11. Null Space Monte Carlo

PEST's null space Monte Carlo (NSMC) functionality is described in PEST documentation and in the PEST book. Briefly, many random parameter sets are generated which "almost calibrate" a model. (The RANDPAR, RANDPAR1, PNULPAR, and possibly PREDUNC7 utilities supplied with the normal version of PEST can be used in preparing these parameter sets). Then, by repeatedly running PEST using its SVD-assist functionality, all of these parameter sets can be adjusted with minimal computational burden so that they calibrate the model to within a user-specified tolerance. (That is, they can all be adjusted so that the objective function associated with each one of them is reduced below a user-specified threshold.)

There is no reason why PEST_HP cannot be used to perform repeated calibration exercises of this type. To automate this process, two batch files can be used – one to initiate repeated runs of the PEST_HP manager, and the other to initiate repeated runs of each of the AGENT_HP agents. The first of these batch files should be run from PEST_HP's working folder. Meanwhile, a copy of the second of these batch files should be placed in the working folder of each agent and run from there.

Figure 11.1 shows an example of a batch file used for running PEST_HP.

```
rem ############################################################
rem Delete an existing record file.
rem ############################################################

del /P record.dat
echo  > record.dat
pause

rem ############################################################
rem Do all the PEST_HP runs.
rem ############################################################

for /L %%i in (1,1,50) do (
parrep nrandom%%i.par base.pst.kp1 base.pst
pest_hp base_svda /h :4004
find /I "ie phi" base_svda.rec >> record.dat
copy base.bpa base.bpa.%%i
copy base_svda.rec base_svda.rec.%%i
timeout /t 2
)
```

Figure 11.1 A batch file used to initiate repeated runs of PEST_HP when implementing PEST's NSMC methodology.

In the example of figure 11.1 a PEST control file named *base.pst* holds base parameters. Randomly generated, null-space projected, parameter sets are housed in parameter value files named *nrandom*.par* where "*" is replaced by 1, 2, 3 etc., these constituting parameter set indices. Random parameter sets are sequentially introduced to the base PEST control file as initial values in this file using the PARREP utility. The super parameter PEST control file is named *base_svda.pst*. The script provided in figure 11.1 runs PEST_HP repeatedly in order to adjust these parameter sets so that each of them fits the calibration dataset better. Normally the NOPTMAX variable in file *base_svda.pst* should be set to 1, or perhaps 2, to place an upper limit on the number of model runs that are committed to this process. After each PEST_HP run is complete, the parameter value file containing adjusted parameters, and the corresponding PEST_HP run record file which documents the inversion process, are copied to files *base.bpa.i* and *base_svda.rec.i* respectively, where *i* is the parameter set index.

The batch file illustrated in figure 11.2 can be placed in each of the agent folders.

```
:label1
agent_hp base_svda /h hostname:4004
timeout /t 2
goto label1
```

Figure 11.2 A batch file used to initiate repeated runs of AGENT_HP.

The batch file depicted in figure 11.2 needs to be run only one; replace *hostname* in this file with the IP address or name of the computer on which the PEST_HP manager is running. On completion of each inversion process, execution of AGENT_HP is re-initiated in readiness for the next inversion process.

Notice the line:

```
timeout /t 2
```

in each of figures 11.1 and 11.2. This WINDOWS system command creates a pause of 2 seconds in the batch processing sequence. This is not essential, but allows a few moments to elapse for manager-agent messaging to catch up with the batch processing sequence; this pause may need to be longer where there are many agents and where network traffic is high.

It is often a good idea to implement Broyden Jacobian updating when using PEST_HP in the NSMC process. As is described in PEST documentation, one of the means through which the NSMC process achieves a high degree of model-run efficiency is through re-use of the same Jacobian matrix for the first iteration of each random parameter set adjustment process. This matrix is usually calculated on the basis of the calibrated parameter set rather than on the basis of any one random parameter set. Parameter-set-specific improvements in this matrix achieved through Broyden updating may allow the first iteration of each random parameter set adjustment process to achieve more than it otherwise would in terms of reducing the objective function.