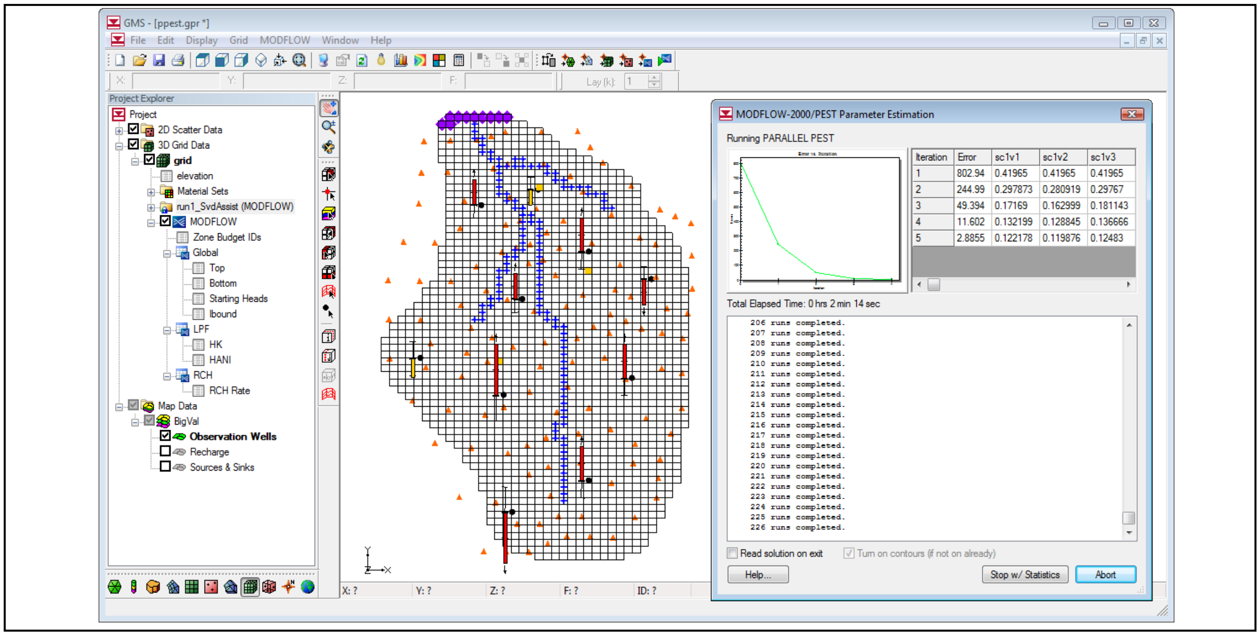
GMS

v. 9.2

GMS 9.2 Tutorial

MODFLOW – Advanced PEST

Pilot Points, SVD-Assist, Parallel PEST



Objectives

Learn how to parameterize a MODFLOW model and run PEST to obtain optimal parameter values. Experiment with truncated singular value decomposition (SVD), SVD-Assist, and parallel PEST.

Prerequisite Tutorials

- MODFLOW - Model Calibration
- MODFLOW - Automated Parameter Estimation
- MODFLOW – PEST Pilot Points

Required Components

- Grid
- Geostatistics
- Map
- MODFLOW
- Inverse Modeling
- Parallel Pest

Time

- 30-60 minutes

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1 Contents

2 Introduction

The *MODFLOW-Automated Parameter Estimation* tutorial describes the basic functionality of PEST provided in GMS. It illustrates how to parameterize a MODFLOW model and run PEST to obtain optimal parameter values. This tutorial describes new PEST features available in GMS starting with version 7.1. These features include: Truncated Singular Value Decomposition (SVD), SVD-Assist, and Parallel PEST.

Each of these features is intended to decrease the amount of time necessary for PEST to complete the optimization process. The SVD options focus on identifying and removing insensitive parameters from the model inversion process, while Parallel PEST speeds up the inversion process by running more models simultaneously.

2.1 Outline

This is what you will do:

1. Open a MODFLOW model and solution.
2. Run PEST using SVD.
3. Run Parallel PEST.

4. Run Parallel PEST using SVD-Assist.

3 Description of Problem

The model we will be calibrating in this tutorial is the same model featured in the *MODFLOW-Model Calibration* tutorial. The model includes observed flow data for the stream and observed heads at a set of scattered observation wells. The conceptual model for the site consists of a set of recharge and hydraulic conductivity zones. These zones will be marked as parameters and an inverse model will be used to find a set of recharge and hydraulic conductivity values that minimize the calibration error. We will utilize two methods for model parameterization: polygonal zones and pilot point interpolation.

4 Getting Started

Let's get started.

1. If necessary, launch GMS. If GMS is already running, select the *File* | *New* command to ensure that the program settings are restored to their default state.

5 Reading in the Project

First, we will read in the modeling project:

1. Select the *Open* button .
2. Locate and open the **Tutorials\MODFLOW\advPEST** directory.
3. Open the file entitled **start.gpr**.

You should see a MODFLOW model with a solution and a set of map coverages. Three of the coverages are the source/sink, recharge, and hydraulic conductivity coverages used to define the conceptual model. The active coverage contains a set of observed head values from observation wells. If you switch to the source/sink coverage, you will notice that an observed flow value has been assigned to the stream network.

~~6 Running PEST with SVD Option~~

~~We will now run PEST with the current model.~~

1. ~~Select the *File* | *Save As* command.~~
2. ~~Enter **run1.gpr** for the file name and select the *Save* button.~~
3. ~~Select the *MODFLOW* | *Run MODFLOW* menu command.~~

~~This model will run for 10 iterations. Depending on the speed of your computer this may take a few minutes. Notice that after 10 iterations the final model error is 109. We will now run the model with the SVD option turned on.~~

4. ~~Select the *Close* button to exit the dialog.~~

5. ~~Select the *MODFLOW | Parameter Estimation* menu command.~~

6. ~~Turn **on** the *Use SVD* option.~~

7. ~~Select the *SVD Options* button.~~

~~This dialog allows the user to edit the values of the MAXSING, EIGTHRESH, and EIGWRITE variables associated with the SVD process. MAXSING is the maximum number of singular values to include in the inversion process. This value is problem dependent. Often a more appropriate approach is to use EIGTHRESH to limit the number of singular values to include in the inversion process. EIGTHRESH is a ratio of lowest to highest eigenvalues at which truncation is implemented. Only those parameters are estimated whose eigenvalue divided by the maximum eigenvalue exceeds EIGTHRESH. Finally, EIGWRITE controls items written to the *.svd file. If the value of EIGWRITE is 1 then a more verbose *.svd file is written. The default values work well for the current model. The user is referred to the PEST Manual pp 8-9 for more information on SVD.~~

8. ~~Select *OK* to exit the *SVD Options* dialog.~~

~~In the interest of time we are going to limit the number of PEST iterations.~~

9. ~~In the *NOPTMAX. Max number of iterations* field enter **5**.~~

10. ~~Select *OK* to exit the PEST dialog.~~

11. ~~Select the *File | Save As* command.~~

12. ~~Enter **run2** for the name of the project and select *Save*.~~

13. ~~Select the *MODFLOW | Run MODFOW* menu command.~~

~~Notice that on this model run PEST was able to complete the run in 5 iterations and the final error was less than 1.0.~~

14. ~~Select *Close* to exit the dialog.~~

~~7~~6 Running Parallel PEST

All of the steps required to run PEST must also be followed to run Parallel PEST. The only additional inputs required by the user are to specify the number of models that can be run simultaneously by PEST as well as a "WAIT" variable. The WAIT variable is described by the PEST documentation as the amount of time that PEST and PSLAVE will pause at certain strategic places in their communication. Normally the default value should work fine. However, if either PEST or PSLAVE reports a sharing violation on your hard drive then you should increase the value of the WAIT variable.

To illustrate Parallel PEST and SVD-Assist we will start with a different project.

1. Select the *File* | *New* command and select *No* at the prompt to save your changes.
2. Select the *Open* button.
3. Locate and open the **Tutorials\MODFLOW\advPEST** directory.
4. Open the file entitled **run1_SvdAssist.gpr**.
5. Select the *MODFLOW* | *Global Options* menu command.
6. Select the *Parameter Estimation* option under *Run options* and select *OK* to exit the dialog.
7. Select the *MODFLOW* | *Parameter Estimation* menu command.
8. Change the *NOPTMAX. Max number of iterations* to **2**.
9. Turn on the *Use Parallel Pest* toggle.
10. Select *OK* to exit the dialog.

~~8~~7 Saving the Project and Running Parallel PEST

Now we will save our project prior to running parallel PEST.

1. Select the *File* | *Save As* command.
2. Locate the **Tutorials\MODFLOW\ppest** folder.
3. Enter **run2_PPest** for the project name and select the *Save* button.
4. Select the *Run MODFLOW* button.

At this point new command prompt windows are created depending on the number of slaves that can run on your computer. These command prompts that are initially minimized are running PSLAVE. Also notice that the *MODFLOW-2000/PEST Parameter Estimation* dialog is available from GMS. This dialog reads the output from Parallel PEST and updates the model error and parameter values for each PEST iteration. If the user selects the *Abort* button from this dialog then all of the Parallel PEST processes will be terminated. In addition, selecting the *Stop w/ Statistics* button will allow Parallel PEST to stop at its current iteration.

Parallel PEST should take a few minutes to run two iterations with the current model. On each of the PEST iterations MODFLOW is run 129 times which is once for each pilot point that is being estimated.

5. Select the *Close* button on the *MODFLOW-2000/PEST Parameter Estimation* dialog.

~~9~~8 Running Parallel PEST with SVD-Assist

Now we will run Parallel PEST again with the SVD-Assist option turned on. This process is particularly advantageous for models that have hundreds or thousands of parameters (such as pilot points).

SVD-Assist involves 3 basic steps. First, PEST runs MODFLOW once for every parameter in order to compute a matrix. This information is used to create super parameters that are combinations of the parameters originally specified. Second, SVDAPREP is run to create a new PEST control file. The options for SVDAPREP are entered by selecting the *SVD-Assist Options* button. For more information on each of these options see the PEST manual in section 8.5.4.2. The most important option entered is the *Specify # super param* and this is set to **No** by default. When this option is set to No, then the information written to the *.svd file will be used to specify the number of super parameters. Third, PEST runs using the new control file written by SVDAPREP. This should result in significantly fewer model runs for each PEST iteration. This often results in an order of magnitude reduction in the number of runs required for each PEST iteration.

1. Select the *MODFLOW | Parameter Estimation* menu command.
2. Change the *NOPTMAX. Max number of iterations* to **15**.
3. Turn on the *Use SVD* and the *Use SVD-Assist* toggles.
4. Select *OK* to exit the dialog.
5. Select the *File | Save As* menu command.
6. Enter **run2_SvdAssist** for the project name and select the *Save* button.
7. Select the *Run MODFLOW* button .

After the first PEST iteration, notice that each PEST iteration now only requires 11 MODFLOW runs instead of 129. When PEST finishes running the error should be around 0.1.

8. Select the *Close* button on the *MODFLOW-2000/PEST Parameter Estimation* dialog.

When PEST runs with SVD-Assist the parameter values are not written to the *.par file because this file contains the values for the super parameters. The base parameter values are written to a *.bpa file.

9. Select the *MODFLOW | Parameters* menu command.
10. Select the *Import Optimal Values* command.
11. Select the **run2_SvdAssist.bpa** file and select *Open*.

~~10~~9 Changing the Regularization Option

We will now change our regularization option to use the *Preferred value regularization* method.

12. Select the *MODFLOW | Parameter Estimation* command.
13. Turn **off** the *Preferred homogeneous regularization* toggle.
14. Turn **on** the *Preferred value regularization* toggle and select *OK*.

~~11~~10 Saving the Project

We are now ready to save and run PEST.

15. Select the *File | Save As* command.
16. Save the project with the name **mfpest_pilot_pref_val.gpr**.

~~11.1~~10.1 Prior Information equations

You can compare the different prior information equations written from GMS by looking at the *.rpf files in the MODFLOW directories. The prior information equations for *Preferred homogenous regularization*, found in mfpest_pilot.rpf should look like the following:

```
pi0 1.0 * log(sc1v1) - 1.0 * log(sc1v2) = 0.0 0.0018556829581 regul_1
pi1 1.0 * log(sc1v1) - 1.0 * log(sc1v3) = 0.0 0.0003314571401 regul_1
pi2 1.0 * log(sc1v1) - 1.0 * log(sc1v4) = 0.0 0.0000983152822 regul_1
```

Notice that these equations define a relationship between the different pilot points. In addition, the weight applied to theses equations changes as shown by the last number written to each line. In contrast, the prior information equations for *Preferred value regularization*, found in mfpest_pilot_pref_val.rpf shown below, have the same weight applied and define a preferred value for each point.

```
pi0 1.0 * log(sc1v1) = -0.877359449863 1.0 regul_1
pi1 1.0 * log(sc1v2) = -0.87738275528 1.0 regul_1
pi2 1.0 * log(sc1v3) = -0.764383137226 1.0 regul_1
```


~~12~~11 Running PEST

We will now run PEST.

17. Select the *Run MODFLOW* button.

PEST will take several minutes to run. When PEST is finished, you will see a message in the text portion of the window and the *Abort* button will change to *Close*.

Once PEST is finished, you can read in the solution.

18. Select the *Close* button. Make sure that the *Read solution on exit* toggle is checked.

You may wish to view the new HK field by importing the optimal values and examining the contours like we did previously.

~~13~~12 Multiple Parameters using Pilot Points

In GMS, pilot points can be used with HK and RCH parameters. Also, you can have multiple HK (or RCH) parameters that use the same or different pilot points. We will now create a second HK parameter and create a new set of pilot points.

19. In the *Project Explorer*, turn **off** the 3D grid.

20. Select the *Hydraulic Conductivity* coverage from the *Project Explorer*.

21. Select the *Select Polygons* tool and double-click the polygon surrounding the river in the middle of the model.

22. Enter a value of **-60.0** for the *Horizontal K* and select *OK*.

23. Right-click on the *Hydraulic Conductivity* coverage and select the *Map To MODFLOW/MODPATH* command.

~~13.1~~12.1 Creating a Second Set of Pilot Points

Now we will create another scatter point set for the new HK parameter. We will again create a 2D grid and convert it to a scatter point set.

24. In the *Project Explorer* right-click on the empty space and then, from the pop-up menu, select the *New | 2D Grid* command.

25. Enter the values shown in the following figure to create the 2D Grid. Make sure to enter **0.5** for the Origin in the Z-Dimension section as this will be the value assigned to the scatter points created from the grid. Also, make sure that the *Grid type* near the bottom of the dialog is set to *Cell centered*.

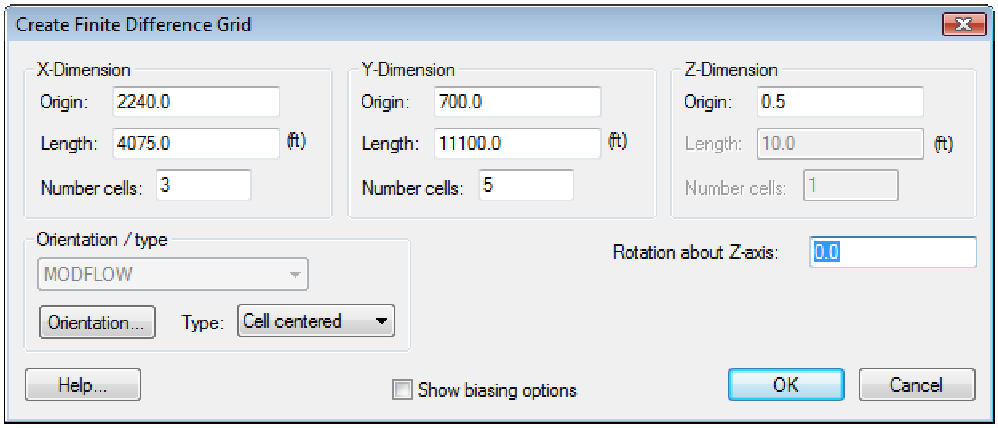

Figure 1. Create 2D Grid dialog.

26. Right-click on the 2D Grid and select the *Convert to 2D Scatter Points* command.

27. Enter **HK_60** for the name of the new scatter set.

28. Right-click on the 2D Grid and select the *Delete* command

~~13.2~~12.2 Creating the New HK Parameter

Now we will create a new parameter for the pilot points that we created.

29. Select the *MODFLOW | Parameters* command.

30. Select the *Initialize From Model* button.

31. Turn on the toggle in the *Param. Est. Solve* column and the *Log Xform* column for the **HK_60** parameter.

32. Turn on the *Pilot Points* option for parameter **HK_60** by selecting the drop down arrow in the *Value* column. Then select **<Pilot points>** from the drop down list.

33. Click on the button above the drop down arrow in the *Value* column for parameter **HK_60**. Make sure that the scatter point set selected in the dialog is **HK_60** and select *OK* to exit the dialog.

~~13.3~~12.3 Using Pilot Points with RCH Parameter

We will also use pilot points to estimate recharge with our model. For the RCH parameter we will use the same set of pilot points that the HK_30 parameter uses but we will create a new data set with starting values for the RCH parameter.

34. Right-click the *Recharge* coverage from the *Project Explorer* and select the *Attribute Table* command.

35. Change the *Feature type* to **Polygons** at the top of the dialog.

36. In the *All* row change the value of *Recharge rate* to **-150.0** and select *OK*.

37. Right-click on the *Recharge* coverage and select the *Map To MODFLOW/MODPATH* command.

Creating New Starting Values for the RCH Parameter

We will create a new data set on the HK scatter set to provide the starting values for the RCH parameter.

38. Select the **HK** scatter point set from the *Project Explorer*.

39. Select the *Edit* | *Data Set Calculator* command.

40. Enter **1e-5** in the *Expression* field and enter **RCH** in the *Result* field.

41. Select the *Compute* button to create a new data set with all values equal to 1.0e-5.

42. Select *Done* to exit the dialog.

Editing the RCH Parameters

Now we will edit the RCH parameters to use pilot points.

43. Select the *MODFLOW* | *Parameters* command.

44. Delete the **RCH_180** and **RCH_210** parameters by selecting the row and then the *Delete* button.

45. Turn on the *Pilot Points* option for parameter **RCH_150** by selecting the drop down arrow in the *Value* column. Then select **<Pilot points>** from the drop down list.

46. Click on the button above the drop down arrow in the *Value* column for parameter **RCH_150**. Make sure that the scatter point set selected in the dialog is **HK** and that the data set is **RCH**.

47. Select *OK* twice to exit both dialogs.

~~14~~13 Saving the Project and Running PEST

We are now ready to save and run PEST.

48. Select the *File* | *Save As* command.

49. Save the project with the name **mfpest_pilot_2zones.gpr**.

When pilot points are assigned to both HK and RCH parameters, the prior information equations for the HK and RCH parameters are assigned to different regularization groups. According to John Doherty, this helps PEST to differentiate weighting amongst pertinent prior information equations (read as: PEST works better with this option).

50. Select the *Run MODFLOW* button.

PEST will take several minutes to run. When PEST is finished, you will see a message in the text portion of the window and the *Abort* button will change to *Close*. Once PEST is finished, you can read in the solution.

51. Select the *Close* button. Make sure that the *Read solution on exit* toggle is checked.

You may wish to view the new HK field by importing the optimal values and examining the contours like we did previously.

~~15~~14 A Note on Highly Parameterized Models

The model that we have just created has over 100 parameters. This is a fairly simple MODFLOW model that converges rather quickly; most real world problems take longer to run. Thus, it may not be practical to run MODFLOW over 100 times for each PEST iteration. However, PEST supports a very innovative method known as SVD-Assist which can dramatically reduce the number of model runs required for each PEST iteration. When you combine SVD-Assist with Parallel PEST it becomes practical to use PEST with models containing hundreds or even thousands of parameters. You can learn more about these methods in the tutorial: *MODFLOW – Advanced PEST*

~~16~~15 Conclusion

This concludes the *MODFLOW – Advanced PEST: SVD, SVD-Assist, Parallel PEST* tutorial. Here are the things that you should have learned in this tutorial:

- GMS supports the SVD option for PEST.
- You can use Parallel PEST from GMS.
- You can run SVD-Assist from GMS by simply turning on the option. When you are using pilot points and you select the *Import Optimal Values* button, a new data set is created for the 2D scatter points.
- You can view the final hydraulic conductivity field calculated by PEST by selecting the **HK** item in the *Project Explorer* below the **LPF** package.
- You can use pilot points with **HK** and **RCH** parameters and assign pilot points to different parameter zones.

