values and total model calls for local search to converge) associated with Examples 1 and 3 using the PEST LM/SLM implementations.

	Full Update (LM)	Broyden Update (SLM)
Final Objective Function Value	60.94	58.49
Number of Total Model Calls	305	347

Figures 5 and 6 are plots of the transformed observed and simulated flows that constitute the final objective function values for the LM and SLM runs from Examples 1 and 3, respectively, using the independent ERDC LM/SLM implementations. The figures provide the interested reader with a means to effectively compare the final objective function values that were obtained in the two examples in terms of a statistical summary (i.e., R^2

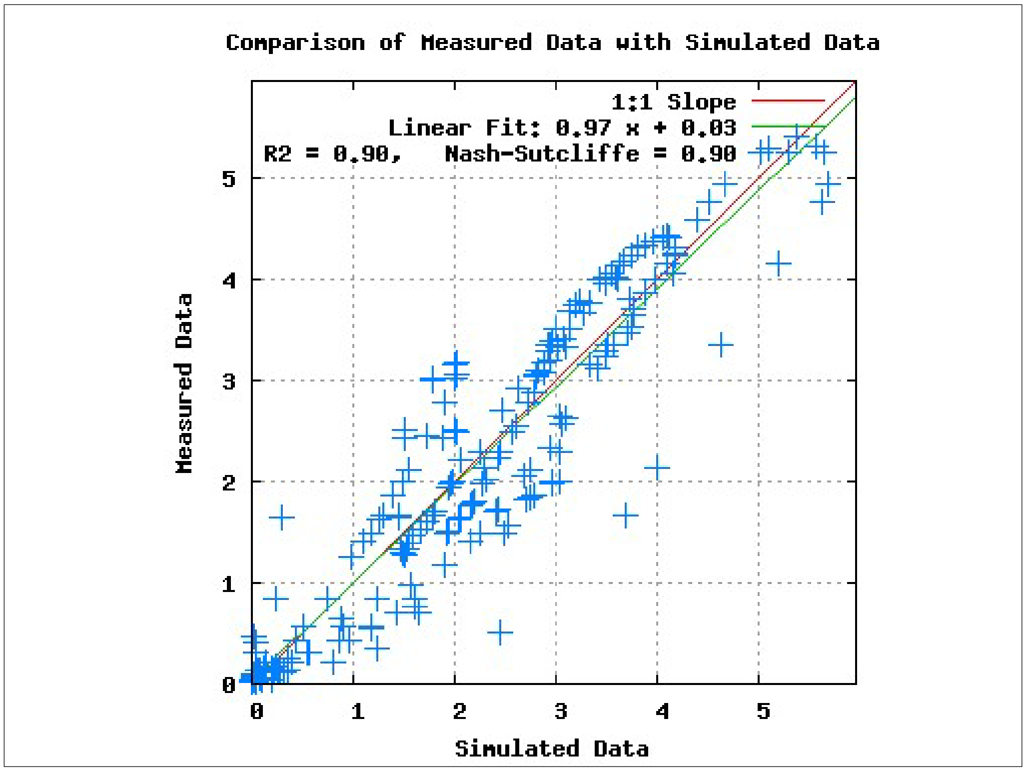

Figure 5. Plot of transformed observed and simulated flows, associated with the final model, for Example 1 using the independent ERDC LM implementation.

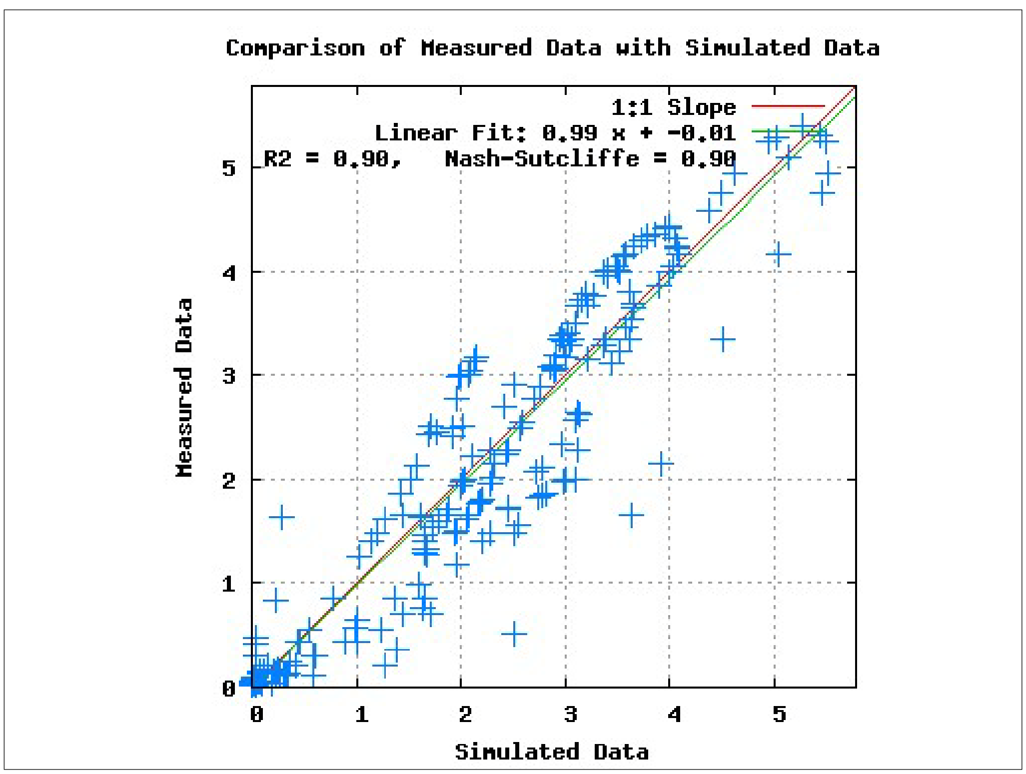

Figure 6. Plot of transformed observed and simulated flows, associated with the final model, for Example 3 using the independent ERDC SLM implementation.

and Nash-Sutcliffe efficiency score) and also by way of a scatter plot of the transformed observed data and its model simulated counterparts. Clearly, there is little difference in terms of fit between the two examples. The PEST SLM implementation required additional model calls to achieve an effectively equivalent model to measurement misfit; whereas, the ERDC SLM implementation obtained an effectively equivalent model to measurement misfit with a highly noteworthy 78 percent reduction in total model calls.

Examining the results that are presented in Table 4, we see that as the number of columns used for cyclic updating increases, so does the total number of model calls required for the local search to converge, of course in each case, with the same convergence criteria imposed. One would expect, but it cannot be guaranteed as there are multiple measures in place to terminate a given LM/SLM local search, that as the number of columns selected for cyclic updating tends to the number of adjustable model parameters (with no measures in place for a full update to occur), that the total number of model calls will tend to the number of model calls required for the LM local search to converge. While not present in this case, the typical pattern is for modest reductions in objective function improvement as one decreases the number of columns used for cyclic updating (Skahill et al., 2010).

Example 7 demonstrated that a minor change to the input control file is all that is required to indicate that forward finite differences will be employed to approximate derivates for the entire duration of the inverse model run. In particular, in Example 7, the fifth entry of each row in the parameter groups section of the input control file was uniformly changed from “switch” to “always_2”. In so doing, derivates calculations were approximated using forward finite differences for the entire duration of the inverse model run; whereas, for previous examples, derivatives calculations initially started out using forward differences, but switched to central derivatives calculations (better accuracy relative to forward differences, but at the cost of twice the number of forward model calls required to estimate the derivate) based on the value of a control data section control file input parameter value. While not demonstrated in this report by way of a specific example, if the fifth entry in the parameter groups section is specified as “always_3”, derivates calculations will be approximated using central finite differences for the entire duration of the inverse model run. With the ERDC LM/SLM implementation, central derivatives can be approximated either in the usual manner ($(f(x+\Delta x)-f(x-\Delta x))/2\Delta x$) or by fitting a parabola through the three points. For all of the examples considered in this report, when central derivatives were used, we fit a parabola to the three points, and this was indicated by the term “parabolic” in the last entry of the parameter groups section of the input control file. If the last entry of the parameter groups section in the input control file is replaced with “outside_pts”, then central derivates will be computed in the usual manner.

Example 8 demonstrated the capacity to effectively reduce the number of adjustable model parameters for a given LM or SLM based local search while using the independent ERDC LM/SLM implementation. In Example 8, it was demonstrated that this is made possible by modifying the input control file in a manner such that the values for some of the parameters that were originally designated in a control file to be adjustable simply piggy-back off of the remaining parameters that in fact are treated as adjustable during a given LM or SLM based local search. Example 9 demonstrated an additional mechanism to reduce the number of adjustable model parameters that will be estimated through modification of the input control file. In particular, Example 9 demonstrated that one can fix what were originally designated to be adjustable model parameters at their initial values. Example 10 demonstrated how to estimate parameter (in)sensitivity and uncertainty at a given location in adjustable model parameter space without performing a local search. One can evaluate parameter (in)sensitivity and uncertainty; albeit local and linear, both during and upon completion of an LM or SLM based local search. With the independent ERDC LM implementations, one can assess these quantities prior to performing what may potentially be a relatively expensive inverse model run. Example 11 demonstrated how one can bias a LM/SLM local search by including prior information; that is, by specifying a preferred parameter state.

4 Summary and Conclusions

In this report, some of the salient features/capabilities of the independent ERDC LM/SLM implementations were demonstrated, by way of eleven examples, using the GCEW GSSHA continuous simulation hydrologic model. This article focuses on the practical application of just one approach that has been developed to support the computer-based calibration of a hydrologic and/or environmental model. Future reports will present the practical application of additional methods (e.g., multilevel single linkage and efficiency enhancements to the CMAES evolutionary strategy) that have been developed to support the computer-based calibration of hydrologic and/or environmental models, likely in a similar manner. Planned research and development efforts are to include the independent ERDC LM/SLM implementations, discussed herein by way of example, directly into the GSSHA simulator. The user of the independent ERDC software implementations of the LM/SLM methods accepts and uses them at his/her own risk. Any questions, comments, and/or concerns regarding the use of the independent ERDC software implementations of the LM/SLM methods with the GSSHA model should be directed to the first author. The interested reader is encouraged to contact the second author with any questions, comments, and/or concerns related to the GSSHA hydrologic simulation model.

References

Baginska, B., W. Milne-Home, and P. S. Cornish. 2003. *Modelling nutrient transport in Currency Creek, NSW with AnnAGNPS and PEST*. Environmental Modelling & Software 18, 801-808.

Bicknell, B. R., J. C. Imhoff, J. L. Kittle, T. H. Jobes, and A. S. Donigian. 2001. *HSPF User's Manual*. Mountain View, CA: Aqua Terra Consultants.

Box, G. E. P., and G. M. Jenkins. 1976. *Time Series Analysis: Forecasting and Control*. San Francisco, CA: Holden-Day.

Broyden, C. G., 1965. A Class of Methods for Solving Nonlinear Simultaneous Equations. *Maths. Comp*. 19, 577-593.

de Groot-Hedlin, C., and S. Constable. 1990. Occam's inversion to generate smooth, two-dimensional models from magnetotelluric data. *Geophysics*, 55(12), 1631-1624.

Doherty, J. 2004. *PEST: Model Independent Parameter Estimation*. Fifth edition of user manual. Brisbane, Australia: Watermark Numerical Computing.

Doherty, J. 2007a. Addendum to the PEST Manual. Brisbane, Australia: Watermark Numerical Computing.

Doherty, J. 2007b. Addendum to the PEST Manual. Brisbane, Australia: Watermark Numerical Computing.

Doherty, J. 2007c. *PEST Surface Water Utilities*. Brisbane, Australia: Watermark Numerical Computing.

Doherty, J., and J. M. Johnston. 2003. *Methodologies for calibration and predictive analysis of a watershed model*. J. American Water Resources Association, 39(2): 251-265.

Doherty, J., and B. E. Skahill. 2006. An Advanced Regularization Methodology for Use in Watershed Model Calibration. *Journal of Hydrology*, 327, 564– 577.

Downer, C. W., and F. L. Ogden. 2003a. *GSSHA user's manual: Gridded surface subsurface hydrologic analysis, version 1.43 for WMS 6.1*. Technical Report. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Downer, C. W., and F. L. Ogden. 2003b. Prediction of runoff and soil moistures at the watershed scale: Effects of model complexity and parameter assignment. *Water Resources Research*, 39(3): 1045.

Frankenstein, S., and G. Koenig. 2004. *Fast All-season Soil STrength (FASST)*. SR-04-1. Hanover, NH: U.S. Army Engineer Research and Development Center, Cold Regions Research and Engineering Laboratory.

Gallagher, M., and J. Doherty. 2007a. Predictive error analysis for a water resource management model. *Journal of Hydrology*, (334), 513–533.

Gallagher, M., and J. Doherty. 2007b. Parameter estimation and uncertainty analysis for a watershed model. Environmental Modelling & Software 22, 1000-1020.

Goegebeur, M., and V. R. N. Pauwels. 2007. Improvement of the PEST parameter estimation algorithm through Extended Kalman Filtering. *Journal of Hydrology*, (337), 436-451.

Gutiérrez-Magness, A. L., and R. H. McCuen. 2005. Effect of Flow Proportions on HSPF Model Calibration Accuracy. J. Hydrologic Engrg. 10, 343-352.

Haydon, S., and A. Deletic. 2007. Sensitivity testing of a coupled Escherichia coli-Hydrologic catchment model. *Journal of Hydrology*, (338), 161-173.

Iskra, I., and R. Droste. 2007. Application of Non-Linear Automatic Optimization Techniques for Calibration of HSPF. Water Environment Research, 79 (6), 647-659.

Kim, S. M., B. L. Benham, K. M. Brannan, R. W. Zeckoski, and J. Doherty. 2007. Comparison of hydrologic calibration of HSPF using automatic and manual methods. Water Resour. Res., 43, W01402, doi:10.1029/2006WR004883.

Kunstmann, H., J. Krause, and S. Mayr. 2006. Inverse distributed hydrological modelling of Alpine catchments. *Hydrology and Earth System Sciences*. 10 (3), 395-412.

Levenberg, K., 1944. A method for the solution of certain problems in least squares. Q. Appl. Math., 2, 164-168.

Madsen, K., H. B. Nielsen, and O. Tingleff. 2004. Methods for Non-Linear Least Squares Problems. Informatics and Mathematical Modelling. Technical University of Denmark.

Maneta, M. P., G. B. Pasternack, W. W. Wallender, V. Jetten, and S. Schnabel. 2007. Temporal instability of parameters in an event-based distributed hydrologic model applied to a small semiarid catchment. *Journal of Hydrology*, 341, 207-221.

Marquardt, D. 1963. An algorithm for least-squares estimation of non-linear parameters. SIAM J. Appl. Math., 11, 431-441.

Menke, W. 1984. *Geophysical Data Analysis*. Orlando, FL: Academic Press Inc.

Misirli, F., H. V. Gupta, S. Sorooshian, and M. Thiemann. 2003. Bayesian recursive estimation of parameter and output uncertainty for watershed models, pp. 113-124, in: Calibration of 20 Watershed Models, edited by: Duan, Q., Gupta, H. V., Sorooshian, S., et al., American Geophysical Union, Washington, DC.

Moore, C., and J. Doherty. 2005. The role of the calibration process in reducing model predictive error. Water Resources Research. 41(5) W05050.

Rode, M., U. Suhr, and G. Wriedt. 2007. Multi-objective calibration of a river water quality model--Information content of calibration data. *Ecological Modelling*, 204, 129-142.

Rose, K. A., B. A. Megrey, F. E. Werner, and D. M. Ware. 2007. Calibration of the NEMURO nutrient-phytoplankton-zooplankton food web model to a coastal ecosystem: Evaluation of an automated calibration approach. *Ecological Modelling*, (202), 38-51.

Santanello Jr., J. A., C. D. Peters-Lidard, M. E. Garcia, D. M. Mocko, M. A. Tischler, M. S. Moran, and D. P. Thoma. 2007. Using remotely-sensed estimates of soil moisture to infer soil texture and hydraulic properties across a semi-arid watershed. Remote Sensing of Environment, (110), 79-97.

Senarath, S. U. S., F. L. Odgen, C. W. Downer, and H. O. Sharif. 2000. On the calibration and verification of two-dimensional, distributed, Hortonian, continuous watershed models. Water Resources Res., 36 (6), 1495-1510.

Skahill, B., and J. Doherty. 2006. Efficient accommodation of local minima in watershed model calibration. *Journal of Hydrology*, (329), 122-139.

Skahill, B. E., and J. S. Baggett. 2006. More Efficient Derivative-based Watershed Model Calibration. Eos Trans. AGU, 87(52), Fall Meet. Suppl., Abstract 1521.

Skahill, B., J. Baggett, S. Frankenstein, and C. W. Downer. 2010. "Efficient Levenberg-Marquardt Method Based Model Independent Calibration." Environmental Modelling & Software (24), 517–529.

Tonkin, M., and J. Doherty. 2005. A hybrid regularised inversion methodology for highly parameterised models. Water Resources Research. Vol. 41, W10412, doi:10.1029/2005WR003995.

Zyvoloskia, G., E. Kwicklis, A. A. Eddebbarh, B. Arnold, C. Faunt, and B. A. Robinson. 2003. The site-scale saturated zone flow model for Yucca Mountain: calibration of different conceptual models and their impact on flow paths. *Journal of Contaminant Hydrology*, 62–63, 731–750.

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13. SUPPLEMENTARY NOTES

14. ABSTRACT
The objective of this technical note is to demonstrate, by way of example(s), how to use the Engineer Research and Development Center (ERDC) implementation of the Levenberg-Marquardt (LM) and Secant LM (SLM) method for model independent parameter estimation to calibrate a Gridded Surface Subsurface Hydrologic Analysis (GSSHA) hydrologic model. The purpose is not to present or focus on the theory which underlies the parameter estimation method(s), but rather to carefully describe how to use the ERDC software implementation of the secant LM method that accommodates the PEST model independent interface to calibrate a GSSHA hydrologic model. We will consider variations of our Secant LM (SLM) implementation in attempts to provide the interested reader with an intuitive sense of how the method works. We will also demonstrate how our LM/SLM implementation compares with its counterparts as implemented in the popular PEST software.

15. SUBJECT TERMS

Calibration	GSSHA
Efficient local search	Secant Levenberg-Marquardt

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