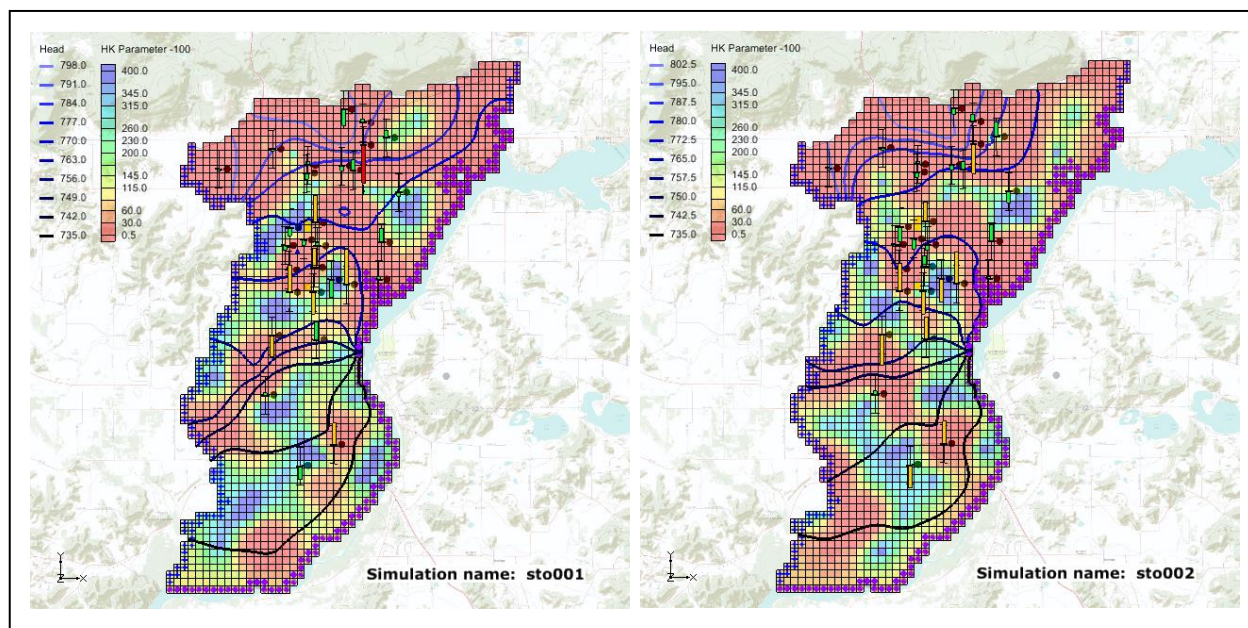


## GMS 10.0 Tutorial

# MODFLOW – Stochastic Modeling, PEST Null Space Monte Carlo I

Use PEST to create multiple calibrated MODFLOW simulations



## Objectives

The PEST Null Space Monte Carlo modeling option for MODFLOW is described. Null Space Monte Carlo is used to create multiple calibrated MODFLOW models.

### Prerequisite Tutorials

- MODFLOW – Advanced PEST

### Required Components

- Grid Module
- Map Module
- MODFLOW
- PEST
- Parallel PEST
- Stochastic Modeling

### Time

- 60-80 minutes

**AQUAVEO™**



<b>1</b>	<b>Introduction .....</b>	<b>2</b>
1.1	Outline.....	3
<b>2</b>	<b>Description of Problem .....</b>	<b>3</b>
<b>3</b>	<b>Getting Started .....</b>	<b>4</b>
<b>4</b>	<b>Reading in the Project .....</b>	<b>4</b>
<b>5</b>	<b>The MODFLOW Run Options .....</b>	<b>7</b>
<b>6</b>	<b>Parameter Options .....</b>	<b>8</b>
<b>7</b>	<b>Saving the Project and Running PEST .....</b>	<b>8</b>
<b>8</b>	<b>Reading in and Viewing the MODFLOW Solutions .....</b>	<b>10</b>
<b>9</b>	<b>Conclusion.....</b>	<b>14</b>
<b>10</b>	<b>Further Reading.....</b>	<b>14</b>

## 1 Introduction

---

GMS supports three methods for performing stochastic simulations: parameter randomization, indicator simulations, and PEST Null Space Monte Carlo. The first two approaches are described in separate tutorials. This tutorial will introduce the PEST Null Space Monte Carlo method.

This tutorial borrows heavily from John Doherty's *PEST Workshop* document. Further, all credit for this approach to quantifying model uncertainty goes to Doherty and his co-authors.

There is always a significant amount of uncertainty associated with a groundwater model. This uncertainty can be associated with the conceptual model or the field data or the input parameters of the model. Some model parameters, such as hydraulic conductivity, are particularly prone to uncertainty. This uncertainty can be reduced by calibrating a model to observation data (monitoring wells, stream flows, etc.). However, even a well-calibrated model can have significant uncertainty associated with it.

The challenge with a groundwater model is to explore the uncertainty while maintaining a calibrated model (i.e., a good fit with field-measured values). The generation of model input parameters that will respect calibration constraints is a time-consuming matter since a parameter estimation exercise must be undertaken for each new set of parameters. However, two tools provided with PEST greatly reduce the amount of time required to perform calibration-constrained Monte Carlo analysis of a groundwater model. The first is the use of SVD-Assist in the calibration process. The second is the pre-calibration null space<sup>1</sup> projection of differences between the stochastic parameter fields and the simplified "calibration parameter field" that is decreed to "calibrate the model." By using both of these utilities, it is possible to obtain parameter sets that respect both the stochastic variability of the subsurface as well as the field-measured values; this is accomplished with only a handful of runs per realization.

---

<sup>1</sup> The null space is comprised of individual parameters, or combinations of parameters, that have no effect on model outputs under calibration conditions. These combinations of parameters can therefore be added to any set of parameters that calibrates the model, thus producing another set of parameters that also calibrates the model.

In this tutorial, the user will start with a calibrated MODFLOW model. Pilot points have been used to estimate hydraulic conductivity (HK), and PEST, running in SVD-Assist mode, was used to calibrate the model. This model will be used as a starting point to create additional calibrated models with different HK fields.

## 1.1 Outline

---

Here are the steps of the tutorial:

1. Open a MODFLOW that has been calibrated using PEST with SVD-Assist.
2. Set up a Null Space Monte Carlo run.
3. Run Parallel PEST with SVD-Assist and Null Space parameter projection for multiple model runs.

## 2 Description of Problem

---

A groundwater model for an unconfined alluvial aquifer in Wisconsin, USA, is shown in Figure 1. The alluvium is highly variable in terms of hydraulic conductivity. In some areas, it is composed of high conductivity, well-sorted gravels, while in other areas it is composed of low conductivity, sandy silts. While the location and description of the model area are accurate, the observation wells used in this exercise are not field-measured values.

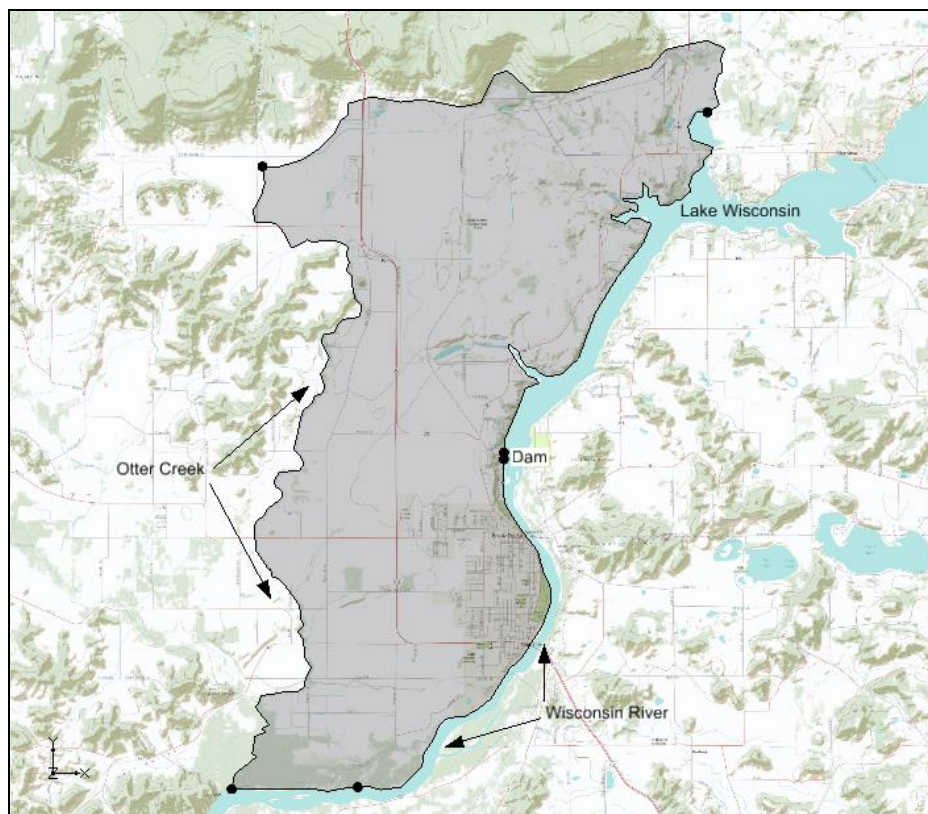


Figure 1 Study area

The model is bounded on the east by Lake Wisconsin and on the south by the Wisconsin River. A stream (Otter Creek) is used as the western boundary. Based on observed heads, it is assumed that a significant amount of recharge occurs along the northern boundary. The aquifer becomes very thin as the user approaches the northern and western boundaries.

### 3 Getting Started

---

Do the following to get started:

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

### 4 Reading in the Project

---

First, read in a project containing the MODFLOW solution:

1. Select the **Open**  button.



2. Locate and open the *Tutorials\MODFLOW\sto\_pest\_nsmc\_I* directory.
3. Select the file entitled “start.gpr.”
4. Click **Open**.

The user should see a one layer MODFLOW model and observation wells similar to the figure below.

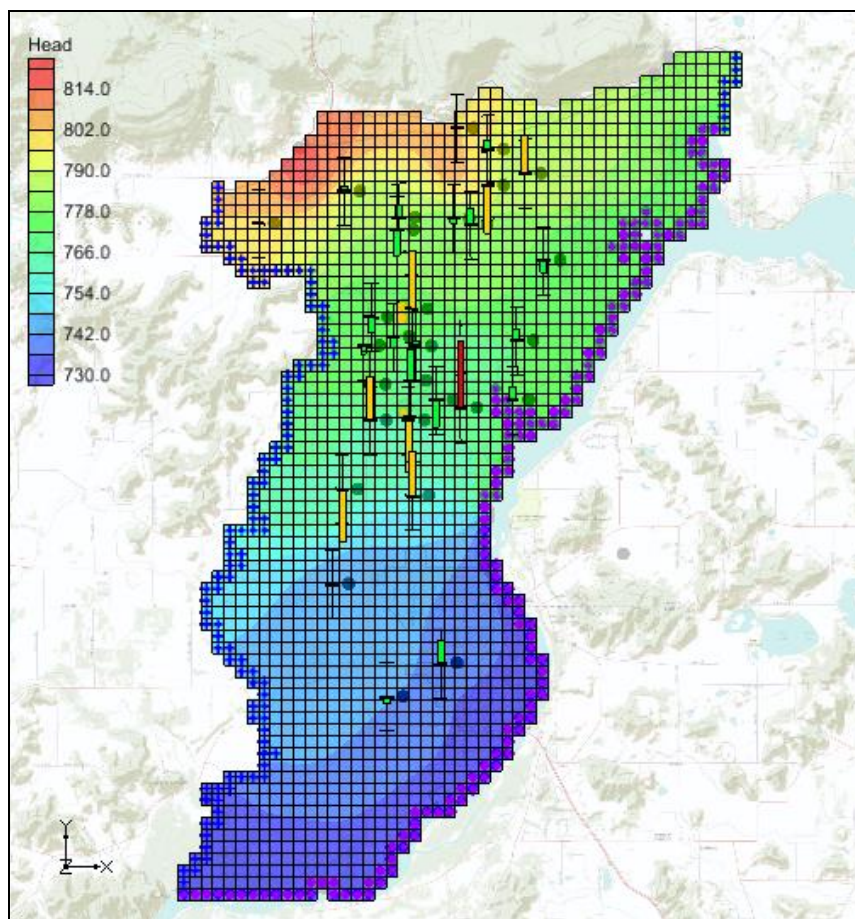







Figure 2 Calibrated MODFLOW model

5. Expand the following items in the Project Explorer:
  - “3D Grid Data”  folder
  - “grid (1)”  item
  - “start (MODFLOW)”  folder
  - “Parameters”  folder.
6. Right-click on the “start (MODFLOW)”  folder and select the properties command to see the error associated with the model.

This model is fairly well calibrated. Notice that the Root Mean Squared Residual for Heads is about 1.33 and that the Sum of Squared Weighted Residual of Heads is about 197.5. Most of the computed heads at the observation wells are within acceptable limits (green targets); several of the observations wells have computed heads just outside of acceptable limits (yellow targets) and one observation well has significant error (red target).

7. Select the **Done** button to exit the dialog.
8. Select the “HK Parameter -100” dataset in the *Project Explorer*. The user’s display should look similar to the figure below.

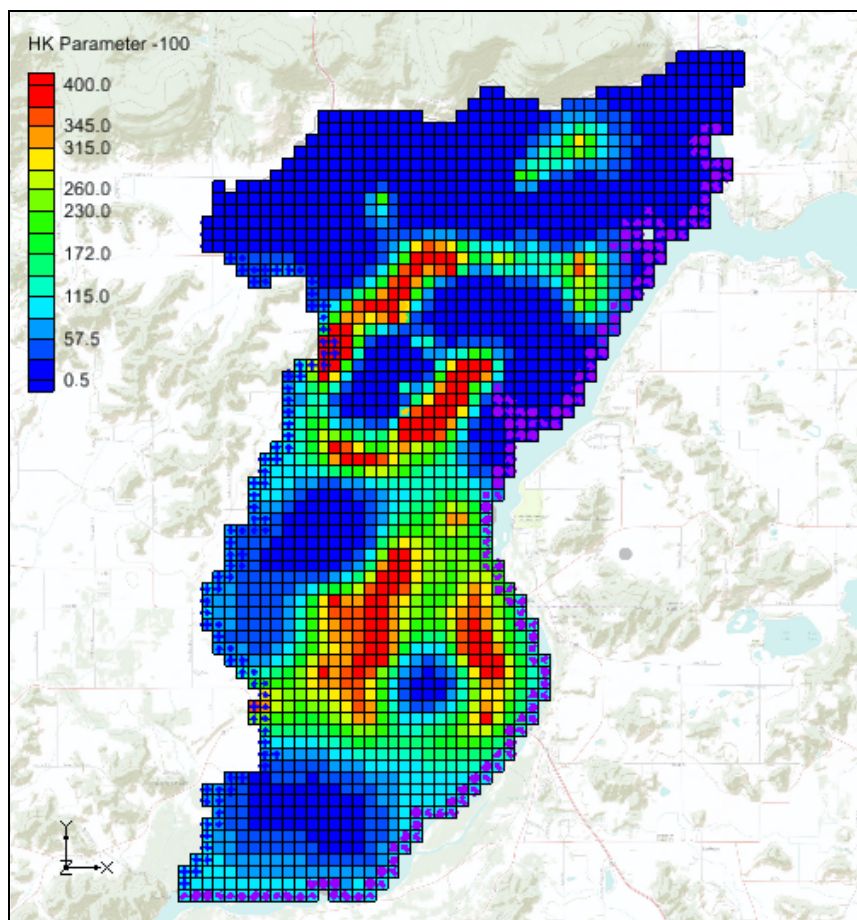


Figure 3 Hydraulic conductivity (HK) field for calibrated model

This model was calibrated using PEST with SVD-Assist and pilot points to estimate the hydraulic conductivity (HK) of the aquifer. The above figure shows the final estimate of HK. As the user runs PEST with the Null Space Monte Carlo method, the user will create different HK fields that will also calibrate the model.

9. Select the “Head” dataset in the Project Explorer.

## 5 The MODFLOW Run Options

---

The user will now set up a Null Space Monte Carlo run. For demonstration purposes, only 3 realizations will be performed. When this is done, the user will have 3 different MODFLOW models with different HK arrays that all calibrate the model.

1. Select the *MODFLOW* | **Global Options** command to open the *MODFLOW Global/Basic Package* dialog.
2. Under the *Run options* section of the dialog, select the *Stochastic Inverse* option.

Notice that the text below the *Stochastic Inverse* option has changed to explain that the stochastic method is *PEST Null Space Monte Carlo*.

3. Select the **Stochastic Options** button to open the *Stochastic Options* dialog.

This dialog is used to change the stochastic options. The other options available in this dialog are explained in separate tutorials. With the data that is currently loaded in GMS, the only stochastic inverse option available is PEST Null Space Monte Carlo. In order to use the Null Space Monte Carlo method, the user must have a model that has already been calibrated using PEST with SVD-Assist.

4. Select the **Options** button next to the *PEST NSMC* option to open the *Monte Carlo Options* dialog.

The user will leave most of the inputs in this dialog at their default values. However, only 3 realizations of our model should be run, and PEST needs an indication of the amount of acceptable error for the model. Furthermore, the user is going to specify the Random seed; this allows the user to replicate the results of the sample solution for this tutorial.

5. Enter “3” for the *Number of realizations*.
6. Enter “200.0” for the *Termination threshold (PHISTOPTHRESH)*. This value tells PEST that it should stop when the total model error is 200 or less. Remember that the total error for this calibrated model was about 197.
7. Enter “Yes” for *RANDPAR – Specify random seed*.
8. Enter “100” for *RANDPAR – Random seed*.
9. Select **OK** to exit the *Monte Carlo Options* dialog.
10. Select **OK** to exit the *Stochastic Options* dialog.
11. Select **OK** to exit the *MODFLOW Global/Basic Package* dialog.

## 6 Parameter Options

---

At this point, the user must select which parameters to vary during the Monte Carlo process.

1. Select the *MODFLOW* | **Parameters** command.
2. Turn on the *Stochastic Randomize* toggle for parameter “HK\_100.”

By turning this option on, the user is specifying that he or she wants to vary the values at the pilot points that estimate the HK\_100 parameter during the Monte Carlo runs.

3. Select the **OK** to exit the dialog.

## 7 Saving the Project and Running PEST

---

Now save the project and run PEST in stochastic mode.

1. Select the *File* | **Save As** command.
2. Change the project name to “sto.gpr.”
3. Click **Save**.
4. Select the *MODFLOW* | **Run MODFLOW** command.

Parallel PEST and MODFLOW are now running in stochastic inverse mode. A dialog comes up from GMS showing the progress of the PEST runs. The user should see something similar to the figure below.



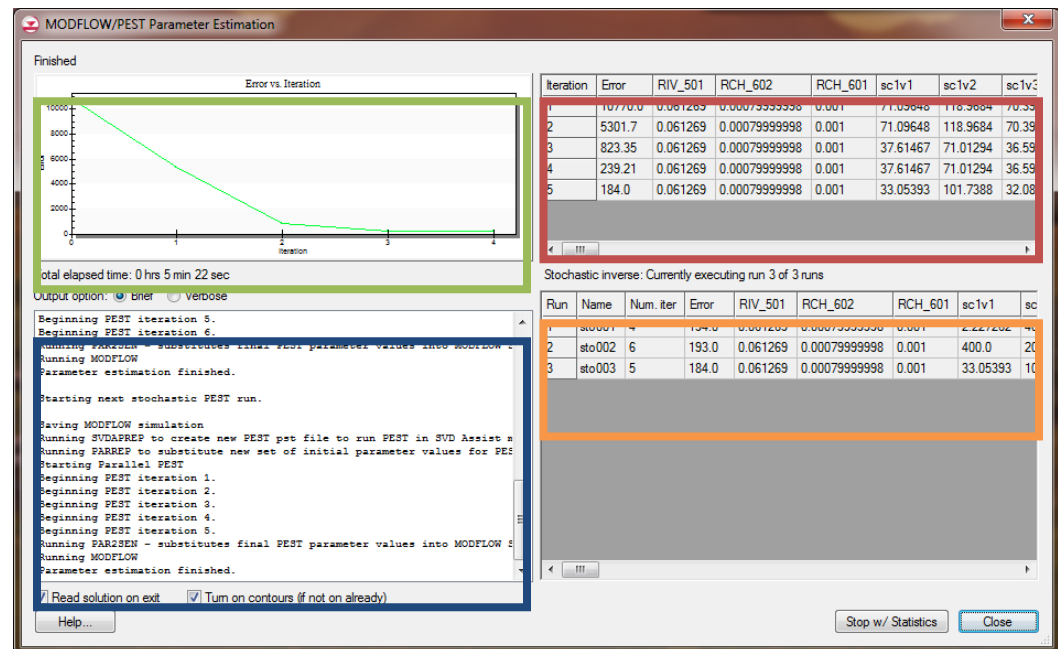


Figure 4 PEST Model Wrapper

The graph (outlined in green above) shows the model error vs. PEST iteration. To the right of the graph is a spreadsheet (outlined in red above) that shows the model error and the parameter values for each PEST iteration. Below the graph is a text window (outlined in blue above) that shows the output that PEST would print to the screen if the user were running PEST from the command line. In the bottom right portion of the dialog is another spreadsheet (outlined in orange above) that shows the results for each realization and includes the number of PEST iterations, the model error, and the parameter values.

There are many steps involved in running PEST with the Null Space Monte Carlo method; GMS runs several PEST utilities to make all of this happen. The following is a list of the steps involved.

1. PEST runs MODFLOW once for each parameter to compute a Jacobian matrix. In this case, the user has a steady state model and is using Parallel PEST, so this step is completed fairly quickly.
2. PPCOV, a PEST utility, is run to generate uncertainty information for the pilot points. The PPCOV utility generates a covariance matrix for the pilot points. This matrix is created using the variogram that is specified as part of the interpolation options for the pilot points. For this reason, kriging must be used with the pilot points if the user wants to use the Null Space Monte Carlo method.
3. RANDPAR, a PEST utility, is run to generate random values for the parameters that are being randomized. This utility generates one file for each realization. For this example, these files will be named “sto000\_random1.par,” “sto000\_random2.par,” and “sto000\_random3.par.”
4. PNULPAR, a PEST utility, is then run to modify the random parameter values through Null Space projection. This utility generates one file for each

realization. For this example, these files will be named “sto000\_random\_nul1.par,” “sto000\_random\_nul2.par,” and “sto000\_random\_nul3.par.” An explanation of how PNULPAR calculates values is given below:

In this process the difference is first taken between each parameter set and the calibration parameter; this difference is then projected onto the calibration null space, and the projected difference re-added to the calibration parameter set. If the model were linear, and if the cutoff between null and solution spaces were sharp, each new parameter set obtained in this way would calibrate the model with an identical objective function to that achieved using the calibration parameter set. However, in general, random parameter sets modified in this manner do not result in perfectly calibrated models, and will thus require adjustment in order that calibration constraints be respected. Such adjustment takes place through alterations made to the calibration solution space (leaving the null space untouched).<sup>2</sup>

5. SVDAPREP, a PEST utility, is then run to create a new PEST input file (pst) using information from the original PEST run in step 1. PEST will then run SVD-assisted parameter estimation, greatly reducing the number of model runs required for each PEST iteration.
6. For each realization, 2 steps are required:
  - a. PARREP, a PEST utility, is run to substitute the parameter values generated by PNULPAR in step 4 for the current realization.
  - b. PEST is launched using the parameter values for the current realization and runs until the objective function is at or below PHISTOPTHRESH or until that maximum number of PEST iterations is reached.

On a reasonably fast computer, this process should finish in about 5 to 15 minutes. If while executing the run, PEST fails for some reason, the user may want to adjust the Parallel PEST wait time to a value of 0.1 (or greater) instead of the default value of 0.001. This is specified in the PEST dialog that can be accessed by selecting the *MODFLOW* / **Parameter Estimation** command.

---

## 8 Reading in and Viewing the MODFLOW Solutions

---

Once all the MODFLOW runs are completed, the user can read in the solutions. Notice that, for this example, the model error for each of the realizations is less than 200; each of these new models is calibrated to the same level of error as our original model.

1. Make sure the *Read solution on exit* toggle is checked.

---

2 John Doherty. PEST Workshop, Regularized Inversion and Predictive Error Variance Analysis. (Corinda, Australia: Watermark Numerical Computing), pp 66.

2. Select the **Close** button.
3. Select **OK** at the prompt to read in all converged solutions.

The user should see a new folder named “sto (MODFLOW)(STO)” in the Project Explorer. Expand this folder and view the individual solutions. Notice how the observation targets change with each solution and that, in general, the targets remain within acceptable error limits. The user should see figures similar to those below.

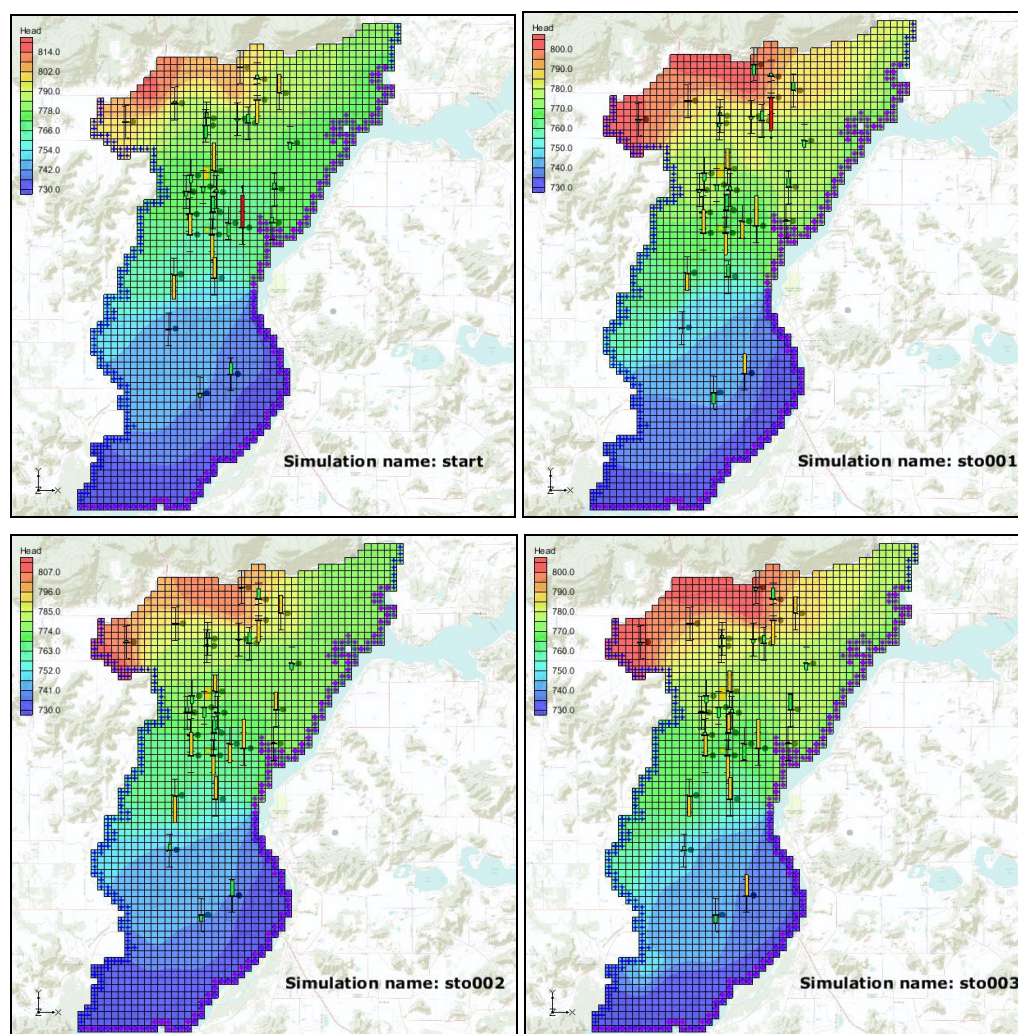


Figure 5 Computed heads from stochastic MODFLOW models

4. Right-click on the “sto (MODFLOW)(STO)” folder.
5. Select the **Statistical Analysis** command.

This creates new datasets based on the MODFLOW outputs. Among the new datasets, the user should see are “mean\_Head,” “min\_Head,” “max\_Head,” and “stdev\_Head.”

6. Select the “stdev\_Head” dataset.

The user should see a figure similar to the one below. Notice that there is very little variability in the computed heads around the locations of the observation points; while in grid cells with no observation points, the user has standard deviation values up to 6.6.

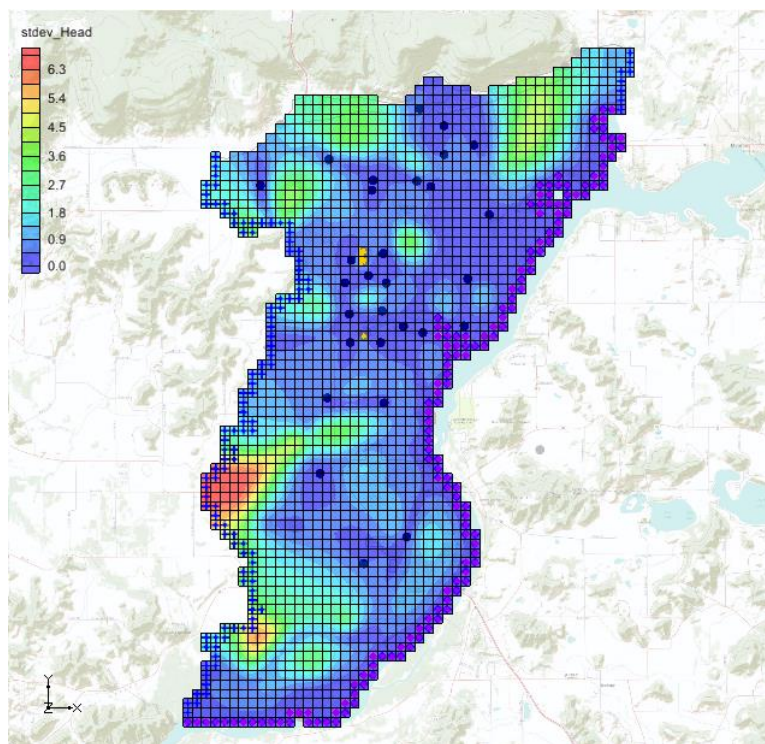




Figure 6 Standard deviation of computed Heads from stochastic MODFLOW models

Now compare HK datasets to see the different HK fields that will still calibrate the model.

7. Select the “HK Parameter -100”  dataset under the “Parameters” folder in the “start (MODFLOW)” folder.
8. Now select the “HK Parameter -100”  dataset under the “sto (MODFLOW)(STO) / sto001 (MODFLOW) / Parameters” folders. Notice the different distribution of HK values.

The following figure shows the different HK fields side by side.



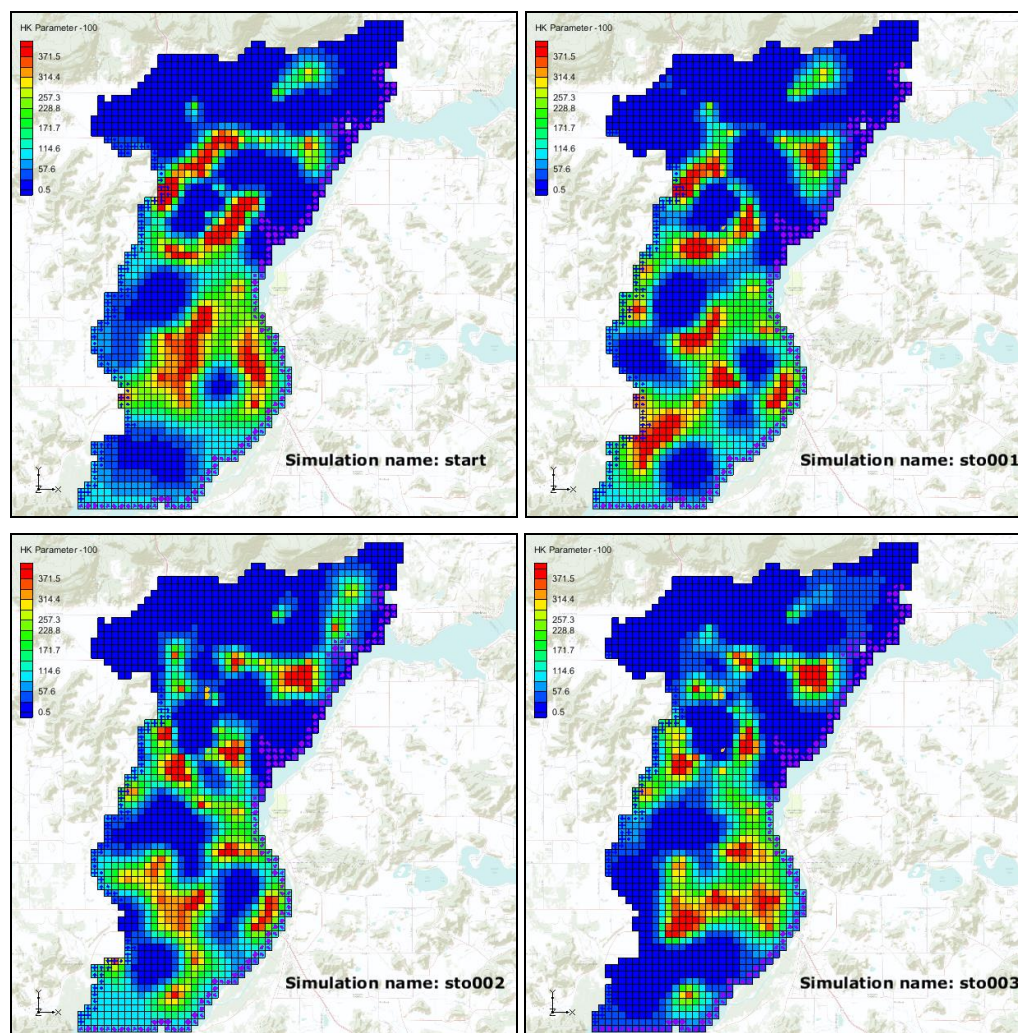





Figure 7 Unique HK fields that calibrate the model

The user can also view statistics about the different HK arrays that calibrate the model. New datasets were created describing the variability in the HK arrays when the user executed the Statistical Analysis command. Datasets show the min, max, mean, and standard deviation of HK for each grid cell. The user can view these datasets to get a feel for how much variability can occur in the HK input array and still result in a calibrated model.

9. Select the “stdev\_HK Parameter -100”  dataset under the “sto (MODFLOW)(STO)” folder in the Project Explorer.
10. Select the “Head”  display theme under the “Display Themes”  folder in the Project Explorer.

The user should see something similar to the figure below. Notice that the maximum standard deviation value for HK is around 224.0. This means that there are areas in this model where the HK value can vary significantly, and yet the model will still match field-measured head values.



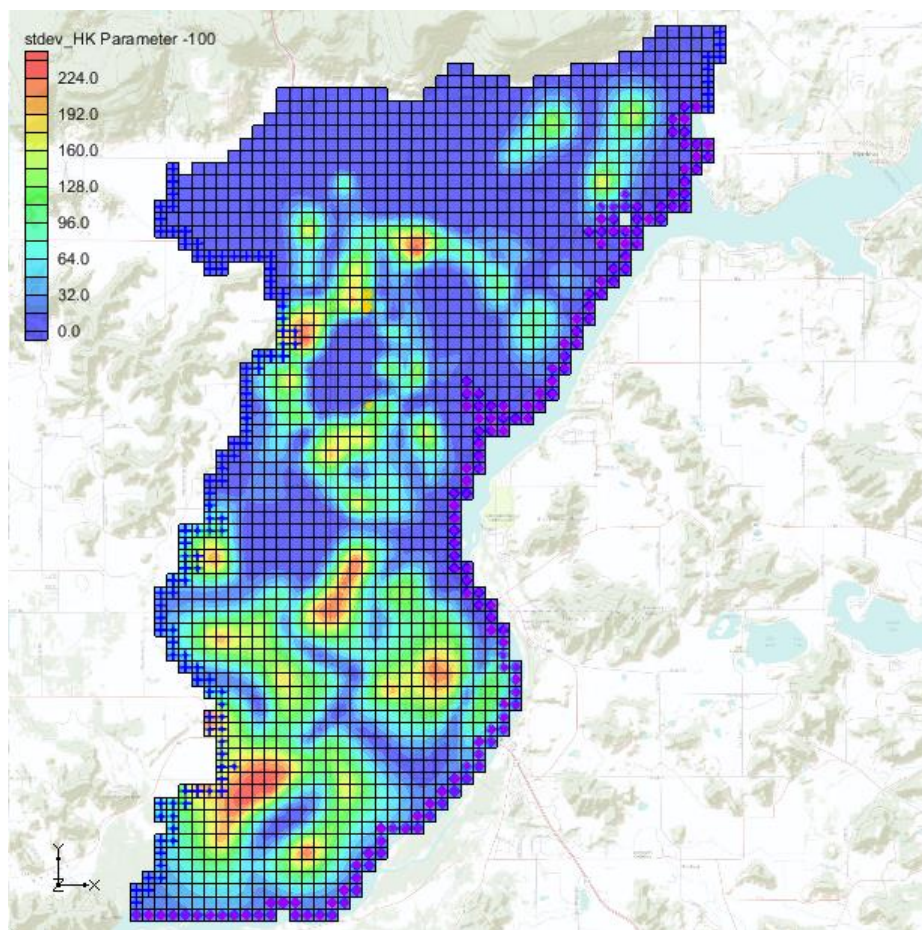


Figure 8 Standard Deviation of HK Input Array

## 9 Conclusion

This concludes the Stochastic Modeling – PEST Null Space Monte Carlo I tutorial. Here are the key concepts in this tutorial:

- It is possible to create multiple calibrated models using the PEST Null Space Monte Carlo approach.
- GMS runs several PEST utilities to automate the process of running the Null Space Monte Carlo method.

## 10 Further Reading

- Doherty, J. PEST Workshop, Regularized Inversion and Predictive Error Variance Analysis. Watermark Numerical Computing, Corinda, Australia, pp. 66.

- Doherty, J. 2005. PEST: Model-Independent Parameter Estimation. Watermark Numerical Computing, Corinda, Australia.
- Doherty, J. 2006. Addendum to PEST Manual. Watermark Numerical Computing, Corinda, Australia.
- Moore, C. and Doherty, J. 2005. The role of the calibration process in reducing model predictive error. *Water Resources Research*, Vol. 41, No 5. W05050.
- Moore, C. and Doherty, J. 2006. The cost of uniqueness in groundwater model calibration. *Advances in Water Resources*, Vol. 29, Issue 4, April, pp. 605–623.
- Tonkin, M. and Doherty, J. 2005. A hybrid regularized inversion methodology for highly parameterized models. *Water Resources Research*, Vol. 41, W10412, doi:10.1029/2005WR003995, 2005.
- Tonkin, M. and Doherty, J. 2007. Efficient nonlinear predictive error variance for highly parameterized models. *Water Resources Research*, Vol. 43, W07429, doi:10.1029/2006WR005348.