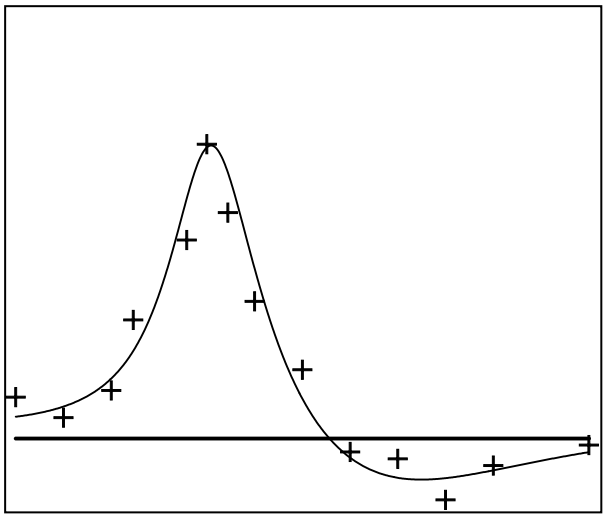
PEST_HP

PEST for Highly Parallelized Computing Environments

Manual for Version 16



Watermark Numerical Computing

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1. Introduction

1.1 General

PEST_HP is a heavily modified version of BEOPEST. Its inversion algorithm is similar to that of PEST (and hence BEOPEST). However parts of that algorithm have been altered to improve its performance when working in conjunction with big models with long run times and questionable numerical stability. Its inversion algorithm has also been tuned for increased efficiency in highly parallelized computing environments such as high performance clusters and the cloud.

There are some elements of PEST functionality which PEST_HP does not possess. In developing PEST_HP, the PEST source code has been renovated, and some of it removed, to make it easier to alter and debug. At the same time, those aspects of the PEST inversion algorithm that pertain to highly parameterized inversion and parallel run management have been enhanced and made considerably more efficient.

The following capabilities of PEST/BEOPEST/Parallel PEST have been eliminated in producing PEST_HP:

- PEST_HP cannot run in "predictive analysis" mode.
- It cannot read an external derivatives file.
- It cannot write a "PEST-to-model-message" file.
- It does not write a resolution data file.
- PEST_HP cannot be started using the "/p1" switch to activate conjunctive parallelisation of the first model run with those required for filling the first Jacobian matrix. However this capability has been replaced with functionality that achieves a similar outcome – see below.
- PEST_HP does not write a sequence of matrix files in which approximations to the posterior parameter covariance and related matrices are recorded during every iteration of the inversion process. (Actually this type of file is available through PEST only if the inversion process is over-determined and unregularised.)
- Manual and automatic user intervention are not supported by PEST_HP.
- PEST_HP does not record the AIC and similar information-theoretic statistics on its run record file. (These are meaningless in contexts of highly parameterized inversion.)
- On completion of an inversion process, PEST_HP does not undertake a final model run using optimised parameters.

Most of the above PEST capabilities are not widely used. Hence contexts in which PEST_HP can work are generally the same as those in which PEST (and BEOPEST/Parallel PEST) can work. PEST_HP reads a normal PEST input dataset. If a PEST control file instructs PEST_HP to undertake processing which it does not support, it ceases execution with an appropriate error message.

The following features are new in PEST_HP. Collectively, they generally result in improved numerical performance of PEST_HP over that of BEOPEST and Parallel PEST when conducting highly parameterized inversion in a highly parallelized computing environment. They also result in

improved reporting of that performance. All of these new features are discussed in the present document.

- During each iteration of the inversion process, PEST_HP calculates a series of Marquardt lambda values on which to base parameter upgrade calculations. The number of selected lambdas depends on the number of cores available for testing parameter upgrades. Each lambda defines a direction in parameter space; these are selected using an enhanced version of the algorithm employed by the traditional PEST. PEST_HP then chooses a number of parameter sets along each of these directions as parameter upgrade candidates. These parameter sets are then distributed to networked cores for parallelized testing. This process keeps otherwise idle cores busy at the same time as it maximizes the chances of finding an improved parameter set, even in difficult numerical circumstances where the integrity of finite-difference-based derivatives may be compromised by model convergence difficulties.
- Optionally, a second round of parameter upgrade calculations and parallelized testing can be undertaken using a Jacobian matrix that is improved through Broyden updating.
- The efficiency of the BEOPEST parallel run manager has been improved. If requested, model runs can be abandoned and/or terminated during the parameter upgrade testing procedure if they are taking too long. Thus if testing of a problematic parameter set promulgates model solver convergence difficulties, the inversion process can continue without having to wait for completion of the afflicted model run.
- In order to reduce idle processor time, and hence to raise parallelization efficiency, the initial model run of the inversion process can be undertaken in a serial computing environment prior to using PEST_HP for implementation of the inversion process in a parallelized environment. This pre-inversion run also internally orders observations recorded in the PEST control file to match the reading sequence encountered in model output files. Where observation numbers are high, the efficiency of reading model output files can be greatly improved through this process.
- The efficiency of imposition of parameter bounds in highly parameterized contexts has been improved.
- PEST's sensitivity reuse functionality has been improved to better accommodate a parallel computing environment.
- PEST_HP delays the onset of higher order finite-difference derivatives calculation if it detects that imposition of parameter change limits have hindered improvements to the objective function.
- PEST_HP provides a continuous record of parallel computing efficiency; it also provides a record of parameter sets that instigate model run failure.
- In undertaking parameter estimation, PEST_HP can optionally write a "run results file" which records parameters and model outputs pertaining to all non-Jacobian model runs. In future versions of PEST_HP the contents of this file will support construction of proxy models.
- The running of PEST_HP can be dedicated solely to production of a run results file based on parameter sets provided in a series of parameter value files. This can facilitate uncertainty analysis, sensitivity analysis and proxy model construction.
- PEST_HP can be instructed to cease execution after a user-specified time has elapsed, regardless of whether the inversion process is complete or not.

- Where multiple commands are used to run a model, or where PEST's observation re-referencing functionality is activated, user-specified numbers written to model output files can instruct PEST_HP to award zero sensitivities of respective model outputs to a parameter that is being varied incrementally for finite-difference derivatives calculation.
- Model-generated files can be distributed to all computing nodes (possibly after local processing) prior to the commencement of each iteration of the inversion process; in some circumstances this can lead to considerably enhanced model execution speeds.
- A PEST_HP-compatible version of the CMAES_P global optimiser has been written. Like PEST_HP and BEOPEST, this uses TCP/IP for communication between the run manager and parallel run agents.
- A PEST_HP control file can cite new parameter types, namely "secondary parameters" and "file-parameters". Use of the former parameter type can replace the PAR2PAR utility as a means of transforming parameters that are estimated through the inversion process to those that are actually used by the model. File-parameters, on the other hand, can only be used with CMAES_HP; they facilitate optimisation under uncertainty.
- PEST_HP provides a novel means of obtaining a Jacobian matrix based on randomized finite differences. This methodology is still in its experimental stages.
- User-specified elements of a Jacobian matrix can be strategically set to zero. This can raise the integrity of a Jacobian matrix that has been filled through random parameter differencing.
- Where a Jacobian matrix is known to possess a blocky structure, PEST_HP can increment multiple parameters simultaneously. This, together with its Jacobian blanking functionality, can considerably reduce the model run burden of filling a Jacobian matrix.
- A new "quick regularisation" option has been provided.

Meanwhile, the following (and many other) advanced features of PEST/BEOPEST/Parallel PEST are retained in PEST_HP.

- SVD-assisted inversion can be employed for estimation of parameters, and for production of calibration-constrained random parameter sets using the null space Monte Carlo methodology.
- One objective function can be traded off against another by running PEST_HP in "pareto" mode.
- Inverse problem solution strategies based on Gaussian elimination, singular value decomposition and LSQR are all supported.
- Multiple options are provided for calculation of regularisation weights, and for determination of comparative inter-regularisation-group weighting when employing Tikhonov regularisation.
- Different command lines can be used to run the model in calculating derivatives with respect to different parameters.
- Observation re-referencing supports use of one or a number of simplified models for calculation of derivatives, while retaining a complex model for testing parameter upgrades.
- Alterations made to members of the PEST suite (versions 15 and above) to promote greater inter-operability with members of the PEST++ suite have also been made to PEST_HP. These include the use of comment lines in a PEST control file. See PEST documentation for details.

PEST_HP can be used interchangeably with PEST, BEOPEST and Parallel PEST. It requires no input data in addition to that required by the normal PEST; hence a PEST input dataset is also a PEST_HP input dataset. However a number of PEST_HP-specific control variables, and three sections, can optionally be added to a normal PEST control file to construct a PEST_HP control file. PEST/BEOPEST/Parallel PEST will cease execution with a pertinent error message if they encounter these new variables and sections. Conversely, PEST_HP will cease execution with an appropriate error message if a PEST input dataset requests functionality which is no longer available in PEST_HP.

Note that the binary restart files written by PEST/BEOPEST/Parallel PEST on the one hand, and by PEST_HP on the other hand, are not compatible with each other. Hence an inversion process which is commenced by one of these programs cannot be completed by the other.

1.2 Terminology

The terms "master" and "slave" are not employed by PEST_HP. These have been replaced by "PEST_HP run manager" and "parallel run agent" (or simply "manager" and "agent") respectively.

1.3 PEST_HP License File

PEST_HP (and CMAES_HP) will only run if a file named *pest_hp.lic* is present in the folder (i.e. the directory) from which the manager is run. You receive this file when you purchase PEST_HP. It contains the (encrypted) name and address that you supplied when you purchased it. These details are recorded at the start of run record files that are written by PEST_HP and CMAES_HP on each occasion that they run.

You can make copies of *pest_hp.lic*. You can then use a copy anywhere where you initiate execution of the PEST_HP or CMAES_HP manager (including the cloud). This file is not required in folders used by PEST_HP agents.

1.4 Using PEST_HP

Use of PEST_HP is very similar to that of BEOPEST. To run the PEST_HP manager based on the contents of the PEST control file *case.pst*, start it using the command:

```
pest_hp case /h :nnnn
```

where *nnnn* is a port number (for example 4004). Note the space character between the "/h" string and the following colon. To run a PEST_HP run agent, use the command:

```
pest_hp case /h hostname:nnnn
```

where *hostname* is the name of the machine on which the manager is running, and *nnnn* is the port number employed by the manager (as provided on the manager's command line) ; alternatively use the IP address of the machine on which the manager is running instead of *hostname*. (Only TCP/IP version 4 is supported at the time of writing.)

As is explained in PEST documentation, each parallel run agent must operate from a different folder. If desired, one of these folders can be the same as that employed by the run manager.

Operation of PEST_HP can be terminated in the same manner as that of PEST and BEOPEST. This can be done brutally by pressing the <Ctl> <C> keys. Alternatively, the PSTOP or PSTOPST command can be issued from another window open to the PEST_HP manager's folder.

A halted PEST_HP run can be resumed using the "/s" switch. This switch must be placed before the "/h" switch. Hence to recommence an interrupted run of the PEST_HP manager based on file *case.pst*, use the command:

```
pest_hp case /s /h :nnnn
```

The "/s" switch is not required for recommencement of execution of a PEST_HP run agent.

The "/i" command line switch and the "/t" command line switch have the same roles for PEST_HP as they do for BEOPEST. The "/i" switch informs the PEST_HP manager that it must read a Jacobian matrix file (i.e. a JCO file) to obtain the Jacobian matrix for use in the first iteration of the inversion process; if started using this switch, PEST_HP prompts for the name of the JCO file which it must read. The "/t" switch allows the user to associate a text string with a particular PEST_HP run; see PEST documentation for details.

A new switch, namely "/hpstart", has been introduced for the use of PEST_HP, as well as that of PEST; it enables the latter to expedite the efficiency of an ensuing PEST_HP run. When employed on the PEST_HP command line, the "/hpstart" option instructs PEST_HP to read a "hp starter file" named *case.hp* (where the PEST control file is named *case.pst*). This file contains information previously recorded during a dedicated PEST run, also initiated using the "/hpstart" command line option, in which the model is run only once. The information contained in file *case.hp* saves PEST_HP from having to conduct an initial model run to calculate the initial objective function and initial model-calculated reference values associated with observations comprising the calibration dataset. Hence, immediately upon commencement of its execution, PEST_HP can initiate parallelization of model runs in order to fill the initial Jacobian matrix. At the same time, where observations number in the tens or hundreds of thousands, PEST_HP's reading of the model-generated counterparts of observations from model output files is accelerated, as observations will have been ordered internally to PEST_HP to match their occurrence in these files. This is further discussed later in this document.

The running of CMAES_HP is similar to that of PEST_HP. See section 12 of this document for details.

1.5 Alternative Version of PEST_HP

Two versions of the PEST_HP executable program are provided. One is named *pest_hp.exe*. The other is named *pest_hp_mkl.exe*. The latter executable program is linked to the Intel Maths Kernel Library. At the same time, the programming associated with a number of numerically-intensive parts of the PEST_HP algorithm have been altered to take advantage of the efficiencies offered by this library. Where the number of parameters and/or observations is large, this can result in much faster execution of PEST_HP.

If you use *pest_hp_mkl.exe* then a DLL named *libiomp5md.dll* must be situated in the folder from which you run *pest_hp_mkl.exe*. Alternatively, it must reside in a folder that is accessible through your computer's PATH environment variable. Many users will already have this DLL resident on their machines. However, because some will not, it is supplied with PEST_HP.

If you use *pest_hp_mkl.exe* instead of *pest_hp.exe* then the commands that are outlined in the previous section should be altered accordingly. However there is little to be gained by using *pest_hp_mkl.exe* as the agent - only as the manager. A *pest_hp_mkl.exe* manager will raise no

objections if it is used in conjunction with a *pest_hp.exe* agent. Where you are using PEST_HP on an office network, this deployment strategy will save you from having to copy *libiomp5md.dll* to machines on which you run agents.

1.6 Parallel Run Management File

Parallel PEST requires that the user provide a parallel run management file. This file must possess the same filename base as the PEST control file, but its extension must be "*.rmf*". BEOPEST does not require a file of this type. However, if this file is present in the directory from which it is run, BEOPEST will read values for the optional PARLAM and RUN_SLOW_FAC variables from this file. In contrast, PEST_HP does not read a parallel run management file at all. As will be discussed below, the PARLAM variable is redundant to parallel run management undertaken by PEST_HP; if desired, the optional RUN_SLOW_FAC variable can be supplied through the PEST control file.

1.7 When Not to Use PEST_HP

PEST_HP cannot undertake serial model runs; runs are always undertaken using a run agent. There is no lower limit on the number of run agents that PEST_HP can use; it can use as few as 1. However its inversion algorithm works best where there are many parallel run agents at its disposal. Ideally there should be at least ten (but hopefully many more), as its performance can be degraded when it works with fewer agents than this. When only a few agents are available it is better to use BEOPEST than PEST_HP.

As presently programmed, the upper limit of PEST_HP agents is set to 2048. If required for a specific application, this can be altered with ease; contact the programmer.

1.8 The "PEST Whisperer"

A new program named PWHISP_HP is supplied with PEST_HP. PWHISP_HP reads PEST_HP input and output files, reflects upon what it sees in those files, and records all its thoughts in a run record file of its own which can be inspected using a standard text editor. PWHISP_HP looks for any elements in PEST_HP setup that may compromise its efficiency, or impair its ability to perform highly parameterized inversion. It suggests to the user ways in which he/she can alter a PEST_HP input dataset, or modify PEST_HP deployment, in order to obtain better results. It tries to answer questions which a modeller may ask during or after a PEST_HP run, especially if he/she is wondering whether PEST_HP could have performed better than it did.

While much of the advice provided by PWHISP_HP is just as applicable to PEST as it is to PEST_HP, PWHISP_HP can only be used with PEST_HP. Because of novel ways in which PEST_HP uses the Marquardt lambda and performs Broyden Jacobian updating, certain aspects of the run record file written by PEST_HP are different from that written by PEST. PWHISP_HP reads the PEST_HP run record file in detail; this is how it makes its assessment of PEST_HP performance. It has not been programmed to read a run record file written by the normal version of PEST.

PWHISP_HP is run using the command:

```
pwhisp_hp case outfile
```

where *case.pst* is a PEST control file and *outfile* is the name for the text file which PWHISP_HP must write. This command can be issued even while PEST_HP is running; you do not have to wait until PEST_HP execution is complete in order to receive advice from the PEST whisperer. If they are

available, PWHISP_HP reads some or all of the following PEST_HP input/output files, recording any suggestions that it can make based on the contents of these files on its own run record file.

- the PEST control file (*case.pst*);
- the PEST run record file (*case.rec*);
- the parameter value file (*case.par*, or *basecase.bpa* if PEST_HP is conducting SVD-assisted inversion);
- the composite sensitivity file (*case.sen*);
- the intermediate residuals file (*case.rei*); and
- the Jacobian matrix file (*case.jco*).

Note the following.

- PWHISP_HP does not offer advice on PEST_HP execution if PEST is run in "pareto" mode. This is because PEST_HP's tasks when running in this mode are very different from when running in "estimation" or "regularisation" modes.
- PWHISP_HP does not offer advice on CMAES_HP execution.
- It is not the intention of PWHISP_HP to repeat suggestions and warnings provided by PESTCHEK. PESTCHEK should be used to check a PEST_HP input dataset before PEST_HP is run. PWHISP_HP seeks verification from the user that this has indeed been done.

1.9 The PEST_HP Cost Estimator

Prior to running PEST_HP on the cloud, costs can be estimated using a utility program named PCOST_HP. PCOST_HP reads a PEST control file to obtain details of a PEST run; it obtains the other information that it needs for cost estimation from the command line. It is run using the command:

```
pcost_hp case runtime agents rate [iteration_override]
```

where

case	is the filename base of a PEST control file;
runtime	(a real number) is the estimated model run time in minutes;
agents	(an integer) is the number of agents that PEST_HP will employ;
rate	(a real number) is the cost per minute per agent for cloud rental; and
iteration_override	(an optional integer) allows you to over-ride PCOST_HP's estimate of the number of iterations that PEST_HP will undertake.

Note that the cost per agent will be less than the cost per rented machine if a number of agents use the same machine. In fact the cost per agent will be the cost per machine divided by the number of agents using each machine.

PCOST_HP lists the outcomes of its calculations to the screen. Figure 1.1 shows an example.

```
Estimated cost without hp starter file = $29.00
Estimated cost with hp starter file    = $27.20

Some specifications:-
  PEST mode of operation                                    : regularization
  Number of adjustable parameters                           : 10
  Jacobian runs per itn before switch to higher order derivs : 10
  Jacobian runs per itn after  switch to higher order derivs : 20
  Parameter upgrade testing runs per iteration              : 5
  Number of upgrade testing cycles per iteration            : 1
  Number of iterations used for cost estimation             : 10
  Number of iterations specified in PEST control file       : 30

Possible idle agents per iteration (in units of model runs):-
  Initial model run (if not using hp starter file)          : 4
  Initial model run (if using hp starter file)              : 0
  Fill Jacobian matrix before switch to higher order derivs  : 0
  Fill Jacobian matrix after  switch to higher order derivs  : 0
  Parameter upgrade testing                                 : 0
```

Figure 1.1 An example of PCOST_HP screen output.

Cost estimates provided by PEST_HP are only approximate. It has no idea how many iterations will be required for completion of the inversion process. So it guesses that the inversion process will reach completion after 8 iterations, unless the NOPTMAX variable in the PEST control file is set to less than this, or unless the settings of the SOFTSTOPHOURS or HARDSTOPHOURS variables (see later in this document) impose an upper time limit on a PEST_HP run. PCOST_HP's calculations are also based on the assumption that the model run time will not vary from the initial estimate provided on its command line. In practice this may not be the case, especially for highly nonlinear models which employ adaptive time stepping for which the run time may be sensitive to the values of model parameters.

Costs may be considerably greater than estimated by PCOST_HP if PEST_HP is asked to run in "regularisation" mode, the number of parameters is high, and many of these parameters hit their bounds. As is explained in documentation of PEST, this situation requires many re-formulations of the inverse problem as pertinent parameters are sequentially frozen at their bounds. Implementation of the numerical steps required to accommodate bounds enforcement may keep the PEST_HP manager busy while agents are standing idle (sometimes for up to an hour if parameter numbers are greater than 10000, observation numbers are high, and many parameters encounter their bounds). PEST_HP cannot predict this. However it does issue a warning message if adjustable parameters number over 2500 and LSQR is not being employed as a solution mechanism for the inverse problem. (Note that, as is explained in section 3 of this document, the time taken by PEST_HP to perform numerically intensive tasks can be considerably shortened if the *pest_hp_mkl.exe* executable program is used instead of the *pest_hp.exe* executable program. The time required to compute a regularisation weight factor can also be considerably reduced if the REG2MEASRAT variable is used to control regularisation; see section 7.12 of this document.)

A warning message is also issued if the setting of the HARDSTOPHOURS or SOFTSTOPHOURS variables affects calculation of estimated PEST_HP running cost. Warning messages are placed under the cost estimate. See figure 1.2.

```
Estimated cost without hp starter file = $120.60
Estimated cost with hp starter file    = $119.60

Warning: estimated costs are limited by HARDSTOPHOURS setting in PST file.

Warning: the manager's run time (and hence the total cost) is unpredictable
as a large number of parameters is being estimated, but LSQR is not being
used as the solution mechanism.

Some specifications:-
  PEST mode of operation                                    : regularization
  Number of adjustable parameters                           : 1100
  Jacobian runs per itn before switch to higher order derivs : 1200
  Jacobian runs per itn after  switch to higher order derivs : 2400
  Parameter upgrade testing runs per iteration              : 100
  Number of upgrade testing cycles per iteration            : 1
  Number of iterations used for cost estimation             : 8
  Number of iterations specified in PEST control file       : 30

Possible idle agents per iteration (in units of model runs):-
  Initial model run (if not using hp starter file)          : 99
  Initial model run (if using hp starter file)              : 0
  Fill Jacobian matrix before switch to higher order derivs  : 0
  Fill Jacobian matrix after  switch to higher order derivs  : 0
  Parameter upgrade testing                                 : 0
```

Figure 1.2 A cost estimate affected by the HARDSTOPHOURS setting, with an accompanying warning message pertaining to use of a large number of parameters.

As was stated above, PCOST_HP does not necessarily assume that the number of iterations required for completion of an inversion process is equal to the value of the NOPTMAX variable supplied in the "control data" section of the PEST control file. NOPTMAX is often set to a high value in order to allow other control variables to establish inversion completion. PCOST_HP assumes that after 8 iterations, the objective function will have been reduced to a value that satisfies the user (in which case he/she will stop execution of PEST_HP him/herself), or to a value that PEST_HP cannot improve (in which case PEST_HP ceases execution itself). If neither of these occurs, then the NOPTMAX setting prevails, of course. The user can provide a value other than 8 for the purpose of cost estimation by entering this number as the value of the optional *itn_override* command line variable. However PCOST_HP will reduce *itn_override* to NOPTMAX if it is greater than NOPTMAX.

If PEST_HP is run in "pareto" mode, PCOST_HP does not assume that 8 iterations will be required for completion of the inversion process because, under these circumstances, PEST_HP traverses the Pareto front rather than undertaking a single inversion exercise. Instead PCOST_HP assumes that PEST_HP will complete its traversal of the Pareto front, and that the number of iterations will therefore be equal to:

(NUM_WTFAC_INC-2)*NUM_ITER_GEN+NUM_ITER_START+NUM_ITER_FIN

(See the PEST manual for definitions of these Pareto control variables.) You can override this number through selection of a value for *itn_override* which is less than this.

Note the following:

- If PCOST_HP encounters an error in the PEST control file which it reads, it ceases execution after writing an appropriate error message to the screen.

- An entry of “na” for any specification quoted by PCOST_HP means “not applicable”. The following conditions (and others) may result in a “na” condition being recorded in PCOST_HP’s screen output:
    - no parameter upgrade calculations are performed because NOPTMAX in the PEST control file is set to -2;
    - the switch to higher-order derivatives is not made because there is no parameter group for which the setting of FORCEN is either “switch” or “switch_5”.
- As is explained later in this document, the number of cycles of parameter upgrade testing can be reduced from two to one by disabling Broyden Jacobian improvement; this is achieved by setting the JACUPDATE variable to zero in the “control data” section of the PEST_HP control file.
- Use of a hp starter file is explained later in this document.

2. Marquardt Lambda Selection

2.1 The Selection Algorithm

In BEOPEST and Parallel PEST, implementation of the "partial parallelization" procedure whereby different values are selected for the Marquardt lambda, and parameter upgrades are calculated and tested using these different Marquardt lambdas, is dependent on the setting of the PARLAM parallelization control variable. According to this setting, the Marquardt lambda selection and parameter upgrade testing procedure can be serial, partially parallel, or fully parallel. Unless PARLAM is set to -9999, an initially parallel procedure can become a serial procedure if one or more parameters encounter their bounds.

The Marquardt lambda selection and parameter upgrade testing procedure undertaken by PEST_HP is always parallel; it never becomes serial, even if some parameters hit their bounds. On all iterations of the inversion process, PEST_HP selects a set of Marquardt lambdas, calculates parameter upgrades using these lambdas, and commissions a set of parallel model runs based on these upgraded parameter sets. If it has enough run agents at its disposal, it also calculates parameter upgrades corresponding to fractional lengths along the upgrade directions defined by different Marquardt lambdas. These fractions can be both greater and less than 1.0, with a fraction of 1.0 corresponding to the optimum length of the parameter upgrade vector according to an assumption of local model linearity. The line search fractions employed by PEST_HP are pre-set; however, on any particular iteration of the inversion process, PEST_HP can adjust them to reflect the distance in parameter space between current parameter values and the closest parameter bound in the direction of each upgrade vector.

Upgraded parameter sets calculated in the manner discussed above are bundled into a set of model runs that are undertaken in parallel. The multiplicity of upgraded parameter sets that require testing occupies computing cores that would otherwise be idle. PEST_HP ensures that the number of parameter upgrades that requires testing is such that the set of parallelized models runs which implement this testing can be undertaken simultaneously in roughly the same time (based on PEST_HP's assessment of the relative computing speeds of agents which are at its disposal). Once these model runs have been completed, PEST_HP processes the results, and selects the best parameter set for potential use in the next iteration of the inversion process. (Note that "best" depends on whether PEST_HP is running in "estimation", "regularisation" or "pareto" mode.)

Optionally, PEST_HP then repeats this process. However before doing so, it improves the Jacobian matrix using a Broyden update procedure informed by the results of the just-commissioned set of parallel model runs. The number of Broyden Jacobian updates which PEST_HP undertakes is set by the JACUPDATE variable supplied in the PEST control file; however it will never exceed the number of parameter upgrade directions determined by the number of Marquardt lambda values just employed (each Marquardt lambda defines a different update direction). Once this new set of parallelized model runs is complete, PEST_HP moves on to the next iteration.

During any iteration of the inversion process, PEST_HP calculates Marquardt lambda values itself. Its choice of the number of lambda values to employ depends on the number of available parallel run agents. However it will never employ less than three Marquardt lambda values, even if this is less

than the number of parallel agents available to it. Furthermore, a user can constrain PEST_HP's choice of the number of Marquardt lambdas to employ in calculating upgrades through use of the PEST_HP-specific UPTESTMIN and UPTESTLIM control variables; see below. In calculating lambda values, PEST_HP ignores variables which control the Marquardt lambda selection procedure provided on the sixth line of the PEST control file. In particular, it ignores the RLAMDA1, RLAMFAC, PHIRATSUF, PHIREDLAM and NUMLAM variables. To make its indifference to the values supplied for these variables explicit, it does not even record them on its run record file. (It is nevertheless wise to choose sensible values for these variables so that PESTCHEK does not complain if asked to review the PEST control file.)

The optional JACUPDATE variable also appears on the sixth line of the PEST control file. If this is set to zero, or omitted from the PEST control file altogether, PEST_HP will not undertake Broyden enhancement of the Jacobian matrix based on the parallelized set of model runs which were carried out to test parameter upgrades. Instead, PEST_HP immediately commences the next iteration of the inversion process wherein it initiates finite-difference calculation of a new Jacobian matrix. Alternatively, if JACUPDATE is set to *N*, then PEST_HP undertakes *N* updates of the Jacobian matrix, based on directions in parameter space corresponding to the *N* most productive Marquardt lambdas. (Updating of the Jacobian matrix in this fashion does not require any model runs. It is an internal numerical procedure that is accomplished quickly; see PEST documentation for details.) If necessary, PEST_HP reduces *N* to the number of Marquardt lambdas that was actually used during the immediately preceding round of parallelized parameter upgrade tests. If you do not know what value to supply for JACUPDATE, set it to a high number such as 999; PEST_HP will then undertake as many Jacobian updates as it can. Alternatively, omit it from the PEST control file in order to forego Jacobian updating altogether. Limited experience to date suggests that on some occasions (particularly when running PEST_HP in "pareto" mode), the second round of parallelized parameter upgrade testing based on a Broyden-improved Jacobian matrix can be worth the trouble. On other occasions it is not, particularly if the number of available parallel run agents is large; in this case there is a greater computational advantage to be gained in re-computing the Jacobian matrix altogether using the just-upgraded parameter set than in trying to improve it in the hope of calculating a better upgrade.

PEST_HP will never undertake more than two rounds of parallelized parameter upgrade testing (and hence one round of Broyden Jacobian updating). Unless there are fewer than three agents at its disposal, each set of parallelized model runs required for parameter upgrade testing will be comprised of model runs which are fewer or equal in number to the number of agents which are at its disposal. The procedure is thus designed to maximize use of otherwise idle computing cores while progressing the inversion process as quickly as possible.

2.2 Upper Upgrade Test Limit

As stated above, when calculating parameter upgrades, PEST_HP selects Marquardt lambdas itself. It also calculates intervals along the parameter upgrade vectors that are computed using these Marquardt lambdas for which new parameters will be generated and then tested using parallelized model runs. The total number of upgraded parameter sets for which model runs can be commissioned is between 120 and 140, the exact number depending on the case. However the final number of parameter upgrades that are tested is restricted to the number of agents which are active. If more agents then this are available, then those agents which are not engaged in

undertaking model runs for the purpose of testing parameter upgrades remain idle during the parameter upgrade testing procedure.

Its capacity to simultaneously test many different parameter upgrades is one of the strengths of the PEST_HP inversion algorithm. However, for some models, the number of runs devoted to upgrade testing may need to be restricted to a smaller number than PEST_HP would normally choose as it attempts to keep all agents busy. On some occasions, for some highly non-linear models, parameter sets that are calculated using very high or very low Marquardt lambdas can induce convergence difficulties in the model's solver. Model instances which employ these parameter sets may then take a long time to run, this holding up the whole inversion process as other agents remain idle while waiting for these runs to finish. While this problem can be addressed to some extent using the RUN_ABANDON_FAC and WIN_MRUN_HOURS variables (see below), its chances of occurrence can be reduced by limiting the number of agents that are actually used in a single round of parallel upgrade testing. This limit applies to both the first round of parameter upgrade testing undertaken immediately after filling the Jacobian matrix, and to the second round of parameter upgrade testing that is commissioned after Broyden Jacobian updating. Upgrade agent limiting can be accomplished using the UPTESTLIM control variable.

The UPTESTLIM variable is optional. If present, it is placed in the "control data" section of the PEST control file – on the sixth line of this file. It can be placed anywhere after the values supplied for RLAMBDA1, RLAMFAC, PHIRATSUF, PHIREDLAM, NUMLAM, and (optionally) JACUPDATE, which also appear on this line. Suppose that you wish to limit PEST_HP to the use of no more than 50 agents when testing parameter upgrades. Then the string "UPTESTLIM=50" should be written on this line. See appendix 1 for an example.

If the number of model runs devoted to parameter upgrade testing is limited in this fashion, then PEST_HP calculates Marquardt lambdas and line search factors in a way that maximizes upgrade testing efficiency while respecting this model run limit. However caution should be exercised in setting an upgrade testing limit. If it is set too low, then some of the benefits of using PEST_HP will be lost.

2.3 Lower Upgrade Test Limit

Sometimes it is useful to set a lower limit on the number of parameter upgrade tests that PEST_HP undertakes, even if it does not have enough agents at its disposal to undertake the necessary model runs in parallel all at once. A user may insist, for example, that at least 20 parameter upgrade tests be undertaken even though PEST_HP may have access to 10 CPU's. He/she may do this in order to gain the benefits of the line search that PEST_HP undertakes along different parameter upgrade directions that are calculated using different Marquardt lambdas. This may prove a fruitful strategy in highly nonlinear inversion contexts.

The UPTESTMIN control variable can be used to set this minimum number of upgrade tests. Its use is almost identical to that of UPTESTLIM. Insert the string "UPTESTMIN=*N*" (where *N* must be replaced by the desired minimum number of upgrade tests) on the sixth line of the PEST control file anywhere after the values supplied for RLAMBDA1, RLAMFAC, PHIRATSUF, PHIREDLAM, NUMLAM, and (optionally) JACUPDATE.

Note that efficiency of computing node usage is maximized if UPTESTMIN is an integral multiplier of the number of agents that PEST_HP is using to supervise model runs.

3. HP Starter File

3.1 The Role of the Starter File

The serial version of standard PEST (including I64PEST, the 64 bit version of PEST) can now be run with a new command line option. This option is "/hpstart". Let us suppose that a PEST control file is named *case.pst*. Then to run PEST with this new option, use the command:

```
pest case /hpstart
```

If initiated using this option, PEST runs the model only once using parameter values supplied in the PEST control file; it then ceases execution. As well as its usual set of output files, PEST writes a binary file named *case.hp*; this is referred to herein as a "hp starter file". This file is used by PEST_HP. If PEST_HP is to be run on another machine, or in the cloud, this file should be placed in the folder used by the PEST_HP manager, and in folders used by all run agents.

When execution of the PEST_HP manager is initiated, the following command can be used:

```
pest_hp case /hpstart /h :4004
```

When the PEST_HP manager is started in this way, it reads file *case.hp*, along with its normal set of PEST input files (i.e. the control, template and instruction files). The information contained in file *case.hp* eliminates the requirement for PEST_HP to undertake an initial model run in which it calculates values for model outputs using parameter values supplied in the PEST control file. (These outputs are used as reference values in finite-difference calculation of the first Jacobian matrix.) Instead, PEST_HP obtains these reference values from the hp starter file. These reference model outputs are also used to calculate the initial objective function, which is reported to the screen and to the run record file.

Because the PEST_HP manager obtains initial reference values from the hp starter file, and because the need for a model run based on initial parameter values is thereby eliminated, it can commence finite-difference calculation of the initial Jacobian matrix immediately upon commencement of execution. All run agents can therefore be immediately put to work; there is no "gap time" in which they are waiting for completion of the initial model run (and thereby losing money if cores have been purchased on the cloud). This is a better option for handling of the initial model run than that provided by the "/p1" command line switch which is supported by BEOPEST, but not by PEST_HP. The "/p1" switch bundles the initial model run with the model runs required for filling of the first Jacobian matrix. Hence this first bundle of runs is comprised of N+1 model runs, where N is the number of adjustable parameters. Filling of the second Jacobian matrix requires only N model runs however, as reference observations used in finite-difference approximations to derivatives are calculated during the preceding Marquardt lambda selection and parameter upgrade testing process. Where inversion takes place in the cloud, this disparity between the number of model runs required to fill successive Jacobian matrices can make selection of an optimal number of processors difficult. Ideally N should be an integer multiple of the number of available processors; no processors are therefore idle as model runs are undertaken for filling of the Jacobian matrix.

(Note that the above logic assumes that one model run is required per adjustable parameter. If derivatives with respect to all parameters are calculated using higher order finite-differences, the same logic applies, as the number of model runs required for filling the Jacobian matrix remains an integer multiple of *N*. The argument breaks down, however, where forward differences are used for some parameters and higher order differences are used for other parameters. It is also invalidated where PEST's observation re-referencing functionality is invoked. This does not erode the value of the hp starter file however.)

PEST_HP run agents also read the hp starter file. However they do not need to be started using the "/hpstart" command line switch; in fact if this switch is provided on an agent's command line, it is ignored (as are any other command line options). Instead, PEST_HP run agents are informed of the fact that they should read a hp starter file by the PEST_HP run manager (if its execution is initiated using the "/hpstart" command line option). The contents of the hp starter file include information which can facilitate the reading of lengthy model output files by run agents. In particular, the PEST_HP agent is informed of the order in which observations are encountered as model output files are read. Where observations number in the hundreds of thousands, and/or where ordering of model outputs corresponding to observations does not coincide with the ordering of observations in the PEST control file, this can reduce the time to read model output files considerably on the first occasion on which they are read by a PEST_HP agent. (Note that if a hp starter file is not employed, then PEST_HP, and all other version of PEST, order observations internally as they read model output files for the first time; their second reading of these files is therefore fast, regardless of the presence, or otherwise, of a hp starter file.)

If either the PEST_HP manager or a PEST_HP agent is asked to read a hp starter file, but the file is not actually present in the folder from which it is run, the absence of this file will be tolerated. The manager will undertake the first model run using a single agent, just as if it had not been requested to read a hp starter file at all. An agent which does not find an expected hp starter file in its folder will read model output files in the usual way, without the benefit of ordering information contained in the hp starter file. Unless observation numbers are very large, this is not a serious disadvantage. Where observation numbers are very large, the benefits of ordering are available on subsequent occasions that model output files are read.

A hp starter file must be written by PEST or I64PEST. It cannot be produced by BEOPEST or Parallel PEST. A serial version of PEST must be used to produce a hp starter file because it stores both reference observations and the ordering of observations in model output files. Where an initial model run is undertaken by BEOPEST or Parallel PEST, the former information is available to the manager whereas the latter information is obtained by an agent. It is therefore difficult to record both sets of information in the same file. Use of a serial version of PEST to write the hp starter file is not a constraint however, as the concept of "parallel" makes little sense when only one model run is undertaken.

If execution of PEST_HP is re-commenced using the "/s" switch, then the presence of a "/hpstart" switch is ignored – except for the fact that the PEST_HP manager instructs its agents to read this file in order to accrue the efficiency gains discussed above where observation numbers are large.

3.2 The "/i" Command Line Option

Execution of PEST_HP can be initiated using the "/i" command line switch. (This switch is also available for PEST, BEOPEST and Parallel PEST.) If started in this way, the PEST_HP manager requests the name of a JCO file which it must read to obtain the initial Jacobian matrix; it does not therefore need to fill this Jacobian matrix using finite-difference-calculated derivatives. See PEST documentation for further details.

If the PEST_HP manager is started with both the "/hpstart" and "/i" command line options, then the need to undertake both the initial model run, and any model runs required for filling of the initial Jacobian matrix, are eliminated. PEST_HP can therefore commence calculation of parameter upgrades using different Marquardt lambdas immediately. However it has been programmed to pause for about a minute before commencing this process; this provides time for all run agents to connect to the manager. As has been discussed above, the Marquardt lambda and line search strategy adopted by PEST_HP for calculation of parameter upgrades depends on the number of available agents.

Note that, as stated above, if PEST_HP is run as an agent rather than as a manager, it ignores all command line options (except the "/h" option through which it learns its agent status and the contact details of its manager).

3.3 SVD-Assist and the "/hpstart" Option

There is nothing to be gained by a PEST_HP manager reading a hp starter file if SVD-assisted inversion is being undertaken. The Jacobian matrix file produced by PEST (or by BEOPEST, Parallel PEST or PEST_HP) as a precursor to initiation of SVD-assisted inversion actually includes reference values for observations. Neither the initial model run, nor model runs required for filling of the first Jacobian matrix, need therefore be undertaken by either PEST_HP or by PEST/BEOPEST/Parallel PEST at the commencement of an SVD-assisted inversion process. Use of the "/hpstart" command line switch therefore has no effect on the operation of the PEST_HP manager, except for the fact that it informs its run agents to expect a hp starter file in their working folders. As is explained above, the agents can then use this file to order observations prior to reading model output files so that the reading of these files can be expedited.

4. Run Results File

4.1 File Contents

As the name implies, a "run results file" records the outcomes of a sequence of model runs. The first line of the file provides the number of parameters and number of model outputs (i.e. observations) which are featured in the file. These coincide with the number of parameters and observations featured in the PEST control file on which a PEST_HP run is based. The run results file then records the names of all of these. Then, for a sequence of model runs, it provides parameter values used for those runs together with model outcomes (i.e. the model-generated counterparts to observations featured in the PEST control file) calculated on the basis of these parameters. (Note that the outcomes of prior information equations are not reported.) The run results file is an ASCII file. Its format is obvious from an inspection of it.

A run results file can serve many purposes. These include uncertainty analysis (where parameter values are randomly selected, or semi-randomly selected using methodologies such as Latin hypercube), global sensitivity analysis (where parameter values follow a Sobol sequence or express trajectories defined by sequential variation of individual parameters), and construction of a proxy model that can partially replace a large, complex model in calibration of the latter. PEST-suite software that is presently under development facilitates production and usage of proxy models for this purpose.

4.2 The RRFSAVE Option

There are two means by which PEST_HP can be instructed to write a run results file. The first is through use of the RRFSAVE variable in the "control data" section of the PEST control file. This variable appears on the tenth line of this file; it must follow the values of the ICOV, ICOR, IEIG and optional IRES variables (these variables are ignored by PEST_HP as it does not write the corresponding files). It can be supplied anywhere following these variables, intermixed with other variables that can also optionally appear on this line (namely VERBOSEREC, JCOSAVEITN, REISAVEITN, PARSAVEITN and PARSAVERUN); see appendix 1 for an example. If the value of the RRFSAVE variable is supplied as "rrfsave", then PEST_HP will record a run results file. Alternatively, if RRFSAVE is supplied as "norrfsave", or omitted altogether, then PEST_HP will not record a run results file.

If recording of a run results file is instigated in this manner, then PEST_HP does not record run results for every single run which it commissions. In particular, results are not saved for model runs which are undertaken for the purpose of finite-difference derivatives calculation because:

1. Too many of these runs are undertaken; and
2. Parameter values are very similar for these runs.

Instead it records outcomes of the following runs:

1. The initial model run;
2. All model runs undertaken for testing of parameter upgrades.

If the name of the PEST control file is *case.pst*, then the run results file saved by PEST_HP is named *case.rrf*.

In complying with the protocol of a run results file, PEST_HP records the reason for which each recorded model run was carried out. Where applicable, this includes the value of the Marquardt lambda and line search factor, and whether or not Broyden Jacobian improvement was implemented. This is followed by the values of all parameters employed for that model run, and the values of model-calculated observations read from model output files recorded on that model run.

In the event of a failed model run, all model output values for that run are recorded as -1.11E35. In contrast, model output values of -1.22E35 indicate an abandoned model run.

4.3 The "/f" Command Line Option

If started with the "/f" command line option, PEST_HP does not undertake parameter estimation at all. Instead it undertakes a series of model runs specifically for the purpose of calculating model outputs using different sets of parameters. These parameter sets must be supplied in a sequence of parameter value files recorded prior to running PEST_HP. They can be constructed using PEST-suite utility programs such as RANDPAR, RANDPAR1 and LHS2PEST; a Sobol sequence parameter set generator is available on request. The protocol for parameter value files is such that a single set of parameters is stored in each file. (See PEST documentation for specifications of this type of file.) PEST_HP expects that these files are named as a sequence with a common filename base. Suppose that the filename base is *sample*. Then the parameter value files must be named *sample1.par*, *sample2.par*, *sample3.par*, etc. The sequence does not need to begin at 1; however there must be no gaps in the sequence. The names of the parameters which appear in each of these files must be the same. They must correspond to parameters that appear in the PEST control file on which basis PEST_HP is run.

Suppose that PEST_HP is started using the command:

```
pest_hp case /f /h :4004
```

Then, upon commencement of execution, PEST_HP reads the PEST control file *case.pst*. It then issues a series of prompts. These prompts, and possible responses to these prompts, are presented below.

```
PEST_HP will run the model repeatedly, using parameter values recorded
 in a sequence of parameter value files. It will record all model-calculated
 observations in a run results file.

 Enter filename base of parameter value files: parval
 Enter first index to use: 101
 Enter last index to use: 200

 Enter parallel run packet size: 50

 Enter name for run results file: record.rrf
```

Responses to the above prompts instruct PEST_HP to read files *parval101.par* to *parval200.par* to obtain 100 sets of parameter values. (If the names of parameters read from these files do not correspond to parameter names recorded in the PEST control file *case.pst*, PEST_HP will cease

execution with an appropriate error message.) The PEST_HP run manager will then tell its agents to carry out model runs based on these parameters. In the above example, parallel model runs will be carried out in packets of 50. (It is the user's responsibility to choose the run packet size in a way that minimizes the chances of agents being idle; the number of agents available for carrying out model runs in this example should thus be 5, 10, 25, 50 or 100.) After each packet of model runs has been completed, PEST_HP calculates objective function components and writes these to the screen and to its run record file; it also records parameter values and model outputs for all runs comprising the packet in the run results file. It then initiates the next packet of parallel model runs.

There is no reason why the run packet size cannot be equal to the total number of parameter sets for which model outputs must be calculated. This is a matter of convenience. Sometimes a useful choice for run packet size is a number which is a small multiple of the number of available run agents. This allows you to view objective functions before the complete set of model runs is finished, thus allowing verification that the model's behaviour is in accordance with expectations. On the other hand, if model run times are sensitive to parameter values, some agents may intermittently become idle while waiting for a packet of model runs to finish because of slow model run times on other agents. Maximum efficiency is thereby gained if the run packet size is equal to the number of runs which must be undertaken.

In the event of model run failure, PEST_HP does not cease execution with an error message if started with the "/f" switch. Nor does it try to repeat a failed model run using another agent. Instead it assumes that the model did not like the parameter set with which it was provided. The objective function is recorded as -1.11E35. All model outputs associated with the offending parameter set are recorded in the run results file as -1.11E35. Model run failure is thus easily recognized.

If an appropriate value is supplied for the RUN_ABANDON_FAC variable in the "control data" section of the PEST_HP control file (see section 7.2.3), PEST_HP will abandon model runs that are requested in any run packet if these runs are unduly late. The role of the RUN_ABANDON_FAC variable in defining "late" when PEST_HP is run with the "/f" command line option is the same as its role in defining "late" where model runs are undertaken for parameter upgrade testing. Model outputs of abandoned runs are all assigned a value of -1.22E35 prior to recording these values in the run results file. The abandoned status of the model run is recorded in the header to the subsection of the run results file in which the results of the abandoned model run are recorded. Meanwhile values of -1.22E35 are recorded for the total objective function, and components of the objective function pertaining to the abandoned model run, in the PEST run record file.

A non-zero WIN_MRUN_HOURS setting (see section 7.2.4) is also respected if PEST is run with the "/f" switch. Agent-terminated model runs are treated as failed model runs. Objective function and model output values recorded in the run record and run results files reflect this status.

As is documented in the PEST manual, a parameter value file supplies values for the PRECIS and DPOINT variables used by PEST for writing numbers to model input files; it also provides the SCALE and OFFSET for each parameter. PEST_HP ignores all of these in reading the sequence of parameter value files to which it is directed when run with the "/f" command line option. Instead, values for all of these variables are obtained from the PEST control file. This frees the parameter value generator which writes the parameter value files from needing to know the values of these control variables.

When the PEST_HP manager is run with the "/f" switch, each agent writes a file named *pest####.pfl* in its working directory on each occasion that it runs the model. This file contains a single entry, namely the name of the parameter value file from which the manager obtained parameter values that pertain to the current model run. If the parameter value filename contains a blank, its name is enclosed in quotes; otherwise it is not. This file is overwritten on each occasion that the agent runs the model.

4.4 Reading a Run Results File

The RRFCALCPSI utility supplied with the standard PEST suite can read a run results file calculated by PEST_HP. It calculates objective function components associated with each observation group. However it adds value to the contents of the run results file by allowing a different PEST control file to be used in calculation of objective function values from that which was used by PEST_HP in the production of this file.

See Part II of the PEST manual for details.

5. Model File Distribution

5.1 General

Suppose that a modeller is calibrating (for example) a steady state groundwater model, or a natural state geothermal reservoir model. The execution speeds of models such as these are much faster if initial pressures provided to the model are close to final pressures. The latter depend, of course, on parameter values. It is PEST_HP's job to adjust these such that model-generated pressures and/or flows (calculated from pressures) match observed pressures and/or flows at measurement sites.

During each iteration of the inversion process through which a model such as this is calibrated, PEST_HP attempts to improve the fit between model-calculated pressures/flows and their measured counterparts. After finite-difference derivatives have been calculated, different parameter upgrades, calculated using different Marquardt lambdas, and different line search fractions along different upgrade directions, are tested on the different computing nodes on which PEST_HP agents are running. The model that is run on one of these nodes employs the best parameters calculated for that iteration. PEST_HP does not know in advance which parameter set will be the best; this becomes apparent after the model which employs this parameter set, and models which employ other parameter sets, have been run by their respective agents, and objective functions associated with all of these parameter sets have been calculated.

The best parameter set achieved during any iteration of the inversion process is used as the starting point for the next iteration. Finite difference derivatives are calculated by varying parameters individually and incrementally from base values comprising this parameter set. Ideally, the initial pressures used by the model for all of these parameter-increment runs should be those calculated on the basis of the best parameter set from the previous iteration. The model runs devoted to finite-difference derivatives calculation should then be fast because solution pressures calculated for incremented parameters should be only incrementally different from initial pressures calculated using base parameters.

One way of achieving this desirable outcome is to employ PEST_HP's observation re-referencing functionality. Thus at the beginning of each new iteration, a special model run is undertaken in which best parameters achieved during the previous iteration are employed. Pressures calculated using this parameter set are then saved as initial pressures for an immediately ensuing model run. This next model run should take very little time; its purpose is to create reference model outputs used in finite-difference derivatives calculation. Meanwhile these same initial pressures should be distributed to every agent at PEST_HP's disposal so that model runs that are undertaken by these agents are also fast. The speed of the finite-difference derivatives calculation process is thus greatly increased.

Note how, in the above procedure, the simulator is run twice when PEST-HP undertakes the re-referencing model run. During both of these runs it employs best parameters from the previous iteration. The first simulation calculates steady-state/natural state pressures based on these parameter values; the second simulation uses these pressures for its initial conditions. In doing so it reproduces the simulation context in which other model runs will be undertaken with parameters incrementally varied from their current values. As stated above, pressures and flows at observation

locations calculated during this second simulation become reference pressures used in finite difference derivatives calculation.

While this approach has been used successfully on many occasions, some problems may arise in its implementation – particularly in the cloud environment. One problem is that of distributing the file which contains initial pressures to agent nodes. The PEST_HP run manager node may not have permission to write to agent nodes. It may not even know where they are! Another problem is that this procedure requires that the model be run using best parameters achieved up to this point in the inversion process at the start of each new iteration (just before commencement of finite-difference derivatives calculation). However this same run has already been done during the previous iteration. Furthermore, all agents other than that which is undertaking the re-referencing run must stand idle while this repeated run proceeds. This does not constitute efficient usage of cloud resources.

These problems can be overcome by using PEST_HP's file distribution functionality. At the end of each iteration of the inversion process PEST_HP can optionally fetch one or a number of files from the node on which the best model run from the previous iteration was carried out. These files are first transferred to the manager's node using TCP/IP – the same protocol as that employed for all other PEST_HP manager-to-agent communication. Then, optionally, the manager can issue a user-specified system command to process these files; this processing is undertaken locally on its own node. Then calculation of finite-difference derivatives commences. However before PEST_HP commissions a model run on any particular agent, it transfers one or a number of files to that agent. These files can be the same as those previously transferred to the manager from the node on which the best model run was carried out. Alternatively, new files calculated by the manager node on the basis of these transferred files can be transferred to each agent node. As before, transfer between manager and agent is completed using TCP/IP. Thus write permission on agent nodes is not required. The model is then run on that agent with a parameter incrementally varied in the usual manner.

This file distribution protocol eliminates the need for the manager to know where the agent is situated. It also eliminates the need for the manager to have read/write permission on the agent's drive. At the same time, this protocol reduces the computational burden of the re-referencing run. An expensive simulation with old starting pressures is no longer required. Instead, the re-referencing simulation can use pressures calculated during the parameter upgrade procedure of the previous iteration as its initial pressures. These same initial pressures are distributed to all agents for finite-difference derivatives calculation.

5.2 PEST Control File

To implement strategic file distribution as outlined above, a new section must be introduced to the PEST control file. This "distribution files" section must be the final section of the file. Figure 5.1 shows specifications of the "distribution files" section of the PEST control file while figure 5.2 shows an example.

```
* distribution files
DISTRIB_TYPE SOURCEFILE_AGENT TARGETFILE_MANAGER [SOURCEFILE_MANAGER TARGETFILE_AGENT]
The above line is repeated up to four times.
command = DISTRIB_MODEL_COMMAND
The above line is optional and can be inserted anywhere in the "distribution files" section.
```

Figure 5.1 Specifications for the "distribution files" section of a PEST control file.

```
* distribution files
2 model.out temp.dat init.dat init.dat
1 model.out init.dat
command = process_outputs.exe
```

Figure 5.2 Example of the "distribution files" section of a PEST control file.

As for any other section of a PEST control file, the "distribution files" section must begin with a header line which provides the name of the section. This line must begin with an asterisk character followed by a space.

Up to six lines of data can follow the "* distribution files" header. The section is considered to finish when a blank line, or the end of the PEST control file, is encountered. Only five lines can follow the section header if a model command is not supplied.

The optional command associated with the "distribution files" section (i.e. DISTRIB_MODEL_COMMAND) can be provided on any of the lines which follow the "* distribution files" section header. However only one such command can be supplied. The line which provides this command must commence with the string "command =". The actual command which the PEST_HP manager will deliver to the operating system must follow this string.

Note the following features pertaining to the protocol of the line which provides the optional system command associated with file distribution.

- The word "command" can be supplied in upper or lower case, or in a combination of the two.
- The "=" character which follows the "command" string can optionally be separated from this string by a space.
- The command which follows the "=" character can optionally be separated from it by a space.
- The text comprising the system command can optionally be surrounded by double quotes.

As for other commands cited in the PEST control file, the text comprising DSITRIB_MODEL_COMMAND of figure 5.1 will be provided to the operating system exactly as written by the user. This command can be the name of a batch file, or the name of an executable program; optionally it can also include command line arguments.

Lines other than that which provides the DISTRIB_MODEL_COMMAND which appear in the "distribution files" section of the PEST control file (there can be a maximum of five of these) must all begin with an integer. This integer must be 1 or 2. This is the value of the DISTRIB_TYPE variable associated with each distribution file.

If DISTRIB_TYPE is set to 1, then the nominated file on the node on which the best model run was achieved during the previous round of parameter upgrade testing is copied to the manager's node; however this file is not distributed to nodes used by other agents. The modeller must therefore organize file distribution to these nodes him/herself. Alternatively, in some parallelization contexts, all model incidences may read this file from the manager's working folder themselves, this obviating the need for distribution of the file to agent nodes. In contrast, if DISTRIB_TYPE is set to 2, the PEST_HP manager first copies the nominated file to its own node from the best-upgrade node, and

then copies it to each agent node, possibly after processing the file using the DISTRIB_MODEL_COMMAND system command.

If DISTRIB_TYPE is set to 1, then two filenames must follow the value of this variable. These are denoted as SOURCEFILE_AGENT and TARGETFILE_MANAGER in figure 5.1. The first is the name of the file that must be copied from the best-upgrade agent's node. The second is the name that will be given to this file on the manager's node. If either of these filenames contain spaces, the filenames should be enclosed in quotes. These names can include (relative) pathnames if desired. In many cases the names given to SOURCEFILE_AGENT and TARGETFILE_MANAGER will be the same, and contain no pathnames; hence the file is simply copied from the working directory (i.e. folder) of the best-upgrade agent to the working directory of the PEST_HP manager.

If DISTRIB_TYPE is set to 2, then four filenames must follow the value of this variable. The first two are identical to those required when DISTRIB_TYPE is set to 1. However the other two are required for copying the file from the manager's node to agent nodes. SOURCEFILE_MANAGER is the name of the file that must be copied from the manager node to all agent nodes. TARGETFILE_AGENT is the name given to this file on agent nodes once it has been copied. In many circumstances SOURCEFILE_MANAGER will be the same as TARGETFILE_MANAGER. However if a DISTRIB_MODEL_COMMAND is run by PEST_HP, then this command may process the TARGETFILE_MANAGER file to produce a new SOURCEFILE_MANAGER file that is appropriate for distribution to agents. While PEST_HP allows this complication, and allows a file copied from the best-upgrade agent's node to be named differently when it appears on the manager's node, there will be many occasions where such complexity is not warranted; there will also be many occasions where no local command is employed to process the copied file. In this case all of the filenames associated with a DISTRIB_TYPE of 2 will be the same.

5.3 Implementation Details

PEST_HP initiates file distribution at the end of each iteration of the inversion process, just before it commences the next iteration (and possibly at the end of the inversion process – see below). First, regardless of the DISTRIB_TYPE setting associated with each distribution file, PEST_HP copies the file from the best-upgrade agent's node to the manager's node. This is done for all distribution files cited in the "distribution files" section of the PEST control file. If this process fails for any of the distribution files, PEST_HP ceases execution with an appropriate error message. After it has transferred all distribution files to the manager's node (recall that there can be up to five of these), PEST_HP issues the optional system command associated with its file distribution functionality (i.e. DISTRIB_MODEL_COMMAND of figure 5.1). It then proceeds to the next iteration.

For distribution files with a DISTRIB_TYPE of 2, PEST_HP does not transfer the pertinent distribution file to an agent's node until just before the next occasion on which it employs that agent to carry out a model run. If there is a failure in this transfer, PEST_HP ceases execution with an appropriate error message.

Activation of file distribution functionality requires some small modifications to normal PEST_HP functionality in order to guarantee the integrity of the inversion process. These modifications are as follows.

- If, during any iteration of the inversion process, the objective function fails to fall, and if this failure triggers PEST_HP's initiation of higher order finite-difference derivatives calculation, PEST_HP will normally commence the new iteration using the best parameters that have been achieved so far during the inversion process, even though they were not achieved during the previous iteration. This strategy cannot be adopted if file distribution functionality is in place because model-generated files associated with the best parameter set will have been lost from the node which employed this parameter set for its model run. Instead, the next iteration employs the best parameter set from the previous iteration despite the fact that this is not the best overall parameter set achieved during the inversion process to date.
- There may be occasions when the PEST_HP run manager loses access to the node of the best-upgrade agent before it can copy files from that agent's node to its own node. (This can happen if the agent disappears from the network, or if PEST_HP has access to less than three nodes.) If this happens, PEST_HP records this state of affairs to the screen and to the run record file; it then continues to the next iteration without file distribution.
- All distribution file transfers are recorded on the run management record file.

Note also the following.

- If more than one file requires distribution, then PEST_HP will allow duplicate names for the SOURCEFILE_AGENT and SOURCEFILE_MANAGER files associated with these different distribution files (though it is unclear why a user would want to do this). However it will not allow duplicate names for the TARGETFILE_MANAGER or TARGETFILE_AGENT filenames associated with different distribution files.
- Even if no source and target files are provided in the "distribution files" section of the PEST control file, a DISTRIB_MODEL_COMMAND can still be supplied. If so, the PEST_HP manager will send this command to the operating system at the close of every iteration of the inversion process.
- PEST_HP cannot be restarted using the "/s" switch if file distribution functionality is activated, as it does not know the status of distribution files on either manager or agent nodes on recommencement of execution. Use the PARREP utility to create a new PEST control file based on optimised parameters from the previous run to restart it under these circumstances.
- PEST_HP cannot be started with the "/f" switch if file distribution functionality is activated as use of this functionality would support no gains in efficiency when PEST_HP is used in this way.
- If TCP/IP communications fail when an agent is receiving a distribution file from its manager, or if PEST_HP, running as an the agent, cannot write the distribution file to its local drive, it ceases execution with an appropriate error message. The agent is therefore lost to the inversion process.

On termination of execution, PEST_HP copies distribution files from the folder of the best-upgrade agent to that of the manager:

- if it can, and
- if parameters underwent improvement on the final iteration of the inversion process.

Success of this operation depends on whether the files that were written by the best-upgrade agent on the last parameter upgrade cycle are still present in that agent's folder. If PEST_HP is able to copy these files back to the manager, if notifies the user through its screen output, its run record file and its run management record file. If not, no message is recorded. In neither case is the DISTRIB_MODEL_COMMAND issued to the operating system.

5.4 File Distribution and Broyden Jacobian Updating

Notwithstanding the extra book-keeping that it requires, PEST_HP does not prevent Broyden updating of the Jacobian matrix if file distribution is activated. This is because conjunctive use of these two items of PEST_HP functionality may be warranted when calibrating large, highly parameterized, nonlinear models such as geothermal reservoir models.

Caution must be exercised in implementing both of these options together, however. In particular, it is advisable that the directory used by the PEST_HP manager should not also be employed by a PEST_HP agent.

During each iteration of the inversion process, pertinent files that are nominated in the "distribution files" section of the PEST control file are copied from the folder used by the agent that supervised the best model run, to the folder used by the PEST_HP run manager, at the end of the first parameter upgrade testing cycle, regardless of whether a second round of upgrade testing takes place following Broyden Jacobian updating. If a second round of upgrade testing does, indeed, take place, files earmarked for distribution are copied to the manager's folder only if the best parameter set obtained during that second testing cycle is an improvement over the best obtained during the previous cycle of parameter upgrade testing (i.e. the cycle of parameter upgrade testing undertaken without a Broyden-updated Jacobian matrix). File distribution from the manager's folder to agent folders (for files with a DISTRIB_TYPE of 2) then takes place as agent nodes are commissioned to undertake model runs at the beginning of the next iteration of the inversion process.

5.5 File Distribution and Randomized Jacobian

File distribution to agent node folders does not occur if PEST_HP is using a randomized Jacobian matrix (see section 9), and the covariance matrix from the previous iteration on which this Jacobian matrix is based is being supplemented with model runs from the present iteration in accordance with the setting of the NRANDREPEAT control variable. Under these circumstances, parameter reference values are unchanged for the next iteration. Hence files copied back to the manager's folder from the best-run agent's folder during the previous iteration cannot be used to provide initial conditions for model runs undertaken during the subsequent iteration of the inversion process as the upgraded parameters from the previous iteration have been rejected (because they did not result in objective function improvement). Instead, reference parameter values employed at the beginning of the previous iteration are retained for the new iteration.

Similar considerations apply to the optional DISTRIB_MODEL_COMMAND system command. Where PEST_HP is not using a randomized Jacobian matrix, this command is issued at the beginning of every iteration of the inversion process because upgraded parameters from the previous iteration are employed as reference values for the ensuring iteration, even if they did not lower the objective function. Where a randomized Jacobian matrix is employed, however, the DSITRIB_MODEL_COMMAND system command is not issued where a reference parameter set persists to the next iteration in accordance with the dictates of NRANDREPEAT functionality.

6. PEST_HP-Specific Output Files

6.1 General

PEST_HP records the same suite of output files that other versions of PEST record (with the exception of file *case.mtt* which provides a linear approximation to the posterior parameter covariance matrix in over-determined parameter estimation contexts). However it records some extra output files (in addition to the optional run results file described in the previous section); these are now described.

6.2 Objective Function Record File

Unless it is run using the "/f" command line switch, PEST_HP writes an "objective function record file" named *case.ofr* (on the assumption that the governing PEST control file is *case.pst*). This file contains a table which links the value of the objective function, and components thereof, to the iteration number of the inversion process. It is updated at the beginning of each iteration. This file is easily imported into a spreadsheet or graphing package for visual tracking of PEST_HP progress.

Where PEST_HP is run in "regularisation" mode, the objective function record file lists values for the measurement and regularisation objective functions, as well as for the objective function components associated with all non-regularisation observation groups. It does not provide objective function values for regularisation groups as these are non-comparable between iterations; they are subject to multiplication by the regularisation weight factor, and to inter-group weight factor adjustment as designated by the value of the IREGADJ regularisation control variable.

Where PEST_HP is run in "estimation" or "pareto" modes, the objective function record file lists values for the total objective function, and for the objective function components associated with all observation groups.

6.3 Parallel Run Efficiency File

Suppose that PEST_HP is run on the basis of the PEST control file *case.pst*. In common with BEOPEST and Parallel PEST, PEST_HP records parallel run management details in a file named *case.rmr* (the parallel run management record file). In contrast to BEOPEST and Parallel PEST however, PEST_HP records an additional "parallel run efficiency file" named *case.rme*. This file contains a table which can be easily imported into a spreadsheet or graphing package for plotting. For each parallel agent, the parallel run efficiency file records:

- the agent's working folder;
- the current status of the agent (active, idle or lost);
- the number of model runs carried out by the agent;
- the number of run failures encountered by the agent;
- the number of times that a run undertaken by the agent was abandoned or assigned to another agent;
- the number of successful model runs carried out by the agent;
- the maximum, minimum and average model run times (in seconds) encountered by the agent;
- the cumulative run time (in seconds) over all model runs undertaken by the agent;

- the cumulative time (in seconds) over which the agent has existed;
- the parallel run efficiency of the agent (calculated by dividing cumulative run time by cumulative existence time).

These statistics need some refinement for cases where different commands can be used to run the model in different circumstances, for example if multiple model commands are employed for the purpose of finite difference derivatives calculation, and/or if observation re-referencing is undertaken. This refinement awaits further PEST_HP development.

The parallel run efficiency file is updated every minute, or at the completion of every parallel package of model runs, whichever happens sooner.

PEST_HP issues a warning message to the screen at the beginning of each iteration of the inversion process if a particular agent has encountered run failures but no run successes. This may indicate that a file is missing or corrupted in that agent's folder.

6.4 Parameter Error File

See section 7.1.2.

7. New and Altered Control Variables

7.1 Model Run Failure

7.1.1 LAMFORGIVE and DERFORGIVE

If the LAMFORGIVE variable on the sixth line of the PEST control file is set to "nolamforgive", or if this variable is omitted from the PEST control file, then BEOPEST and Parallel PEST will cease execution with an appropriate error message if an agent reports model run failure for a particular set of updated parameters. But first the BEOPEST or Parallel PEST run manager asks that the run be repeated by another agent; if failure is repeated, the manager ceases execution with the pertinent error message. Alternatively, if LAMFORGIVE is set to "lamforgive", then BEOPEST/Parallel PEST will not repeat the offending model run. Instead they will declare that the objective function corresponding to the offending set of parameters is very high; this provides a signal to the inversion process that this part of parameter space is unproductive.

PEST_HP ignores the LAMFORGIVE setting (or absence of LAMFORGIVE setting) provided by a user in the PEST control file. It sets LAMFORGIVE internally to "lamforgive".

PEST_HP does not ignore the setting of the DERFORGIVE variable provided in the PEST control file, however; instead, it treats this variable in the same way that BEOPEST and Parallel PEST treat it. If DERFORGIVE is set to "noderforgive" (or omitted from the PEST control file), then model run failure during filling of the Jacobian matrix causes PEST_HP to repeat the run and then, if failure occurs again, terminate execution with an appropriate error message. Alternatively, if DERFORGIVE is set to "derforgive", PEST_HP does not repeat the failed model run using another agent. Instead it declares the sensitivities of all model outputs to the incremented/decremented parameter to be zero. It does not cease execution; it continues to fill the Jacobian matrix by processing other model run outcomes.

7.1.2 Record of Offending Parameter Sets

PEST_HP records all parameter sets which precipitate model run failure in a "parameter error file" named *case.per* (assuming that the PEST control file on which the current PEST_HP run is based is named *case.pst*). Offending parameter sets are listed using a format which is not unlike that of a parameter value file. Hence, with a little cutting and pasting, a parameter value file is readily built using any of the offending parameter sets recorded in a parameter error file. The PARREP utility can then be employed to populate a new PEST control file using these parameters. NOPTMAX can be set to zero in the new PEST control file; PEST can then be run to reproduce the problem.

When PEST_HP is employed to undertake SVD-assisted inversion then, as is documented in the PEST manual, the inversion process is based on so-called super parameters. In the event of model run failure, PEST_HP records the values of not only super parameters, but also of base parameters, in its parameter error file. The latter can be PARREPed into the base parameter PEST control file to reproduce the model run problem in the manner described above. It may not be possible to reproduce the problem by PARREPing super parameters into the super parameter PEST control file as definition of super parameters can change during the course of the inversion process.

7.2 Handling of Overdue Model Runs

7.2.1 General

Sometimes model runs can take longer than expected to reach completion. Where parallel model runs are distributed across a local network, this may happen because the computer on which a local agent is running has been given other work. Alternatively, it may be perceived that the model is taking a long time to run because network communications between the manager and the pertinent agent have broken down. A third alternative is that the parameter set on which the model run is based may be creating convergence difficulties for the model solver. The first two of these occurrences are unlikely in a cloud environment. The third can sometimes happen where model runs are being undertaken for the purpose of testing parameter upgrades. Under these circumstances the parameter sets on which the different model runs are based can be very different.

PEST_HP adopts two different strategies for the handling of late model runs; the strategy that is adopted on any particular occasion depends on the reason for which model runs are being undertaken. When derivatives are being calculated, PEST_HP re-assigns overdue model runs to alternative agents which have already completed the model runs assigned to them. (Note that model run re-assignment can be prevented, if desired, in ways described below.) On the other hand, where a packet of model runs is initiated for testing a variety of updated parameter sets, and where one or more of these parameter sets delays completion of the packet because of problematic solver convergence, PEST_HP can be instructed not to wait for such overdue model runs (if they are "overdue enough"). Instead, it abandons the troubled agents until they have completed these overdue runs (and ignores the results of those runs), while advancing to the next iteration of the inversion process wherein PEST_HP commences filling of a new Jacobian matrix. Furthermore, if the JACUPDATE control variable is set to greater than zero (so that Broyden Jacobian updates are undertaken during each iteration of the inversion process prior to initiating a second round of update-testing model runs), PEST_HP internally re-sets this control variable to zero. This action is undertaken under the premise that the run-time cost of testing a second set of parameter updates during each iteration of the inversion process is likely to be increased considerably by agents becoming bogged down with problematical model runs.

These options, together with a third option whereby a run agent can terminate a model run if it takes longer to execute than a pre-set time limit, are now discussed in greater detail.

7.2.2 The RUN_SLOW_FAC Variable

BEOPEST and Parallel PEST read the value of a variable named RUN_SLOW_FAC from the Parallel PEST run management file (named *case.rmf* where the PEST control file is named *case.pst*). However PEST_HP does not read a run management file; the value of RUN_SLOW_FAC can instead be supplied on the sixth line of the PEST control file. Recall from the PEST manual that RUN_SLOW_FAC is used to calculate the elapsed time at which a model run is deemed to be overdue; in assuming the worst (namely communications failure with the pertinent run agent), the run manager then assigns the overdue model run to the fastest available idle agent. The elapsed time at which a model run is deemed to be overdue is calculated as RUN_SLOW_FAC times the anticipated model run time on the agent to which the model run is assigned.

As is discussed above, in contrast to BEOPEST and Parallel PEST, PEST_HP commissions an alternative agent to re-commence an overdue model run only where model runs are being undertaken for the

purpose of finite-difference derivatives calculation. Where model runs are being undertaken in order to test parameter upgrades, PEST_HP handles overdue model runs in a different way; this is governed by the RUN_ABANDON_FAC variable discussed in the following subsection.

If a value for RUN_SLOW_FAC is not supplied by the user, PEST_HP uses a default value of 5.0. Use of such a high factor is based on the premise that in a cloud computing environment communication between the manager and its agents is unlikely to fail. Furthermore, all computers used for carrying out model runs are likely to have similar speeds. If, on a particular occasion, a model run is overdue, this is likely to be an outcome of the parameters with which the model was provided for that run. There is thus no need to undertake the same model run using an idle agent, as the outcome of that run is unlikely to change when using the new agent.

RUN_SLOW_FAC can be set to a different value if desired. To assign an alternative value to RUN_SLOW_FAC, add the string:

```
run_slow_fac = value
```

to the sixth line of the PEST control file following the value of the NUMLAM (and optional JACUPDATE) variable. This is the same line of the PEST control file as that on which the strings "lamforgive" and "derforgive" can also be provided. (Note that, as stated above, "lamforgive" is ignored by PEST_HP, as its model run forgiveness behaviour when commissioning model runs to test parameter upgrades is governed by internal settings and/or by the RUN_ABANDON_FAC variable.) In the string "run_slow_fac = *value*", *value* represents a number greater than 1.0. PEST_HP will accept a space on either side of the "=" symbol when reading this string; alternatively, spaces can be omitted. The string can be placed anywhere following NUMLAM (and optionally JACUPDATE), interchangeably with the "lamforgive" and "derforgive" strings. See appendix 1 for an example.

As stated, provision of a value for RUN_SLOW_FAC is optional.

BEOPEST and Parallel PEST have been modified to allow reading of RUN_SLOW_FAC where it is supplied in the manner described above. However for BEOPEST and Parallel PEST, a value supplied for this variable in the run management file over-rides a value supplied for this variable in the PEST control file.

Note that if PEST_HP's first attempt to run the model at the very beginning of the inversion process leads to failure, PEST_HP will not repeat that run using a different agent. It assumes that a mistake has been made in model setup; accordingly, it terminates execution with an appropriate error message.

7.2.3 The RUN_ABANDON_FAC Variable

PEST_HP does not re-assign late model runs to other agents if a packet of model runs has been commissioned for the testing of parameter upgrades. As has already been discussed, the parameter upgrade testing process has been designed to finish quickly so that PEST_HP can move on to the next iteration of the inversion process with agent idleness minimized. However it is not impossible that certain updated parameter sets may precipitate interminably slow model execution speeds. An appropriate setting of the RUN_ABANDON_FAC variable can instruct PEST to abandon inordinately delayed model runs and move on to the next iteration of the inversion process. The RUN_ABANDON_FAC variable instructs PEST_HP to treat the agent as lost until the recalcitrant

model run is complete. Once this occurs, the respective agent is then "brought back into the fold" and assigned a model run appropriate to PEST_HP's current task. Meanwhile, as stated above, if the optional JACUPDATE variable is set to a number greater than zero, PEST_HP sets this variable to zero to reduce the chances of losing agents again.

The means through which a value is supplied for RUN_ABANDON_FAC is very similar to that for which a value is provided for RUN_SLOW_FAC. To assign a value to RUN_ABANDON_FAC, add the string:

```
run_abandon_fac = value
```

to the sixth line of the PEST control file following the value of the NUMLAM (and optional JACUPDATE) variable; see appendix 1 for an example. The protocol is identical to that for RUN_SLOW_FAC. Note, however, that a RUN_ABANDON_FAC value of 0.0 deactivates run abandonment. (The same happens if no value is supplied for RUN_ABANDON_FAC at all.) If it is not assigned a value of 0.0, then RUN_ABANDON_FAC must be provided with a value of 1.2 or greater (preferably greater than 2.0); if not, PEST_HP will cease execution with an appropriate error message.

The way in which the RUN_ABANDON_FAC variable is employed in parallel run management is a little different from that in which the RUN_SLOW_FAC variable is employed Suppose that the slowest model run of the present package has taken *N* seconds to complete. RUN_ABANDON_FAC will abandon all non-completed runs after a further *N* × RUN_ABANDON_FAC seconds have elapsed if no further runs have reached completion in the meantime. However if, over this time, another model run reaches completion, then *N* is re-set and a new agent-abandonment threshold is calculated. (It is apparent from this strategy that tolerance for late model runs increases as PEST_HP discovers that lateness is the norm for the current parallel run package.)

7.2.4 The WIN_MRUN_HOURS Variable

In the Windows version of PEST_HP, a time limit can be placed on how long a model is allowed to run, regardless of the reason for carrying out this run. This variable is not available in the LINUX version of PEST_HP. In the LINUX environment, you can limit model execution times yourself using the *timeout* system command when running the model.

By way of example, suppose that you wish to terminate execution of the model if it runs for more than 30 minutes. (This can serve as a defence against excessive execution time caused by model solver convergence difficulties.) Then the following string should be added to the sixth line of the PEST_HP control file, anywhere following the value of the RLAMFAC variable:

```
win_mrun_hours = 0.5
```

This informs the PEST_HP run manager that it must instruct its agent to terminate a model run if that run takes longer than 0.5 hours. Once an agent has terminated execution of the model, it attempts to read the model's output files in the usual manner. Naturally, these will be incomplete, so a run failure will be reported back to the run manager. The run manager then treats the expired run as it does any other failed model run.

Note the following:

- If the value of WIN_MRUN_HOURS recorded in the PEST control file used by the run manager differs from that recorded in a PEST control file read by a run agent, the value in the run manager's PEST control file takes precedence. Similarly, if a value for WIN_MRUN_HOURS is not supplied in the PEST control file that is read by an agent, but is recorded in that which is read by the run manager, the run manager instructs its agents to terminate model runs once their allotted time has expired, and agents will obey.
- If the value supplied for WIN_MRUN_HOURS in the PEST control file read by the manager is less than or equal to zero, then model run termination functionality is disabled.
- If WIN_MRUN_HOURS is set to a positive number, then DERFORGIVE is automatically activated. That is, model run failure (or model run termination) is forgiven when calculating finite-difference derivatives.
- Model run termination acts independently of model run abandonment. A run can be abandoned by the PEST_HP run manager. However it will not be terminated by the agent until the WIN_MRUN_HOURS model expiry time has elapsed. Run abandonment is done by the manager while run termination is a local affair, implemented by run agents using a run-time limit provided by the manager.

It is important to note that when WIN_MRUN_HOURS is set to a positive number, PEST_HP uses the *CreateProcess()* function from the Windows API rather than a system() call to run the model. This function has certain idiosyncrasies. The following requirements of the command supplied in the "model command line" section of the PEST control file must be respected.

- Do not use the "<" character in the model command to direct the model to read keyboard input from a file. Similarly, do not use the ">" character to direct model output to a file (or to "nul"). If this is a requirement for running the model, place the command to run the model in a batch file, which is then run by the *CreateProcess()* function as the model command.
- If you run a batch file as the model command, be sure to include the ".bat" suffix in the command; the *CreateProcess()* function does not add this suffix itself.

7.3 Termination of PEST_HP

7.3.1 General

Reasons for graceful termination of PEST_HP execution include (but are not limited to) the following. (See the PEST manual for a description of pertinent variables.)

- NOPTMAX iterations have elapsed since execution of PEST_HP began.
- The (measurement) objective function is less than PHISTOPTHRESH.
- Parameter estimates have not improved over the last NPHISTP iterations. (Parameter "improvement" depends on whether PEST_HP is running in "estimation" or "regularisation" mode.)
- The measurement objective function is below PHIMACCEPT (unless REGCONTINUE is set to "continue".)
- The objective function has decreased by less than a relative amount of PHIREDSTP over NPHISTP successive iterations. (When run in "regularisation" mode the objective function in question may be the regularisation or measurement objective function, this depending on the value of the latter in relation to PHIMLIM.)

- The relative change in no parameter has exceeded RELPARSTP over NRELPAR successive iterations.
- The (measurement) objective function has fallen below PHISTOPTHRESH.

In many contexts of PEST_HP usage, it is better to stop PEST_HP yourself than to wait for one of these termination criteria to be met, especially if paying for time on the cloud. As the writer of PEST (and as its longest and most devoted user), I normally set termination criteria tightly in order to avoid premature cessation of PEST execution. However I monitor the progress of PEST myself. When it appears unlikely that further PEST execution will result in a further lowering of the objective function, I terminate it. (The easiest way to stop PEST_HP is to press <Ctl-C> when focussed on the PEST_HP manager window.) The exception to this rule may be when PEST_HP is running in "regularisation" mode and REGCONTINUE is set to "continue". In this case I am seeking the lowest regularisation objective function that I can, commensurate with PEST_HP achieving a measurement objective function of PHIMLIM. If the measurement objective function is below PHIMLIM, then I may allow PEST_HP to raise it to PHIMLIM while lowering the regularisation objective function a little further.

7.3.2 New Termination Criteria

PEST_HP accepts two variables, beyond those which are used by other versions of PEST, that control termination of its execution. These are the HARDSTOPHOURS and SOFTSTOPHOURS variables. Either of these variables can be used, or neither of them can be used. However they cannot be used together.

Suppose that SOFTSTOPTHOURS is provided with a value of 24.0. Then the PEST_HP manager will cease execution on the first occasion that it begins a new iteration of the inverse process following the passing of 24 hours since the commencement of its execution. Thus an upgraded parameter set is calculated before cessation of execution, and no model runs are wasted. When the PEST_HP manager then ceases execution, it signals all of its agents to also cease execution. Unless an agent is preoccupied in supervising an abandoned model run, it ceases execution immediately upon reception of this signal. In contrast, if it is undertaking an abandoned model run it cannot receive this signal until the run is complete; thereupon it ceases execution. Alternatively, it may terminate the model itself after WIN_MRUN_HOURS have elapsed.

If HARDSTOPTHOURS is set to 24.0, then the PEST_HP manager will cease execution 24 hours after commencement of its execution; regardless of the current status of the inversion problem solution process. There may be a slight delay however if parameter numbers are high and PEST_HP is engaged in laborious parameter update calculations. Upon cessation of its own execution, the PEST_HP manager signals to its agents to also cease their execution. However they will not receive this signal until the model runs which they are supervising are complete. (These can be stopped manually, of course, if desired.)

If PEST_HP ceases execution because of a SOFTSTOPHOURS or HARDSTOPHOURS timeout, then its execution can be easily resumed by restarting it using the "/s" switch.

7.3.3 Specifying Values for Timeout Variables

Values are provided for the SOFTSTOPHOURS or HARDSTOPHOURS variables by including the string

softstophours = *value*

or

hardstophours = *value*

anywhere on the ninth line of the PEST control file (the same line that is used by other PEST termination control variables); *value* must be replaced by a number specifying PEST_HP timeout time in hours. See appendix 1 for an example.

7.4 User-Prescribed Insensitivity

7.4.1 General

Like PEST and BEOPEST, PEST_HP supports the use of different model commands for running the model in order to calculate finite-difference derivatives with respect to different parameters. This occurs if the NUMCOM variable in the "control data" section of the PEST control file is set to a number greater than 1, and/or if PEST's observation re-referencing functionality is activated. In the former case, the command index that is associated with each parameter must be recorded in the "parameter data" section of the PEST control file; meanwhile the model commands themselves are listed in the "model command line" section of the PEST control file.

The use of different model commands to run a model for finite-difference calculation of sensitivities with respect to different parameters can be useful where models are complex, take a long time to run, and have many parameters. This functionality allows a modeller to forego the running of all components of a complex model when calculating derivatives for some parameters; for these parameters, only a shorter version of the model may need to be run when calculating sensitivities with respect to those parameters.

For example, suppose that a modeller wishes to calibrate a composite steady state and transient groundwater model. Suppose also that the model domain is populated with pilot points used for representation of both permeability and storage coefficient parameters. Suppose further that the transient component of the calibration process is focussed on a small part of the model domain in which one or a number of pumping tests was conducted, and that storage coefficient pilot points are restricted to this area. A modeller may set up two models as follows:

- model 1, in which both the steady state and transient components of the model are run; it is presumed that this model runs slowly because of its transient component.
- model 2, in which just the steady state component of the model is run; it is presumed that model 2 runs quickly.

It is important to note that when running model 2, the outputs of the transient component of the model must somehow be provided with values, as PEST expects to read all model output files using the instruction set which was constructed for this purpose. This same instruction set is used to read model-generated observations following all model runs.

The modeller may instruct PEST to run model 1 only when calculating finite-difference derivatives for storage coefficient parameters and for permeability parameters associated with pilot points which are situated close to the sites of the pumping tests. For all other parameters, model 2 is employed for finite-difference derivatives calculation. Let us refer to the first group of parameters as type 1 parameters and the second group of parameters as type 2 parameters.

A problem with this scheme in versions of PEST other than PEST_HP, is that the modeller must find a way of ensuring that sensitivities of transient model outputs with respect to type 2 parameters are zero. (Sensitivities of storage parameters to steady state model outputs are automatically zero.) One way to achieve this is to employ PEST's observation re-referencing functionality. The model run undertaken for re-referencing purposes would be comprised of both the steady state and transient models (i.e. model 1). Transient outputs of this re-referencing run would then be saved to a special file. Model 2 would copy the contents of this special file to the expected transient model output file on every occasion that it is run during the same iteration of the inversion process. These model outputs would therefore remain unchanged from their iteration-specific reference values as type 2 parameters are incrementally varied. Sensitivities of these outputs to type 2 parameters would therefore be zero.

While this scheme would be effective, it is somewhat cumbersome to implement. It becomes even more cumbersome to implement in a parallel environment where the transient output file produced during the re-referencing run must be copied to the working directories employed by all parallel run agents. (Note that PEST_HP's file distribution functionality could help here.)

"User-prescribed zero sensitivity" functionality implemented in PEST_HP can be of assistance in situations such as these. When using this option, there is no need to invoke PEST_HP's observation re-referencing functionality. (Note however that observation re-referencing is not precluded when deploying user-prescribed zero sensitivity functionality.) Instead, the modeller can program model 2 to endow all expected transient model outputs with a single, specific, value. (This can also be implemented using a "copy" command run through the model 2 batch file.) This single value (designated as ZEROSENVAL) instructs PEST_HP that the sensitivities of all model outputs which are assigned this value with respect to the parameter that is being incrementally varied are zero.

7.4.2 Implementing User-Prescribed Insensitivity

User-prescribed zero sensitivity functionality is implemented by adding a string such as the following to line 8 of the PEST control file, somewhere following the value of the PHIREDSWH variable (interspersed, if necessary, with other variables which can also be recorded on this line).

```
zerosenval = -1.11e29
```

This string instructs PEST_HP to interpret a model output value of -1.11E29 as a directive that it must award a sensitivity of zero to all model outputs that have this value to the parameter that is being incrementally varied on the pertinent model run. A modeller can select this value him/herself. However its absolute value must be less than 1E30. At the same time, he/she must ensure that pertinent model outputs have this exact value. In the above string, the spaces before and after the "=" symbol are optional.

If user-prescribed zero sensitivity functionality is operative, the user must ensure that a value of ZEROSENVAL (-1.11E29 in the above example) is not recorded by the model except when it is run for the purpose of finite-difference derivatives calculation. If PEST_HP detects this value on the initial model run, on a model run undertaken for observation re-referencing purposes, or on a run undertaken for testing parameter upgrades, it will cease execution with an appropriate error message.

7.5 Sensitivity Reuse

As is described in PEST documentation, PEST's sensitivity re-use functionality can be activated by providing the string "senreuse" on the eighth line of the PEST control file. Optionally a "sensitivity reuse" section can also be provided in the PEST control file in order to assign values to control variables which govern the operation of PEST's sensitivity reuse functionality. If this section is not supplied, then PEST provides default values for these control variables itself.

Experience demonstrates that reusing the sensitivities of relatively insensitive parameters, rather than re-calculating them during every iteration of the inversion process, can sometimes realize spectacular savings in model runs. However at other times the gains in overall model run efficiency are not so great, especially if model outputs used in the calibration process are highly nonlinear with respect to some or all of the model's parameters; in cases such as these, the reduced cost per iteration achieved through sensitivity reuse may be outweighed by an increase in the number of iterations required to lower the objective function.

Where PEST_HP is deployed in a highly parallelized environment such as a computing cloud, then model run reductions should be achieved in packets that are equal to the number of available run agents at PEST_HP's disposal (this is normally equal to the number of deployed cores). Ideally, a modeller should choose the number of agents available to PEST_HP such that the number of model runs required for filling of the Jacobian matrix is an integral multiple of these agents. Uncontrolled reductions in the number of model runs required for filling the Jacobian matrix precipitated by application of PEST's sensitivity reuse functionality may result in some agents being idle for a while. It would be far better if these agents were calculating sensitivities, even if it transpires that some of these sensitivities exert little influence on ensuing parameter upgrade calculations.

During each iteration of the inversion process in which sensitivity reuse is possible, PEST_HP first identifies parameters which are candidates for sensitivity reuse in the same manner that PEST, Parallel PEST and BEOPEST identify these parameters, i.e. through their reduced composite sensitivities in comparison with other parameters. PEST_HP then counts the number of run agents that are currently at its disposal. If necessary, it then increases the number of parameters for which finite-difference calculation of derivatives will take place until the number of agents is an integral multiple of the number of model runs which will be carried out. In doing this, it accommodates the finite difference derivatives settings provided in the "parameter groups" section of the PEST control file, and whether or not the inversion process has reached the stage where higher order derivatives are being calculated instead of forward derivatives.

Suppose, for example, that 500 parameters are being estimated, and that PEST_HP is employing 50 agents. Suppose further that, during one particular iteration of the inversion process, sensitivity reuse functionality decrees 120 parameters to be insensitive enough to forgo finite-difference re-calculation of their derivatives during this iteration. If, at this stage of the inversion process, derivatives are being calculated using forward differences only, then PEST_HP will only reuse sensitivities for 100 parameters instead of 120 parameters in order to prevent 20 agents from being idle during part of the Jacobian matrix filling process. Of the 120 parameters for which it had previously decided that re-calculation of finite-difference derivatives should be foregone, it reinstates those which, according to previous iterations, are likely to be the most sensitive.

Note the following restrictions on the use of sensitivity reuse functionality (in all versions of PEST).

- A prematurely terminated PEST run cannot be restarted using the "/s" switch if sensitivity reuse functionality is engaged. This is because sensitivities pertaining to the previous iteration of the inversion process are not recorded in the run restart file, as this would make that file unduly long.
- If sensitivity reuse functionality is activated, a covariance matrix cannot be supplied for any observation group that is not comprised entirely of prior information. This is because use of an observation covariance matrix can cause "crossover" in composite parameter sensitivities, possibly introducing sensitivity to otherwise insensitive parameters. In contrast, if usage of covariance matrices is restricted entirely to prior information equations, this poses no problems for sensitivity reuse. Sensitivities of prior information equations to parameters do not require calculation through finite differencing.

7.6 Suspension of Observation Re-referencing

Suppose that a modeller is using PEST_HP's file distribution functionality for hastening execution speed of a steady state groundwater model or natural state geothermal reservoir model during calibration of this model. In this context, file distribution may be employed in conjunction with PEST_HP's observation re-referencing functionality. Thus, after distribution of an initial state file, a special model run may be undertaken prior to running the model many times for filling of the Jacobian matrix. This special model run will be undertaken for the purpose of providing a set of reference observations based on newly upgraded parameters and the newly distributed initial state file, before these parameters are sequentially subject to incremental variation for the purpose of finite-difference derivatives calculation.

File re-distribution for this purpose is required at the beginning of each iteration of the inversion process except the first. Ideally, carrying out of the complementary observation re-referencing run should therefore be prevented during the first iteration of the inversion process. This run will not do any harm. However it takes up computing resources for no good reason (especially if the short steady state run is accompanied by an ensuing transient run).

Observation re-referencing can be prevented during the first iteration of the inversion process by placing the string "orr_not_first" on the fifth line of the PEST control file following the "obsereref" string. "Orr_not_first" stands for "observation re-referencing – not in first iteration".

Note the following:

- If the "orr_not_first" string is supplied while the "obsreref" string is not supplied on the fifth line of the PEST control file, PEST_HP will cease execution with an appropriate error message.
- Because of the way in which it operates, observation re-referencing cannot be suspended during the first iteration of an inversion process in which more than one model command is employed for finite difference derivatives calculation with respect to different parameters. If an attempt is made to do this, PEST_HP will cease execution with an appropriate error message.

7.7 Alternative LSQR Settings

The roles of the LSQR_ATOL, LSQR_BTOL, LSQR_CONLIM and LSQR_ITNLIM variables are explained in PEST documentation. In general, the lower are the values ascribed to LSQR_ATOL and LSQR_BTOL,

and the higher are the values ascribed to LSQR_CONLIM and LSQR_ITNLIM, the longer will the LSQR solution process take. A more precise solution to the equations which PEST uses to solve the linearized inverse problem can often be found with tighter settings for these variables.

Where parameters number in the thousands and observations number in the tens of thousands, the LSQR solution process may take a few minutes. (Nevertheless it is far faster than singular value decomposition). Unfortunately, if PEST_HP is run in "regularisation" mode (as it should be when estimating many parameters), the linearised inverse problem may need to be solved many times during each iteration of the overall inversion process in order to estimate the optimal regularisation weight factor for use during that iteration. This can add considerably to the overall length of the inversion process. To make matters worse, parallel run agents are standing idle while repeated solution of the linearised inverse problem is taking place to refine the regularisation weight factor.

This process can be hastened by using looser convergence criteria for calculation of the best regularisation weight factor to use during each iteration of the inversion process; see PEST documentation of the WFFAC and WFTOL regularisation control settings. Alternatively, or as well, PEST_HP can be asked to use looser LSQR settings when undertaking linearized testing of a regularisation weight factor than when actually solving for a parameter upgrade.

Figure 7.1 shows the "lsqr" section of a PEST control file. Values for LSQR_ATOL, LSQR_BTOL, LSQR_CONLIM and LSQR_ITNLIM are supplied on the third line of this section.

```
* lsqr
 1
 1e-4 1000 10000
 0
```

Figure 7.1 The "lsqr" section of a PEST control file.

Figure 7.2 shows this same section of the PEST control file in which alternative values are provided for LSQR control variables for use in calculating the regularisation weight factor. These alternative values must follow the string "alt_regwt". The presence of this string on this line of the PEST control file notifies PEST_HP that alternative values for LSQR control variables follow. (Note that, to avoid confusion, PEST_HP will not allow any text other than "alt_regwt" to follow the values of the normal LSQR control variables on this line of the PEST control file.)

```
* lsqr
 1
 1e-4 1000 10000 alt_regwt 1e-4 100 1000 4
 0
```

Figure 7.2 The "lsqr" section of a PEST control file in which alternative LSQR control variables are provided.

The final entry on the third line of the PEST control file fragment shown above is the value of the variable LSQR_STOPITER. This (integer) number specifies a PEST inversion iteration number. Once this iteration of the inversion process has been reached, PEST_HP no longer uses the alternative LSQR control variables when undertaking linearized testing of iteration-specific regularisation weight factors. Set this to a negative value or zero if you wish that PEST_HP never uses the alternative LSQR control variables for this purpose; set it to a very high number if you wish that PEST_HP always uses these variables for linearized regularisation weight factor testing. (Note that when the REGCONTINUE regularisation control variable is set to "continue", it is good to revert to the use of

the tighter LSQR settings for linearized weight factor testing after a few iterations of the inversion process have elapsed.)

Another means through which the speed of the LSQR solution process can be considerably sped up is through use of the *pest_hp_mkl.exe* executable program in place of *pest_hp.exe*. See section 1.5 of this manual.

An alternative, much faster but approximate, means of calculating the regularisation weight factor is available through the REG2MEASRAT regularisation control variable. This is now discussed.

7.8 High-Speed Regularisation

As is discussed in the previous section, when PEST is run in "regularisation" mode, it calculates a regularisation weight factor during every iteration of the inversion process. It uses a linear approximation to the inverse problem to evaluate a factor that will allow the measurement objective function achieved through the current iteration to approximately equal a user-supplied target measurement objective function; the latter is supplied as the PHIMLIM regularisation control variable. Unfortunately, as has been discussed, calculation of the regularisation weight factor in this fashion can be a numerically intensive procedure, especially where parameter and/or observation numbers are high. Additionally, this calculation can be unreliable when a Jacobian matrix is approximate (as occurs when it is calculated using random or simultaneous parameter increments; see sections 9 and 10 of this document).

A variable named REG2MEASRAT can be added to the first line of the "regularisation" section of a PEST control file. Provision of a non-zero value for this variable instructs PEST_HP to forego the laborious calculation of the regularisation weight factor in the manner described above, and to replace it with a far simpler means of calculating this weight factor. The user-supplied value of REG2MEASRAT must follow the string "reg2measrat="; note that spaces can surround the "=" symbol if desired.

REG2MEASRAT must be greater than or equal to zero; it must also be less than 1.0. A value of zero disables REG2MEASRAT functionality so that the regularisation weight factor is calculated by PEST_HP in the usual manner. Provision of a non-zero value for REG2MEASRAT instructs PEST_HP to endow the regularisation weight factor employed for the current iteration with a value that ensures that the regularisation objective function is equal to REG2MEASRAT times the value of the measurement objective function at the beginning of the iteration.

Figure 7.3 shows the "regularisation" section of a PEST control file in which a non-zero value is provided for REG2MEASRAT. Omission of this variable from a PEST control file effectively endows it with a value of zero.

```
* regularisation
   0.1       0.105      .1    reg2measrat=0.1
 1.0   1.0e-10    1.0e10
 1.3   1.0e-2     1
```

Figure 7.3 "Regularisation" section of a PEST control file in which a value is supplied for the REG2MEASRAT control variable.

Use of the REG2MEASRAT control variable to govern calculation of the regularisation weight factor does not affect PEST_HP's termination criteria when it is run in "regularisation" mode. In particular,

PEST_HP will terminate execution if the measurement objective function falls below PHIMLIM (the target measurement objective function); hence the setting of PHIMLIM matters, even if it has no effect on the way in which the regularisation weight factor is calculated. Note also that "REGCONTINUE" is automatically set to "nocontinue", regardless of its user-supplied setting, if REG2MEASRAT is set to a value greater than zero.

There is an idiosyncrasy associated with use of a non-zero value for REG2MEASRAT which deserves attention. Often the regularisation objective function is zero during the first iteration of an inversion process. This is certainly the case if the ADDREG1 utility is used to add regularisation to a PEST control file. Under these circumstances the regularisation objective function cannot be adjusted to be a user-defined fraction (i.e. REG2MEASRAT) of the current measurement objective function. So PEST_HP does not adjust it at all. Hence, when building a PEST control file, a user should attempt to assign measurement and regularisation weights in a manner that reflects "measurement noise" on the one hand, and the innate variability of parameters on the other hand. If a covariance matrix derived from a variogram is employed instead of weights for regularisation-embodying prior information equations (as is easily achieved using the PPCOV* family of utilities supplied with the PEST Groundwater Data Utility suite), then regularisation weighting will be correct. Meanwhile, an appropriate level of "measurement noise" can be back-calculated from the level of model-to-measurement fit that the user hopes to attain through the regularised inversion process.

7.9 Switching to Higher Order Derivatives

If the FORCEN control variable assigned to any parameter group in the "parameter groups" section of a PEST control file is set to "switch", then PEST will switch from two point derivatives to higher order derivatives if, on any iteration of the inversion process, the objective function fails to improve by a relative amount of more than PHIREDSWH. However, the iteration at which the switch occurs can be postponed using the NOPTSWITCH variable. This prevents wastage of model runs where the objective function was not lowered as much as it otherwise would have been if the parameter upgrade vector had not been shortened through a parameter encountering its RELPARMAX, FACPARMAX or ABSPARMAX(N) change limit. (Note that a rise in the objective function will always precipitate the switch to higher order derivatives, regardless of the NOPTSWITCH setting.)

The NOPTSWITCH variable is optional. If you do not supply a value for this variable in the PEST control file, then PEST will switch to higher order derivatives calculation as early as at the end of the first iteration of the inversion process if the relative objective function reduction achieved during that iteration is less than PHIREDSWH. Unfortunately, this is not an uncommon occurrence. Furthermore, a limited fall in the objective function during the first iteration does not necessarily signify the need for more precise derivatives. More often than not, it reflects the fact that some parameters need to change a long way from their initial values in order to have an effect on the objective function, but that the length of the parameter upgrade vector was limited by RELPARMAX, FACPARMAX or ABSPARMAX(N).

PEST_HP has been programmed to recognize this situation. If the user does NOT supply a value for NOPTSWITCH (which is most often the case), then PEST will not switch to higher order derivatives at the end of the first or second iteration of the inversion process if any parameter encounters its RELPARMAX, FACPARMAX or ABSPARMAX(N) change limit during these iterations, as long as there was at least some improvement in the objective function. There are many occasions where

preventing the premature onset of higher order derivatives calculation in this fashion can provide efficiency benefits that extend beyond these initial iterations. It is often in the first and second iterations that parameters need to change the most, and are hence most likely to encounter parameter change limits. On subsequent iterations they may not need to change as much in order to support a considerable lowering of the objective function. PEST_HP may therefore not need to switch to higher order derivatives until much later in the inversion process.

Note however that if NOPTSWITCH receives a value in the PEST control file, this value will be respected by PEST_HP; it will not switch to higher order derivatives calculation until the end of the NOPTSWITCH-nominated iteration unless the objective function fails to fall at all during a particular iteration. Note also that if NOPTSWITCH is set to 1 or 2, then PEST_HP will not over-ride the onset of higher order derivatives calculation at the end of these iterations if the objective function fails to fall by more than PHIREDSWH during these iterations because of change-limiting of the parameter upgrade vector; it only suppresses the onset of higher order derivatives calculation following limited objective function improvement during these iterations if NOPTSWITCH is omitted from the PEST control file, or is set to a value of zero by the user.

7.10 Marquardt Lambdas for SVDMODE Equal to 2

7.10.1 Calculating Parameter Upgrades

When the SVDMODE variable in the PEST control file is set to 2, PEST undertakes singular value decomposition of $\mathbf{Q}^{1/2}\mathbf{J}$ where **J** is the Jacobian matrix and **Q** is the weight matrix. **Q** is often diagonal, with elements equal to the squares of user-supplied weights. However **J** can also include Tikhonov regularisation which may be accompanied by one or more covariance matrices. In that case **Q** includes the inverse of these matrices as well.

With SVDMODE set to 2, PEST computes parameter upgrades $\delta\mathbf{k}$ using the equation:

$$\delta\mathbf{k} = \mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1\mathbf{Z}^t\mathbf{Q}\mathbf{h} \qquad (7.1)$$

where **V** and **S** are obtained through singular value decomposition of $\mathbf{Q}^{1/2}\mathbf{J}$ as:

$$\mathbf{Q}^{1/2}\mathbf{J} = \mathbf{U}\mathbf{S}\mathbf{V}^t \qquad (7.2)$$

The "1" subscript on **V** and **S** in equation 7.1 signifies truncation at an appropriate singular value index. Normally the truncation point is chosen using the EIGTHRESH variable provided in the "singular value decomposition" section of the PEST control file. If so, truncation is such that the ratio of lowest to highest retained singular value squared is no smaller than EIGTHRESH. A suitable value for EIGTHRESH is about 5×10^{-7}. This is the value which prevents numerical noise incurred through finite difference calculation of elements of the Jacobian matrix from unduly contaminating estimated parameters.

7.10.2 Marquardt Lambda Values

Implementation of Marquardt lambda functionality is different when SVDMODE is set to 2 from its implementation for other inverse problem solution methods.

Let the current value of the Marquardt lambda be signified as λ. A number λ_a is added to all diagonal elements of $\mathbf{S}^{-2}$. λ_a is calculated from λ using the following formula:

$$\lambda_a = \lambda \times \mathbf{S}^{-2}_{(1,1)} \times \text{EIGTHRESH} \qquad (7.3)$$

In equation 7.3 $\mathbf{S}^{-2}_{(1,1)}$ is the first diagonal element of $\mathbf{S}^{-2}$. That is, it is the inverse squared of the first singular value. If the current value of λ is above 1.0, the addition of λ_a to all diagonal elements of $\mathbf{S}^{-2}$ ensures that the truncation point moves far to the right, perhaps so far to the right that there is no truncation at all (which can only happen if observations and prior information equations outnumber parameters). If λ is high enough, $\delta\mathbf{k}$ is effectively calculated using the method of steepest descent. On the other hand, as λ falls below 1.0, the truncation point is shifted dramatically to the left. If λ is low enough, the truncation point is determined solely by EIGTHRESH.

It should be noted that where Tikhonov regularisation is employed in solution of an ill-posed inverse problem, singular values do not fall to zero (if Tikhonov regularisation achieves the purpose for which it is intended). It should also be noted that, as the inversion process progresses, PEST_HP centres its selection of Marquardt lambdas on those which it believes from experience in calculating upgrade vectors so far, will be most effective in achieving maximum reduction of the objective function.

Limited experience to date suggests that this methodology for use of the Marquardt lambda when SVDMODE is set to 2 works well when using a randomized Jacobian matrix (see section 9), and when solving highly nonlinear, highly ill-posed inverse problems.

7.11 BOUNDSCALE and JACUPDATE

Versions of PEST other than PEST_HP disable Broyden Jacobian updating if the BOUNDSCALE variable is set to "boundscale" in the "control data" section of the PEST control file. As is described in PEST documentation, the scaling of parameters according to their respective bounds intervals serves a number of useful purposes. These include a higher likelihood of obtaining estimates of parameters which are of minimized error variance, and a higher likelihood of calculating those estimates with numerical stability.

The PEST_HP inversion algorithm has been amended such that incompatibilities between Broyden Jacobian updating and parameter bounds interval scaling have been removed. Note however that, as for other versions of PEST, parameter bounds interval scaling cannot be implemented unless singular value decomposition or LSQR is used as a solution device for the inverse problem (which is recommended practice).

7.12 The UPTESTMIN and UPTESTLIM Variables

See sections 2.2 and 2.3 of this document for a description of the role of the UPTESTMIN and UPTESTLIM variables in limiting the number of model runs employed for testing parameter upgrades.

7.13 Model Run Failure

When using PEST_HP in conjunction with a complex model, there can be occasions where the model fails to run properly when provided with a certain set of parameters. Despite gross errors in its calculations, the model may nevertheless write its expected output files; however the numbers which it records on these files may be nonsense.

If this occurs during testing of parameter upgrades, its occurrence is normally indicated by a very high objective function. This does not trouble PEST_HP. It simply ignores the run; hopefully a more

reasonable objective function can be achieved with an alternative set of parameters. However if this occurs during filling of the Jacobian matrix in response to incremental variation of a parameter, then the outcome will probably be an abnormally high set of sensitivities of model outcomes with respect to that parameter. This normally renders calculation of a useful parameter upgrade vector impossible, as the Jacobian matrix possesses one or a number of singular values which are very much higher than the others. PEST_HP then attempts to adjust the parameters that resulted in model run failure, while ignoring all other parameters. At best, this can lead to no improvement in the objective function; at worst it can promulgate a significant deterioration in the objective function. Experience has demonstrated that, under some circumstances, it can even result in failure of the algorithm that calculates parameter upgrade vectors (this is from the LAPACK family), whereby it gets lost in an infinite loop. Obviously, this situation must be avoided at all costs.

PEST_HP provides two variables that have been designed to detect and/or alleviate this situation. These variables are named JCOWARNTHRESH and JCOWARNZERO. Both of these should be set to a suitably high value; a value of at least 1E20 is suggested.

Suppose that JCOWARNTHRESH is set to 1E20. Then, immediately after filling the Jacobian matrix, PEST_HP warns the user (on its screen and on its run record file) if the absolute values of any Jacobian matrix elements are greater than 1E20. It will, in fact, count the number of elements whose values exceed this threshold and report this number.

Suppose that JCOZEROTHRESH is set to 1E20. Then not only will PEST_HP count the number of Jacobian matrix elements whose absolute values are greater than this threshold and report this to the screen and to its run record file; it will also alter the values of these elements to zero. Thus it may be possible for an unattended PEST_HP run to make progress, despite intermittent model run failure when filling the Jacobian matrix.

Values for JCOWARNTHRESH and JCOZEROTHRESH must be placed on the eighth line of the PEST control file. This is the line that begins with the value of the PHIREDSWH control variable. Figure 7.4 shows an example.

```
* control data
restart estimation
     104      14      13       0       6
     1     2 single  point  2   0   0
 10.0  -3.0  0.3  0.03  10 999  uptestmin=15
 10.0  10.0  0.001
 0.1  noaui jcowarnthresh=1.0E10 jcozerothresh=1.0E30
 30  0.005  4  4  0.005  4
 1  1  1
```

Figure 7.4 "Control data" section of a PEST control file in which values are supplied for the JCOWARNTHRESH and JCOZEROTHRESH control variables.

Note the following usage details:

- PEST_HP will allow values to be supplied for one or both of JCOWARNTHRESH and JCOZEROTHRESH.
- Values supplied for each of these variables must be zero or greater. A value of zero disables the variable.

- The default value for JCOZEROTHRESH is 0.0. The default value for JCOWARNTHRESH is 1e30.
- If positive values are supplied for both JCOWARNTHRESH and JCOZEROTHRESH, PEST_HP insists that the value supplied for JCOZEROTHRESH exceed that supplied for JCOWARNTHRESH.
- PEST_HP does not check prior information sensitivities against the JCOWARNTHRESH and JCOZEROTHRESH thresholds, as these are supplied directly by the user.

8. Stopping and Re-Starting PEST_HP

8.1 Resumption of Execution

Execution of the PEST_HP manager can be terminated abruptly by typing <Ctl-C> in the run manager window. Inadvertent termination of PEST_HP execution can follow power or network failure. Alternatively, its execution can be prematurely terminated in a more gentle manner using the PSTOP or PSTOPST commands; see below.

If execution of PEST_HP is prematurely terminated in any of these ways, it can be restarted using the "/s" switch. If its execution was terminated while undertaking model runs required for filling of the Jacobian matrix (normally the most time-consuming part of the inversion process), PEST_HP will re-commence execution at exactly the same location in its processing sequence as that at which its execution was previously terminated. It will read the outcomes of model runs previously undertaken for filling of the Jacobian matrix from its restart file; it will then complete the filling of this matrix by instructing its agents to undertake the remaining model runs.

If execution of PEST_HP is terminated while model runs are being undertaken for the purpose of testing parameter upgrades, PEST_HP will re-commence execution at that point of its processing sequence where upgrade calculation commenced. Normally, this does not constitute a degradation of efficiency because (as is described in section 2 of this document) PEST_HP often undertakes only one set of parallel runs during that phase of the inversion process in which upgraded parameter sets are calculated and tested. If PEST_HP execution is inadvertently terminated while these runs are being undertaken, they would need to be re-initiated anyway. Nevertheless, if model run times are significantly different for different parameter sets, there will be some wastage of model runs if PEST_HP execution was terminated after some model runs had been completed but before others had been completed. However this potential for run loss must be balanced against the fact that a restarted PEST_HP may not have the same number of agents at its disposal as the previously terminated PEST_HP. The Marquardt lambda selection strategy may therefore be different between the old and new PEST_HP runs.

If Broyden Jacobian updating is activated, then restart functionality presently implemented by PEST_HP will indeed result in the need to repeat the set of model runs based on the unimproved Jacobian matrix if cessation of execution occurred while model runs were being undertaken based on parameter upgrades calculated using the Broyden-improved Jacobian matrix.

If execution of PEST_HP was inadvertently terminated after commencement of execution using the "/f" command line switch, then its execution can be resumed using the "/s" switch, just as for a PEST_HP run that was undertaken for the purpose of solving an inverse problem. In this case execution of the re-started run should also be initiated using the "/f" switch. For example, if the PEST_HP manager was originally started using the command:

```
pest_hp case /f /h :4004
```

then an interrupted run should be restarted using the command:

```
pest_hp case /f /s /h :4004
```

If restarted in this manner, PEST_HP does not prompt for the names of the parameter value files which it must read, nor for the size of a parallel run packet, as it did on its original run. Instead, it obtains this information from its restart file; it then recommences its run at that point in its processing sequence at which its execution was previously terminated. Information calculated during the resumed run is appended to the original run record and run results files (as if execution of PEST_HP had never been interrupted in the first place).

8.2 Stopping and Pausing

In common with normal PEST and BEOPEST behaviour, the typing of "pstop" or "pstopst" in another command line window open to the PEST_HP manager's folder instigates cessation of PEST_HP execution; run agents cease execution when the model runs which they are respectively supervising are complete. If stopped using the "pstop" command, cessation of execution of the PEST_HP manager is immediate. If stopped using the "pstopst" command, the manager records information pertinent to the current inversion process at the end of the run record file before ceasing execution. In either case, execution of the prematurely terminated PEST_HP run can be resumed using the "/s" command line switch as discussed above.

As for the normal PEST and BEOPEST, execution of PEST_HP can be paused and resumed using the "pause" and "unpause" commands. As for the "pstop" and "pstopst" commands, these commands must be issued from a command line window which is open to the PEST_HP manager's folder.

8.3 Special Considerations for the "/f" Switch

If PEST_HP is run using the "/f" switch, so that it records the outcomes of a sequence of model runs in a run results file, then its execution can be terminated using either the "pstop" or "pstopst" commands in the manner described above. However the PEST_HP manager responds slightly differently to each of these two commands. If stopped using the "pstop" command, cessation of the PEST_HP manager's execution is immediate. However if stopped using the "pstopst" command, the manager empties the parallel run register before ceasing execution. Thus model output values corresponding to model runs comprising the latest run packet which have already been completed are recorded in the run results file; meanwhile, corresponding objective functions are recorded in the run record file and written to the screen.

If stopped using the "pstop" or "pstopst" commands, PEST_HP execution can be resumed using the "/s" switch, together with the "/f" switch in the manner described above. However if execution of PEST_HP was terminated using the "pstopst" command, some information will be duplicated in both the run record and run results files upon resumption of PEST_HP execution, namely the outcomes of model runs comprising part of an interrupted run package which were actually completed prior to termination of the previous PEST_HP run. As stated above, these model run outcomes are recorded in these PEST_HP output files in accordance with its programmed response to the "pstopst" command.

9. Randomized Jacobian

9.1 Introduction

This section describes functionality included in PEST_HP that, at the time of writing, is somewhat experimental in nature and is still under development. It's use may allow progress to be made in difficult parameter estimation settings where parameter numbers are large and the dimensionality of the calibration solution space is small. This progress comes at a price, however, as use of the methodology described herein is not designed to achieve a minimum error variance solution to the inverse problem of model calibration. Instead, because parameter upgrade directions are not necessarily confined to the calibration solution space, null space parameter components are introduced to parameters as they are upgraded. This is not desirable when parameter adjustment is being undertaken in pursuit of the so-called "calibrated parameter field". However the methodology may present opportunities for efficient adjustment of random parameter fields in order to satisfy calibration constraints. In this latter case, the introduction of null space components to parameter fields is not only tolerable, but is in fact desirable.

9.2 Overview

In its normal operation, PEST_HP approximates differentials comprising a Jacobian matrix using finite parameter differences. Under these circumstances, filling of the Jacobian matrix requires at least as many model runs as there are adjustable parameters. Where an inverse problem is ill-posed, the Jacobian matrix can then be processed using a subspace method such as singular value decomposition (SVD). SVD reduces parameter space dimensionality by selecting combinations of parameters for estimation in place of individual parameters. In doing this, it formulates a full-rank Jacobian matrix from the original Jacobian matrix that complements the new solution subspace. The original Jacobian matrix is column rank-deficient, this being a consequence of the fact that it has a null space.

Methods such as randomized SVD have received a considerable amount of attention in the recent numerical methods literature; see, for example, Halko et al (2011) for a review. Use of randomized methods is based on the premise that a Jacobian matrix that is employed in solution of an ill-posed inverse problem need only have a rank that is as large as that of the matrix which SVD will ultimately derive to estimate values for a limited number of estimable parameter combinations. The rank of this matrix is equal to the number of parameter combinations which are thus estimated (i.e. to the dimensionality of the parameter solution space). Construction of a matrix which is rank-sufficient in terms of the dimensionality of the calibration solution space, but rank deficient in terms of the number of adjustable parameters featured in the inverse problem, can be achieved if random combinations of parameters are employed to determine the range space of the matrix. The dimensionality of its range space is equal the number of parameter combinations which can be estimated, and hence to the dimensionality of the solution space. The number of sampled parameter sets required to define this space need only be slightly greater than the dimensionality of the solution space.

Enhancements to PEST_HP described in this appendix provide functionality which is similar in some respects to randomized SVD methods, while recognizing that filling of the Jacobian matrix is necessarily undertaken using individual model runs based on individual parameter sets; with

PEST_HP these runs are parallelized. Once a rank-deficient approximation to the Jacobian matrix has been calculated using these parameter sets, solution of the inverse problem can then be undertaken using any of the methods normally employed by PEST_HP. Where a problem is ill-posed, methods of choice will normally be singular value decomposition or LSQR, with Tikhonov regularisation recommended to assist in achieving a solution to the inverse problem whose error variance is minimized according to a modeller's chosen criterion.

The algorithm employed by PEST_HP for randomized filling of the Jacobian matrix is now described.

9.3 Filling the Jacobian Matrix: Theory

If a model is linear, its action can be represented by a matrix. Let this matrix be designated as **Z** when the model is run under calibration conditions. Model outputs that correspond to members of the calibration dataset are represented by the vector **o**. Let the vector **k** represent model parameters. Then:

$$\mathbf{o} = \mathbf{Z}\mathbf{k} \tag{9.1}$$

Suppose that elements of **k** are randomly generated based on a covariance matrix D(**k**) (which we distinguish from C(**k**) which is often used in PEST and related documentation to denote the prior parameter covariance matrix). Then the joint covariance matrix of **o** and **k** can be computed as:

$$\mathrm{C}\left(\begin{bmatrix}\mathbf{o}\\ \mathbf{k}\end{bmatrix}\right) = \begin{bmatrix}\mathbf{Z}\\ \mathbf{I}\end{bmatrix}\mathrm{D}(\mathbf{k})\begin{bmatrix}\mathbf{Z}^{\mathrm{t}} & \mathbf{I}\end{bmatrix} \tag{9.2}$$

On carrying out the matrix products implied in equation 9.2, and extracting the pertinent submatrix from the resulting full matrix, we find:

$$\mathrm{C}(\mathbf{o},\mathbf{k}) = \mathbf{Z}\mathbf{D}(\mathbf{k}) \tag{9.3}$$

where C(**o**,**k**) expresses covariances between the elements of **o** and those of **k**. From (9.3):

$$\mathbf{Z} = \mathrm{C}(\mathbf{o},\mathbf{k})\mathrm{D}^{-1}(\mathbf{k}) \tag{9.4}$$

For a nonlinear model, **Z** is replaced by the Jacobian matrix **J**, this constituting a local linearization of the action of the model at the set of parameters achieved at a certain stage of the inversion process; we denote this set as $\underline{\mathbf{k}}$.

An empirical estimate of C(**o**,**k**) can be obtained by running the model using different random realizations of **k** centred on $\underline{\mathbf{k}}$. The covariance between the *i*'th element of **o**, o_i, and the *j*'th element of **k**, k_i, is then calculated as:

$$C(\mathbf{o},\mathbf{k})_{i,j} = \frac{\sum (o_i - \underline{o}_i)(k_j - \underline{k}_j)}{N} \tag{9.5}$$

where the summation is undertaken across all random parameter sets. Note that *N* rather than (*N*-1) is employed in the denominator of equation 9.5 as $\underline{o}_i$ and $\underline{k}_j$ are known. As stated above, the latter is the optimised value of k_j from the previous iteration of the inversion process (i.e. its current

reference value); meanwhile the former is the *i*'th element of **o**, the vector of reference model outputs calculated using current reference parameters **k**.

As implemented in PEST_HP, D(**k**) is a diagonal matrix. Each element of the diagonal is the variance (square of standard deviation) of the respective, locally randomized, parameter. Hence, in calculation of the covariance matrix featured in equation 9.3, individual parameters comprising elements of the vector **k** are considered to be statistically independent of each other. Furthermore, it is anticipated that parameter standard deviations will be small. (However larger standard deviations can be chosen if desired.) These will normally be of similar magnitude to the increments that would otherwise be used for calculation of a Jacobian matrix using finite parameter differences. The use of small standard deviations serves two purposes:

1. Elements of the matrix **Z** (the local Jacobian matrix) calculated using equation 9.4 are a better approximation to true derivatives than if parameter randomization was based on a larger standard deviation; this accelerates solution convergence of the inverse problem.
2. For some models (for example geothermal reservoir models run under natural state conditions, and groundwater models run under steady state conditions), execution speed can be dramatically increased if initial conditions supplied to the simulator's solver approximate the actual simulated condition. PEST_HP can provide these initial conditions from previously-calculated solution conditions, and update them during every iteration of the inversion process, using its file distribution functionality. However solution conditions determined during a previous iteration of the inversion process can only serve as useful initial conditions for the next iteration of that process if random parameter variations from their current reference values are restricted in size.

The methodology described above for calculating an approximation to **Z** is not unlike that described by Chen and Oliver (2013) to support their Jacobian-enhanced, ensemble Kalman smoother scheme. However in their case parameter randomization plays two roles. Firstly, it is employed to create parameter fields which constitute an evolving ensemble which is used to quantify parameter and predictive uncertainty. Secondly, the outcomes of model runs conducted using these parameter fields are employed in equations that are not unlike those discussed above to compute an approximation to the Jacobian matrix on which modification of these parameter fields is based. An important difference between the Chen and Oliver randomization scheme and that described in the present document is that parameter variances employed in the present scheme are much smaller than those used by Chen and Oliver. Furthermore, in the present case, random parameter sets are generated for use in model runs that are dedicated solely to construction of an approximate Jacobian matrix. The latter is then used to adjust a single parameter field to better satisfy calibration constraints.

As has already been mentioned, the method also bears some resemblance to randomized algorithms which are used for singular value decomposition of large matrices. A major difference between these methods and that described herein is that randomization is used to build an approximation to the Jacobian matrix herein, rather than to decompose it. However if the model to which PEST_HP is linked possesses an adjoint solver, so that "backward" model runs can be undertaken to directly compute matrix multiplications involving $\mathbf{Z}^t$, the distinction between these two roles can fade. Algorithms described by Halko et al (2011) and Tropp et al (2016) could then be employed for rapid calculation of upgrade vectors without the subspace misalignment problems that afflict the present methodology.

9.4 Filling the Jacobian Matrix: Practice

PEST_HP employs a normal probability distribution to generate random parameter values. The mean value of each parameter is its current reference value (i.e. the best parameter value inherited from the parameter upgrade process conducted during the previous iteration). Standard deviations employed in generating random values for parameters are discussed below.

In implementing the above theory, the modeller is faced with the choice of how many random parameter sets *N* to use in building a diminished rank approximation to the Jacobian matrix. There are two factors at play here. The larger is *N*, the better will the empirical covariance matrix computed using equation 9.5 approximate the true covariance matrix. On the other hand, the whole purpose behind construction of a randomized Jacobian matrix is to reduce the numerical burden of parameter estimation. Therefore, *N* should ideally be significantly smaller than the number of adjustable parameters. In practice, *N* must be at least as large as the dimensionality of the calibration solution space; theoretically, it should be slightly larger than this, as a small amount of parameter redundancy provides a better guarantee that the range space of **Z** is properly represented by model outcomes calculated using these parameters.

It is up to the modeller to choose a value for *N* that reconciles these two conflicting demands. The problem of choosing *N* is exacerbated by the fact that the dimensionality of the solution space may not be known in advance. PEST_HP accommodates uncertainty in choosing a suitable value for *N* by allowing it to increase, on an as-needed basis, as the inversion process progresses. See below.

As discussed above, ideally, standard deviations employed in generation of random parameter values should be small. However if they are too small, then round-off errors can diminish the integrity of covariances calculated using equation 9.5. Numerical errors in C(**o**,**k**) can be exacerbated by model solver convergence difficulties; the resulting "model output noise" can impair the numerical integrity of small differences of large quantities. PEST_HP calculates the standard deviation for each parameter as the increment that the parameter would have if two-point (rather than three or five point) finite-difference derivatives were employed to fill the Jacobian matrix. The PEST control variables which determine these increments pertain to parameter groups, and are thus recorded in the "parameter groups" section of the PEST control file. These are the DERINC, DERINCLB, and INCTYP variables. However PEST_HP allows parameter standard deviations calculated in this way to be multiplied by a user-specified factor that is applied to all parameter groups. Hence they can be made as large or as small as a user desires. Alternatively, values for DERINC, DERINCLB and INCTYP can be chosen specifically to achieve desired standard deviations.

When calculating random values for parameters, PEST_HP ensures that these values do not transgress parameter bounds. If, at a particular stage of the inversion process, the current reference value for a parameter is at its upper or lower bound, the sign of the random-to-reference parameter difference is reversed if necessary to ensure that its random value moves away from this bound rather than crossing it. On the other hand, if a parameter is not at its bound, but the random value of a parameter lies above the parameter's upper bound or below the parameter's lower bound, then the random value ascribed to the parameter is adjusted to coincide with the bound.

On some iterations of a PEST_HP inversion process based on randomized Jacobian matrices, a set of upgraded parameter values may be computed which do not, in fact, lower the objective function. In this case PEST_HP can reject the upgrade and use the next iteration of the inversion process to

refine the C(**o**,**k**) covariance matrix calculated during the preceding iteration. Thus the number of parameters *N* used in equation 9.5 is doubled, or trebled, or even quadrupled, this depending on the number of successive iterations that are dedicated to the task of improving this matrix. At the same time, failure to achieve an improved parameter set on a particular iteration can trigger an increase in the value of *N* employed in successive iterations of the inversion process.

Optionally, the covariance matrix calculated during a given iteration of the inversion process can incorporate part of the covariance matrix calculated during the previous iteration. This may help reduce errors in this matrix incurred by use of a small number of random parameter samples in its calculation. It can also help reduce calibration-induced parameter and predictive bias; see below. However there is penalty to be paid for doing this. For a highly nonlinear model, and/or for an inverse problem that is profoundly ill-posed, this strategy may compromise PEST_HP's ability to calculate up-to-date Jacobian matrices which support continuous objective function improvements in difficult objective function terrains.

As for normal operation of PEST_HP, a modeller can implement Broyden updating of the Jacobian matrix based on model outputs determined during a single round of parameter upgrade testing. Theoretically, deficiencies in this matrix can thereby be partially rectified. A second round of parameter upgrade testing is then undertaken using the improved Jacobian matrix.

PEST_HP allows a modeller to commence the inversion process using randomized Jacobian calculation, and then finish it using standard finite-difference derivatives to fill the Jacobian matrix. If *N* is small (presumably chosen as such because the null space of **Z** is large), the number of runs required per iteration increases dramatically when the switch is made to finite-differences because a model run must then be undertaken for every adjustable parameter. (More model runs than this need to be undertaken if higher-order finite differences are employed for filling of the Jacobian matrix). On the other hand, a more accurate Jacobian matrix may hasten progress of the inversion process.

The PEST_HP control variables which govern random and Jacobian calculation are now discussed.

9.5 Control Variables

9.5.1 Reading the Control Variables

Variables which control the action of PEST_HP's randomized Jacobian functionality are read from a section of the PEST control file that is dedicated to holding these variables. This section is named the "randomized jacobian" section. This section must have six lines, the first being a header line. The variables comprising the remaining five lines are listed in figure 9.1. An example is provided in figure 9.2.

```
* randomized jacobian
RANDOMJAC  RANDOMSEED
NRANDSETSTART NRANDSETINC NRANDSETFIN
RANDINCFAC  NRANDREPEAT EMPIRICSTD
RANDJACRETAIN
SWITCH_TO_FD PHIREDFD NOPTSWITCHFD  REPEATTOL
```

Figure 9.1 Variables appearing in the "randomized jacobian" section of a PEST control file.

```
* randomized jacobian
1     222                 #RANDOMJAC  RANDOMSEED
18    12     30           #NRANDSETSTART NRANDSETINC NRANDSETFIN
10.0     4    1           #RANDINCFAC  NRANDREPEAT EMPIRICSTD
0.5                       #RANDJACRETAIN
1   0.1    4   5          #SWITCH_TO_FD PHIREDFD NOPTSWITCHFD  REPEATTOL
```

Figure 9.2 An example of the "randomized jacobian" section of a PEST control file.

The "randomized Jacobian" section must be placed between the "control data" and "parameter groups" sections of a PEST control file. Other sections (such as "singular value decomposition", "simultaneous parameter increments" and "sensitivity reuse") can also appear between the "control data" and "parameter groups" sections of a PEST control file. There is no prescribed ordering for these sections if more than one of them is present.

The roles of these variables are now discussed in detail.

9.5.2 RANDOMJAC

This variable (an integer) must be set to either 0 or 1. If it is set to 0, then randomized Jacobian calculation is disabled; hence derivatives are calculated using finite differences in the normal PEST_HP manner. Alternatively, if RANDOMJAC is set to 1, then randomized Jacobian calculation is enabled.

9.5.3 RANDOMSEED

RANDOMSEED is the seed for the random number generator. Select any integer greater than zero.

9.5.4 NRANDOMSTART, NRANDOMINC, NRANDOMFIN

All of these variables are integers. They all pertain to the variable *N* featured in equation 9.5.

NRANDOMSTART is the initial value of *N*.

If, during a particular iteration of the inversion process, the value of the objective function is at or above the lowest value that has been achieved so far during the inversion process (with current inversion circumstances dictating whether this pertains to the measurement or regularisation objective function if PEST_HP is running in "regularisation" mode), then *N* is increased by NRANDOMINC ("INC" stands for "increment"). However *N* will never be allowed to increase above NRANDOMFIN ("FIN" stands for "finish").

Some of the matters which need to be considered when selecting values for these variables are discussed in the previous subsection. In addition to the theoretical and numerical considerations discussed therein, a further practical matter requires consideration. PEST_HP employs a suite of agent nodes to carry out model runs. Sometimes these nodes will have been purchased from a cloud provider. In most inversion circumstances, under-utilization of agent nodes serves no purpose. Hence, at any stage of the inversion process, the value of *N* should be an integral multiple of the number of available agents.

9.5.5 RANDINCFAC

In generating random numbers for filling of the C(**o**,**k**) covariance matrix, PEST_HP decrees all adjustable parameters to be statistically independent. The mean value of each parameter is its reference value at that particular stage of the inversion process. The standard deviation ascribed to each parameter is equal to the increment that it would have been assigned if derivatives were computed using two-point finite parameter differences. As stated above, these increments are

controlled by the DERINC, DERINCLB and INCTYPE control variables that are assigned to parameter groups.

Standard deviations calculated for all parameters using the DERINC, DERINCLB and INCTYPE control variables can be multiplied by RANDINFAC. RANDINFAC is a real number whose value must be greater than zero.

9.5.6 NRANDREPEAT

If, in a particular iteration of the inversion process, parameter values do not improve (i.e. the objective function does not fall if running in "estimation" mode, or the measurement/regularisation objective function does not fall if running in "regularisation" mode), then PEST_HP can be instructed to retain existing parameter values for the next iteration of the inversion process while continuing to build the covariance matrix which was the focus of its previous iteration. With an increased number of parameter samples, the quality of the covariance matrix should improve, so that a better approximation to the Jacobian matrix can then be obtained through equation 9.4. The integer variable NRANDREPEAT dictates how many such repetitions are allowed. Set it to a value such as 999 to place no limit on the number of repetitions; based on experience gained at the time of writing, this is recommended practice.

Let us suppose that NRANDREPEAT is set to 4, and that on iteration 5 of the inversion process the objective function does not improve. Then PEST will continue to improve the covariance matrix over iterations 6, 7, 8 and 9 unless, on any of these iterations, the objective function improves, in which case it accepts the updated parameter set and moves on to the next iteration. Meanwhile, the number of random parameter sets employed per iteration may increase in accordance with NRANDSETINC and NRANDSETFIN settings. Alternatively, if the objective function has not improved by the end of iteration 9, then PEST_HP accepts the updated parameter set calculated during this iteration and moves to iteration 10 with this updated parameter set as the new reference parameter set; it does this in spite of the fact that the objective function suffers an increase. It is important to note, however, that parameters will not be temporarily frozen in this manner again unless the objective function reaches a new low (i.e. lower than at the start of iteration 5 in this example). Hence the objective function may "bounce around" during subsequent iterations unless a new objective function minimum is found if lack of accuracy of the C(**o**,**k**) covariance matrix is responsible for lack of progress of the inversion process. (This action could be prevented if PEST_HP was programmed to re-freeze parameters at an elevated objective function value if this value cannot be improved during a particular iteration. However PEST_HP makes no attempt to be a "global optimiser"; erratic behaviour of the objective function should be taken as an indication that settings which govern behaviour of the randomized Jacobian process need to be altered, or that use of a randomized Jacobian matrix has taken the inversion process as far as it can go.)

When setting a value for NRANDREPEAT, values of PEST-HP control variables which govern termination of the inversion process should be borne in mind. This is further discussed below.

9.5.7 EMPIRICSTD

EMPIRICSTD stands for "empirical standard deviation". This is an integer variable whose value should be 0 or 1.

The diagonal elements of the D(**k**) covariance matrix appearing in equations 9.3 and 9.4 are the squares of standard deviations of respective parameters. The diagonal elements of D^{-1}(**k**) appearing in equation 9.3 are the reciprocals of the squares of these standard deviations.

As has already been discussed, parameter standard deviations employed by PEST_HP are increments that would otherwise be used in finite-difference derivatives calculation (multiplied by RANDINCFAC). The reciprocals of these standard deviations can be used directly in equation 9.4. Alternatively, standard deviations used in this equation can be calculated empirically from the random values that were actually generated for respective parameters. The empirical standard deviation σ_i of parameter k_i is calculated as:

$$\sigma_i = \sqrt{\frac{\sum \left(k_i - \underline{k}_i\right)^2}{N}} \qquad (9.6)$$

As for equation 9.5, *N* rather than *N*-1 appears in the dominator of equation 9.6 because the value of $\underline{k}_i$ is its current reference value.

Sometimes, if *N* is small, the empirical value of a parameter's standard deviation calculated using equation 9.6 can differ significantly from its theoretical value. This also occurs if a parameter is near its upper or lower bound; as was discussed above, random values generated for bound-limited parameters are altered by PEST_HP to respect these bounds.

Set EMPIRICSTD to 0 to use theoretical, increment-derived parameter standard deviations in equation 9.4; set it to 1 to employ equation 9.6 for calculation of parameter standard deviations.

9.5.8 RANDJACRETAIN

This real variable should be set to a value between 0.0 and 1.0. It governs how much of the covariance matrix calculated during the previous iteration of the inversion process is retained in calculating the covariance matrix for the current iteration. Note, however, that if NRANDREPEAT is set to 1 or greater, and the objective function did not fall during the previous iteration, then (as was discussed above) the entirety of the previous covariance matrix is retained in calculating the covariance matrix for the current iteration. However if the objective function did, in fact, fall during the previous iteration, or if it rose during the previous iteration and the NRANDREPEAT count was exceeded, then the setting of RANDJACRETAIN can inform PEST to retain part of that matrix.

Suppose that RANDJACRETAIN is set to 0.25. Then the total covariance matrix for a particular iteration of the inversion process is calculated as the weighted average of that computed for that iteration using equation 9.5 and that computed during the previous iteration. Weights used in this averaging process are 1.0 and 0.25 respectively.

Set RANDJACRETAIN to 0.0 to suppress carryover of the covariance matrix between iterations.

9.5.9 SWITCH_TO_FD, PHIREDFD, NOPTSWITCHFD and REPEATTOL

If, during a particular iteration of an inversion process based on randomized Jacobian matrices, the objective function does not fall by a relative amount of PHIREDFD, then PEST_HP can switch to finite difference calculation of the Jacobian matrix. This occurs if the integer variable SWITCH_FD is set to 1; a setting of 0 prevents this occurrence.

Suppose that PHIREDFD is set to 0.1 and that SWITCH_FD is set to 1. Then if the objective function does not fall by a factor of 0.1 of its current value, the switch will occur. If PEST is running in "regularisation" mode, then PHIREDFD is applied to either the measurement or regularisation objective function depending on the current value of the measurement objective function in relation to the value of the target measurement objective function PHIMLIM. Obviously, PHIREDFD is a real variable. Its value should be set to somewhere between 0.0 and 1.0, preferably closer to the former than the latter.

The integer variable NOPTSWITCHFD protects PEST_HP from prematurely switching to costly finite-difference derivatives calculation. The switch to finite-difference derivatives calculation will not occur before the iteration specified as the value of this integer variable.

If, on a particular iteration, the objective function does not fall at all, then this will trigger a switch to finite-difference derivatives calculation if SWITCH_FD is set to 1. However if the switch is made immediately, PEST_HP does not have a chance to improve the objective function in its next iteration through covariance matrix enhancement in accordance with the user-supplied setting of NRANDREPEAT. PEST_HP does not make the switch to finite-difference derivatives calculation until REPEATTOL iterations of covariance matrix enhancement have elapsed. REPEATTOL is an integer variable that should be set to 0 or greater; however it must not be greater than NRANDREPEAT. (REPEATTOL stands for "repeat tolerance").

If SWITCH_TO_FD is set to 1, then PEST prints the words "random Jacobian" or "finite-difference Jacobian" to the screen, and to its run record file, at the start of each new iteration of the inversion process on the same line as it prints the words "OPTIMISATION ITERATION NO. *N*". A user is thus immediately aware of which of these methodologies is being employed to fill the Jacobian matrix at any time.

9.6 Accommodating Other PEST_HP Functionality

9.6.1 Incompatibilities

Randomized Jacobian functionality cannot be employed under any of the following circumstances.

- PEST_HP is undertaking SVD-assisted parameter estimation, or is run in "pareto" mode;
- The PEST_HP control file instructs PEST_HP to employ different commands for running the model when calculating finite-difference derivatives with respect to different parameters;
- Split slope analysis is used for accommodation of poor numerical derivatives;
- Sensitivity re-use functionality has been enabled;
- Parameter bounds sticking functionality has been enabled.

If you attempt to violate the first two of the above conditions, PEST_HP will cease execution with an error message. In the other three cases, PEST_HP disables the offending functionality itself.

As yet, PEST_HP's restart capabilities have not been upgraded to include random Jacobian calculation.

The PEST Whisperer (PWHISP_HP) is not yet programmed to read or understand the contents of a PEST control file recorded by PEST_HP when employing randomized filling of the Jacobian matrix.

Nor can the PCOST_HP cost calculator estimate the number of model runs required for parameter adjustment based on a randomized Jacobian.

9.6.2 Adjustments to Other Functionality

9.6.2.1 Observation Re-Referencing

If the NRANDREPEAT control variable is set to a positive number then, as is discussed above, if parameter values are not improved during a particular iteration, they are retained for use in the subsequent iteration. Under these circumstances observation re-referencing functionality is disabled for the subsequent iteration, as re-use of the same parameter values implies re-use of the same observation reference values.

9.6.2.2 File Distribution

If file distribution functionality is enabled, the same applied to this. That is, no file distribution takes place at the start of a new iteration if parameters from the previous iteration are being re-used. As is usual PEST_HP practice, user-nominated files are copied from the best-performing agent's directory to the run manager's directory on termination of execution; however this is only done if parameters were improved during the final iteration of the inversion process.

9.6.2.3 DERFORGIVE

If, during the Jacobian-filling phase of an inversion iteration, the model fails to run to completion while employing a random set of parameters, PEST_HP does not cease execution. In accommodating model run failure in this way, its behaviour is thus similar to finite-difference filling of the Jacobian matrix with a DERFORIGVE setting of "derforgive"; in fact, PEST_HP internally sets DERFORGIVE in this manner. Because the model produces no useable outputs under these circumstances, the covariance matrix of equation 9.5 is not updated in the way that it would be updated if the model run was a success. This lowers the accuracy of this matrix; at the same time, it may reduce the subspace of parameter space in which parameter upgrade vectors lie.

If, on any iteration of the inversion process, all Jacobian-filling model runs fail, PEST_HP ceases execution with an appropriate error message.

9.7 Experience to Date

9.7.1 Solution Method

PEST_HP offers the following methods for calculation of upgraded parameters (see PEST documentation for details):

- Gaussian elimination;
- Singular value decomposition with SVDMODE set to 1;
- Singular value decomposition with SVDMODE set to 2;
- LSQR.

Any of these methods can be used in conjunction with a randomized Jacobian matrix; the means through which the Jacobian is calculated, and use of that Jacobian in calculating parameter upgrades, are independent of each other. However some solution methods appear to be more forgiving of an approximated Jacobian matrix calculated using a small number of random parameter values than other methods.

Experience to date suggests that singular value decomposition with an SVDMODE setting of 2 works best with a randomized Jacobian matrix. However if parameter numbers are very high, the numerical cost of singular value decomposition may be too high to countenance. In this case, there is no choice but to employ LSQR. However, to ease its computational burden, the number of iterations that it employs for solution of the inverse problem (LSQR_ITNLIM) should be set to a number that is commensurate with NRANDSETFIN.

9.7.2 Tikhonov Regularisation

Tikhonov regularisation provides the means through which expert knowledge can contribute to the inversion process. Such expression can promulgate a solution to the inverse problem which approaches that of minimum error variance.

As is extensively described in PEST documentation, in its implementation of Tikhonov regularisation PEST calculates a factor for regularisation weights which attempts to ensure that the measurement objective function attains, but does not undercut, a user-specified target measurement objective function. This weight factor is re-computed during every iteration. Local linearization of the model (i.e. the Jacobian matrix) is required for its calculation. Where the Jacobian matrix is only approximate, the weight factor can only be approximate. Furthermore, its value may undergo significant changes from iteration to iteration in accordance with random variation of the Jacobian matrix.

Experience to date suggests that PEST_HP performs satisfactorily when using a randomized Jacobian matrix if an inverse problem includes Tikhonov regularisation. However while PEST_HP may be able to achieve an appropriately-set measurement objective function target, it may not be able to lower the regularisation objective function to as low a value as it could if a finite-difference Jacobian were employed.

Experience has also shown that this problem can be ameliorated to some extent if the PHIMACCEPT regularisation control variable is set a little higher than when using finite-difference derivatives for filling of the Jacobian matrix – perhaps 5 percent to 10 percent higher than PHIMLIM. Once the measurement objective function has fallen below PHIMACCEPT, PEST_HP then concentrates on lowering the regularisation objective function. The can result in a much more acceptable parameter field than would otherwise be the case. In particular, the estimated parameter field is not as "bumpy" as it would otherwise be because of null space entrainment - a problem to which use of a randomized Jacobian is particularly susceptible.

An alternative to determination of a regularisation weight factor based on the value of PHIMLIM is to use the REG2MEASRAT regularisation control variable as a basis for calculation of this factor. While this is fast, it is also approximate. However a simplified calculation of the regularisation weight factor in this manner is less prone to errors incurred by use of a rank-deficient Jacobian matrix to support linearization of the inverse problem; the Jacobian matrix is not used for calculating the regularisation weight factor when the latter's calculation is based on REG2MEASRAT.

9.7.3 Retainment of Previous Covariance Matrix

For both practical and conceptual reasons, RANDJACRETAIN should be set to a value that allows the covariance matrix used to calculate a low-rank approximation to **Z** using equation 9.4 to inherit characteristics from random parameter sets generated during previous iterations. If this is not done,

the low column rank matrix **Z** calculated using this equation will possess a solution space (orthogonal complement to its null space) that is likely to be somewhat misaligned with the true solution space of the inverse problem, for it can only be comprised of the space spanned by the most recent set of random parameter vectors. Provided that the number of these parameter sets is equal to, or exceeds, the dimensionality of the solution space, solution space misalignment will not necessarily compromise the ability of the inversion process to achieve a good fit with the calibration dataset. However considerable entrainment of null space parameter components will be associated with estimation of parameters. Parameters may therefore be accompanied by considerable calibration-induced bias. To the extent that model predictions show null space dependency, they too may be accompanied by calibration-induced bias.

By accumulating parameter covariance matrices that were computing using random parameter sets generated during previous iterations, the rank of **Z** calculated using equation 9.4 will be larger than if it was computed from the limited number of parameter sets generated during the current iteration. This provides the PEST_HP inversion process with the means to define a solution space which is more closely aligned with the true solution space of the inverse problem.

Based on limited experience to date, NRANDREPEAT values of between 0.3 and 0.8 appear to work well. A large value for this variable dilutes the ability of the most recent parameter samples to reflect re-definition of **Z** arising from model nonlinearity. A small value may promulgate null-space entrainment for reasons just outlined.

9.7.4 Broyden Jacobian Updating

Experience to date suggests that in some inversion contexts Broyden Jacobian updating can enhance PEST_HP's performance dramatically when it is employing randomized Jacobian matrices. However there are other cases where it does not.

If Broyden Jacobian updating is not employed, this seems to result in slower, but steadier, progress of the inversion process, particularly when employing Tikhonov regularisation. In the latter case, regularisation objective functions appear to be lower for a given measurement objective function than if Broyden updating of the Jacobian matrix is employed. This, of course, is desirable, as Tikhonov regularisation poses the inverse problem as a constrained minimization problem, in which the regularisation objective function is minimized subject to the measurement objective function attaining its user-specified target.

9.7.5 Termination Criteria

When using a randomized Jacobian matrix it may be necessary to employ more forgiving termination criteria than when using a finite-difference Jacobian matrix. In particular, NPHISTP, NPHINORED and NRELPAR should be set higher than NRANDREPEAT so that PEST_HP can commit the appropriate number of iterations to improving the empirical covariance matrix of equation 9.5 while the objective function does not improve and parameter values remain the same. At the same time, NOPTMAX may need to be set higher than it normally would. If more iterations are required to reduce the objective function to a certain level, this does not constitute a diminution of inversion efficiency if each iteration requires a comparatively small number of model runs because randomized Jacobian matrices are employed.

10. Jacobian Blanking and Simultaneous Increments

10.1 General

This section continues the theme of the previous section in describing PEST_HP functionality that supports building of a Jacobian matrix using fewer model runs than there are adjustable parameters. This is achieved by endowing more than one parameter with an incremental variation when undertaking Jacobian-filling model runs. The previous chapter described the use of random parameter increments to achieve this purpose. The present chapter focuses on the use of simultaneous parameter increments.

Simultaneous incrementation (as distinct from random incrementation) of more than a single parameter when undertaking a model run for the purpose of finite-difference derivatives calculation requires "blockiness" of the Jacobian matrix. That is, it requires that the set of model-generated counterparts to observations (these being simply referred to as "observations" herein) that are sensitive to some parameters are different from the set of observations that are sensitive to other parameters. If observation-to-parameter sensitivities are such that they are not completely block-isolated in this way, they can be rendered such through strategic zeroing of insensitive elements of a Jacobian matrix. Regardless of whether it occurs naturally, or through strategic zeroing of insensitive elements, use of simultaneous parameter increments requires concomitant use of a "blanking matrix" to ensure that variation of a particular model output in response to variation of multiple parameters is not misinterpreted as sensitivity of that output to more than a single one of the varied parameters.

Use of a blanking matrix can also raise the integrity of a Jacobian matrix computed using random parameter increments. As is described in the previous section of this manual, PEST_HP supports the use of random parameter increments through its "randomized Jacobian" functionality. Through the use of random parameter increments, the number of model runs required per iteration of an inversion process can be reduced to slightly greater than that of the dimensionality of the solution space of the inverse problem on which PEST_HP usage is based. However the dramatic decrease in model run requirements accrued through use of a randomized Jacobian matrix is accompanied by certain costs. These are as follows.

- While progress in lowering an objective function may be high during early stages of an inversion process based on randomized Jacobian matrices, progress at later stages of this process may be compromised by the introduction of spurious correlations between some model outputs and some parameters, especially where true sensitivities of some model outputs to some parameters approach zero. The greater the number of random parameter increment vectors that are used to compute the Jacobian matrix, the smaller will be this effect. However use of a large number of random parameter increment vectors incurs a numerical cost. If the number of random parameter increments approaches the number of adjustable parameters, the benefits of using random parameter increments to fill a Jacobian matrix vanish.
- Parameter upgrades are calculated as linear combinations of parameter increment vectors. Where the number of random parameter increment vectors is equal to, or slightly greater than, the dimensionality of the inverse problem solution space, it is highly probable that

they collectively span a space onto which any solution space vector has a non-zero projection; hence the objective function can be lowered. However it is most unlikely that an objective-function-reducing parameter upgrade vector, calculated as a linear combination of these random parameter increment vectors, does not have a substantial null space component. The upgrade vector is therefore likely to exhibit calibration-induced bias.

Strategic Jacobian matrix blanking can reduce both of these costs. In doing this, it performs a similar role to that of "localization" in improving the performance of an iterative ensemble smoother.

10.2 The JCOBLANK Utility

10.2.1 Simultaneous Parameter Increments

A utility program named JCOBLANK has been added to the standard PEST suite. As is described in Part II of the PEST manual, this program performs two tasks. They are:

1. Construction of a blanking matrix;
2. Design of a model run schedule for finite-difference filling of a Jacobian matrix using simultaneous parameter increments.

The blanking matrix file and simultaneous increment file that are written by JCOBLANK can be read by PEST_HP. Hence PEST_HP can implement a simultaneous parameter increment strategy devised by JCOBLANK.

JCOBLANK can build a blanking matrix in two ways. One option is to employ a "zeroing file". Through this type of file, a user directly identifies Jacobian matrix elements that must be blanked. Alternatively, JCOBLANK can use an existing Jacobian matrix file (i.e. a JCO file) as a basis for blanking; under these circumstances it constructs a blanking matrix that zeroes elements of the Jacobian matrix file whose weighted sensitivities are low compared to other elements of this matrix. In either case, the greater the number of weighted Jacobian elements that are blanked, the greater is the chance that remaining elements of the Jacobian matrix have enough of a "blocky" structure to support design of a model-run-efficient simultaneous parameter increment strategy.

It is important to remember that gains in model run efficiency attained through use of simultaneous parameter increments may compromise the integrity of a Jacobian matrix. This may slow the progress of an inversion process, and may introduce bias to estimated parameters. This effect is likely to be most significant for highly nonlinear models for which model output sensitivities to parameters are functions of the values of the parameters themselves.

While JCOBLANK is documented in part II of the PEST manual, some aspects of its functionality that are pertinent to PEST_HP's implementation of simultaneous parameter increments are now briefly discussed.

10.2.2 Observation Weights

Ideally, rows of a Jacobian matrix for which observation weights are zero should be blanked when this matrix is used as a basis for the design of a simultaneous parameter increment strategy. This is because rows pertaining to observations with zero weight can be omitted from a Jacobian matrix with no adverse consequences for an inversion process. Blanking of zero-weighted rows prevents non-zero sensitivities in these rows from compromising potential blockiness of the Jacobian matrix,

and hence development of an efficient simultaneous parameter increment strategy. JCOBLANK automatically blanks zero-weighted rows of a Jacobian matrix if it builds a blanking matrix from this matrix. However it does not automatically blank zero-weighted Jacobian matrix rows if it follows instructions provided in a zeroing file. It is thus the user's responsibility to ensure that zero-weighted rows are blanked through the instructions which he/she provides in this file if this is his/her desire. There may, indeed, be occasions where blanking of zero-weighted rows is not desirable. This occurs if an inversion process "carries" one or a number of model predictions for which linear uncertainty analysis will later be undertaken.

10.2.3 Simultaneous Increment Strategy

Design of a simultaneous increment strategy can be a numerically intensive procedure. Optimization of this strategy (i.e. reducing the number of model runs required for filling a blocky Jacobian matrix) can be even more numerically intensive. JCOBLANK uses a rather simple algorithm for development of a simultaneous increment strategy. It begins the process by inspecting the first column of the Jacobian matrix. It then determines whether another adjustable parameter can be incremented conjunctively with the parameter associated with this first column by visiting subsequent columns of the Jacobian matrix in order to ascertain whether all non-zero sensitivities in one of these columns are non-overlapping with those of the first column. If it finds such a column, the parameter that is associated with this column is co-assigned to the first Jacobian-building model run. JCOBLANK then continues its inspection of Jacobian matrix columns; however now it looks for a column of the Jacobian matrix whose non-blanked elements have no coincidence with non-blanked elements of columns associated with the two parameters that have been assigned to the first model run. If it finds such a column, then another parameter is designated as being simultaneously incremented during the first Jacobian-building model run. This column-search procedure continues until all Jacobian columns have been visited; the parameter composition of the first model run is thereby completely determined. JCOBLANK then repeats this process to determine the parameter composition of the second model run. And so on.

This strategy is reasonably efficient. However its outcomes may depend on the order in which Jacobian columns are visited. In particular, the parameter composition of different Jacobian filling model runs may be different if Jacobian columns are visited in a random order rather than in a sequential order. In contrast to JCOBLANK, PEST_HP employs a random visitation order of Jacobian matrix columns when it is asked to devise a simultaneous parameter increment strategy (see below). Hence the simultaneous increment strategy which it devises may be different from that devised by JCOBLANK, even if they are based on the same Jacobian matrix. Furthermore, neither of these strategies can be guaranteed to be that which minimizes the total number of simultaneous model runs required for finite-difference filling of a blocky Jacobian matrix.

10.2.4 Blanking Re-Visited

Before it devises a simultaneous parameter increment strategy, JCOBLANK actually builds a blanking matrix based on sensitivities that it finds in the Jacobian matrix. In accordance with user instructions, Jacobian matrix elements with low sensitivities are blanked in order to enhance blockiness of this matrix. The simultaneous increment strategy that it devises is based on this blanking matrix.

Once it has devised a simultaneous parameter increment strategy based on the blanking matrix, JCOBLANK can be asked to review the blanking matrix. The simultaneous parameter increment strategy that it devised using the above algorithm may not require that all blanked elements of a

blanking matrix remain blanked. Hence, if asked to do so, JCOBLANK unblanks elements of the blanking matrix whose blanking is nonessential for support of the simultaneous parameter incrementation strategy which it has just devised. PEST_HP does this automatically when it devises its own simultaneous parameter increment strategy; see below.

10.2.5 Multiple Command Lines

If the NUMCOM variable in the "control data" section of a PEST control file is set to a number greater than 1, then PEST and PEST_HP employ different commands to run a model when calculating sensitivities with respect to different parameters. The index of the command that is used to run the model for a specific parameter is supplied through the DERCOM variable that is associated with each parameter in the "parameter data" section of the PEST control file.

If a model employs multiple command lines, the simultaneous parameter increment strategy devised by JCOBLANK and PEST_HP respect this. That is, only parameters that employ the same model command are incremented simultaneously.

10.2.6 Prior Information

Both JCOBLANK and PEST_HP ignore prior information when they build a blanking matrix, and then devise a simultaneous parameter increment strategy on the basis of that matrix. Because sensitivities of prior information equations are directly supplied through the prior information equations themselves, they do not require calculation through finite parameter differencing. Efficiency of their calculation does not therefore benefit from a simultaneous parameter increment strategy as these sensitivities do not require calculation at all.

10.2.7 Covariance Matrices

If a covariance matrix is assigned to an observation group which does not exclusively pertain to prior information, then JCOBLANK does not perform Jacobian blanking and evaluation of a simultaneous parameter increment strategy if it is asked to base these on an existing Jacobian matrix. This is because JCOBLANK actually works with a weighted Jacobian matrix under these circumstances. The relationship between Jacobian rows and weights is invalidated by the use of a covariance matrix that applies to multiple observations.

10.3 PEST_HP and Simultaneous Parameter Increments

PEST_HP can read a blanking matrix from a so-called "blanking file". It can also read a file containing a simultaneous parameter increment strategy from a so-called "simultaneous increment file". These files must complement each other; they may both have been written by JCOBLANK. PEST_HP uses the contents of the simultaneous increment file to allocate parameter increments to Jacobian-filling model runs. Then, after the Jacobian matrix has been filled using these model runs, it blanks this matrix using information obtained from the blanking file; as stated above, this eliminates confusion in attribution of model output sensitivities to parameters.

PEST_HP can itself be asked to create a blanking matrix based on the latest Jacobian matrix that it has calculated, and to formulate a simultaneous parameter increment strategy based on this blanking matrix. These are used to assist it in building the next Jacobian matrix. PEST_HP constructs the blanking matrix by identifying elements of low absolute value in the Jacobian matrix that it has just filled; in doing this, it employs an identical algorithm to that used by JCOBLANK when it is asked to build a blanking file based on an existing Jacobian matrix. After it has formulated a simultaneous

parameter increment strategy based on this blanking matrix, PEST_HP saves a blanking file and a simultaneous increment file for use in the next iteration of the inversion process (and possibly in iterations following that).

Note the following aspects of PEST_HP's behaviour in building a blanking matrix, and in designing a simultaneous parameter increment strategy.

1. Rows of the Jacobian matrix corresponding to observations that are assigned weights of zero are blanked. If a PEST control file is "carrying" zero-weighted observations as predictions for later use in linear predictive uncertainty analysis, the blanking of these rows of the Jacobian matrix will invalidate this analysis.
2. PEST_HP's algorithm for construction of a simultaneous parameter increment scheme is similar to that of JCOBLANK. However in determining which parameters to increment on a particular model run, it visits columns of the Jacobian matrix in random order. Furthermore, the visitation order varies between the different occasions on which it devises a simultaneous parameter increment strategy.
3. The random number seed which governs PEST_HP's random column visitation order is set internally. It can be re-set by providing a seed to the RANDOMSEED control variable in the "randomized jacobian" section of the PEST control file. This does not require activation of randomized Jacobian functionality; RANDOMJAC can be set to zero in this section of the file, thereby de-activating this functionality.
4. Because PEST_HP visits columns of the Jacobian matrix in random order and JCOBLANK visits these columns in sequential order, a simultaneous parameter increment strategy devised by PEST_HP may differ from that devised by JCOBLANK if the latter program is provided with the same Jacobian matrix.
5. Once it has devised a simultaneous parameter increment strategy, PEST_HP alters the blanking matrix so that it conforms with this strategy (see above). Hence no blanking takes place beyond that which is required to complement the simultaneous parameter increment strategy.
6. If simultaneous parameter increments are employed in building a Jacobian matrix, PEST_HP disables sensitivity re-use and parameter bounds sticking if either of these have been enabled through settings supplied in the PEST control file.
7. As is usual practice, if the NOPTMAX control variable appearing in the "control data" section of a PEST control file is set to -1 or -2, PEST_HP ceases execution after filling the Jacobian matrix. If the SIMINCCALC control variable (see below) is set to 1, then PEST_HP also constructs a blanking matrix and devises a simultaneous parameter increment strategy before ceasing execution; as is described below, these are stored in appropriately-named blanking and simultaneous increment files. If desired, these files can be used on subsequent PEST_HP runs in which the SIMINC control variable is set to 1; however they must first be renamed (see below).

10.4 PEST_HP Control Variables

10.4.1 Section in PEST Control File

A new section has been introduced to the PEST_HP control file. This section is labelled "* simultaneous parameter increments". It must be placed between the "control data" and "parameter groups" sections of a PEST control file. Other sections (such as "singular value decomposition", "randomized jacobian" and "sensitivity reuse") can also appear between the "control data" and

"parameter groups" sections of a PEST control file. There is no prescribed ordering for these sections if more than one of them is present.

Figure 10.1 shows variables which are featured in the "simultaneous parameter increments" section of a PEST_HP control file. Figure 10.2 shows an example.

Note that, at the time of writing, PESTCHEK tolerates the presence of this section, but does not check its contents. The PSTCLEAN utility removes this section from a PEST control file in order to render that file inoffensive to the normal versions of PEST and BEOPEST.

```
* simultaneous parameter increments
BLANKJCO    SIMINC
BLANKFILE
SIFILE
SIMINCCALC
FRACOBS FRACPAR FULLJCOITN SIMINCACCEL MINSIMINC MATCHAGENTS
```

Figure 10.1. Specifications of the "simultaneous parameter increments" section of a PEST control file.

```
* simultaneous parameter increments
1 1                              #BLANKJCO   SIMINC
blanking_file = blank.jcz        #BLANKFILE
si_file = siminc.dat             #SIFILE
1                                #SIMINCALC
.5  .5  5  1 95 1  #FRACOBS FRACPAR FULLJCOITN SIMINCACCEL MINSIMINC MATCHAGENTS
```

Figure 10.2. Example of a "simultaneous parameter increments" section of a PEST control file.

10.4.2 Variables

The role of each of the variables appearing in the "simultaneous parameter increments" section of a PEST control file is now discussed.

BLANKJCO

BLANKJCO is an integer variable which must be set to 0 or 1. Set it to 1 to instruct PEST_HP to read a blanking file and to use the contents of this file to blank every Jacobian matrix that it calculates. Note that Jacobian matrix blanking does not necessarily require that simultaneous parameter increments be employed for filling of the Jacobian matrix. As is stated above, Jacobian matrix blanking can be used to raise the integrity of a Jacobian matrix calculated using random parameter increments.

Unless PEST_HP calculates its own blanking matrix (which occurs when the SIMINCCALC control variable is set to 1), the blanking file read by PEST_HP when BLANKJCO is set to 1 will normally have been written by the JCOBLANK utility. The name of this file is assigned to the BLANKFILE control variable. PEST_HP reads, and then re-reads, this file during every iteration of the inversion process just after it has undertaken the model runs required for filling of the Jacobian matrix.

As is usual practice, if PEST_HP is started with the "/i" command-line switch, it reads an existing Jacobian matrix for use in the first iteration of the inversion process. This matrix is <u>not</u> blanked, regardless of values assigned to the BLANKJCO and SIMINC control variables.

SIMINC

SIMINC, an integer variable, must be set to 0 or 1. If it is set to 1, PEST_HP obtains a simultaneous parameter increment strategy from a user-nominated simultaneous increment file; it employs this strategy during every iteration of the inversion process. The name of this file is assigned to the SIFILE

control variable. Normally this file will have been written by the JCOBLANK utility. PEST_HP reads, and then re-reads, this file during every iteration of the inversion process just before it commissions the model runs required for filling of that iteration's Jacobian matrix.

If SIMINC (or SIMINCCALC) is set to 1, PEST_HP requires that the FORCEN variable for all parameter groups be set to the same value, this being either *always_2*, *always_3*, *switch*, or *always_5*. If different parameter groups have different FORCEN settings, the number of model runs used for calculation of derivatives of model outputs with respect to different parameters differs between parameters. This makes design of a simultaneous parameter increment strategy difficult. Actually, a FORCEN setting of *always_2* may be suitable for most occasions. While this setting precludes the attainment of increased derivatives precision through use of higher order finite differences, this may not matter too much as use of simultaneous parameter increments together with concomitant Jacobian element blanking also reduces the precision of finite-difference derivatives.

If SIMINC is set to 1, PEST_HP will object if BLANKJCO is not also set to 1.

BLANKFILE
BLANKFILE is the name of the Jacobian blanking file which PEST_HP reads if BLANKJCO is set to 1. As is illustrated in figure 10.2, its name must follow the string "blanking_file =" on the second line of the "simultaneous parameter increments" section of a PEST control file. Spaces can optionally surround the "=" sign. If BLANKJCO is set to 0, it is not necessary for the name of a file to follow the "blanking_file =" string, for its name is disregarded under these circumstances. If the name of the blanking file contains a space, its name should be enclosed by quotes.

The blanking file whose name is assigned to the BLANKFILE control variable must be a binary file; its name must have an extension of "*.jcz*". Normally this file will have been written by JCOBLANK. However it must not be named *case.jcz* where *case* is the filename base of the PEST control file, for this name is reserved for the blanking file that PEST_HP writes and reads if SIMINCCALC is set to 1.

SIFILE
SIFILE is the name of the simultaneous increment file which PEST_HP reads if SIMINC is set to 1. As is illustrated in figure 10.2, its name must follow the string "si_file =" on the second line of the "simultaneous parameter increments" section of a PEST control file. Spaces can optionally surround the "=" sign. If SIMINC is set to 0, it is not necessary for the name of a file to follow the "si_file =" string, for its name is disregarded under these circumstances. If the name of the simultaneous increments file contains a space, its name should be surrounded by quotes.

The simultaneous increment file whose name is supplied to the SIFILE control variable will normally have been written by JCOBLANK. This file must not be named *case.sif*, were *case* is the filename base of the PEST control file. This name is reserved for the simultaneous increment file which is written and read by PEST_HP if SIMINCCALC is set to 1.

SIMINCCALC
Set this integer variable to 1 to inform PEST_HP that it must periodically calculate a blanking matrix and devise a simultaneous parameter increment strategy itself. If PEST_HP devises a simultaneous parameter increment strategy during any particular iteration of the inversion process, it does so immediately after it has filled the Jacobian matrix pertaining to that iteration. First it determines a blanking matrix based on weighted sensitivities recorded in the Jacobian matrix that it has just

calculated. This matrix is recorded in a file named *case.jcz*, where *case* is the filename base of the PEST control file. Then, based on this blanking matrix, PEST_HP devises a simultaneous parameter increment strategy for use during one or more subsequent iterations. It stores this strategy in a simultaneous increment file named *case.sif*, where *case* is the filename base of the PEST control file.

Note that just after PEST_HP has devised a simultaneous parameter increment strategy, it re-examines the blanking matrix on which basis this strategy was devised. If it is possible to unblank some elements of this matrix while maintaining the integrity of the simultaneous parameter increment strategy, then it does so. As was discussed above, this can increase the precision of (simultaneous) finite-difference derivatives calculation.

If SIMINCCALC is set to 1, PEST_HP does not use a PEST_HP-calculated simultaneous parameter increment strategy to fill the Jacobian matrix that it calculates during the first iteration of the inversion process. If SIMINC is set to 0, this matrix is filled in the normal way; that is, all parameters are incremented individually. Alternatively, if SIMINC is set to 1, the Jacobian matrix used in the first iteration is filled using a simultaneous parameter increment strategy supplied in a file whose name is ascribed to the SIFILE control variable; the Jacobian matrix is then blanked using the blanking matrix supplied in a file whose name is ascribed to the BLANKFILE control variable. The Jacobian matrix computed during all iterations identified by the value of the FULLJCOITN control variable (see below) is computed in this same way. During all of these iterations, however, PEST_HP evaluates its own blanking matrix and simultaneous parameter increment strategy based on the thus-computed Jacobian matrix if SIMINCCALC is set to 1. These are stored in files *case.jcz* and *case.sif* for use in subsequent iterations; existing versions of these files are thus over-written.

FRACOBS and FRACPAR

PEST_HP calculates a blanking matrix from a Jacobian matrix in the same way that JCOBLANK does. (Unlike JCOBLANK, however, PEST_HP does not optionally read a zeroing file to obtain blanking information.) First PEST_HP blanks all rows of the Jacobian matrix for which observation weights are zero. Then, for each row, it ascertains the weighted sensitivity of highest absolute value. Any elements within this row whose absolute weighted sensitivities are less than FRACOBS times this maximum value are then blanked. The same operation is then performed for each column of the weighted Jacobian matrix using FRACPAR as the governing variable. FRACOBS and FRACPAR should both lie between 1.0 and 0.0 (inclusive); they are real variables.

Note that prior information sensitivities are not blanked. Note also that the blanking matrix and simultaneous parameter increment strategy devised by PEST_HP during any iteration of the inversion process are not used until the ensuing iteration.

FULLJCOITN

As stated above, if SIMINCCALC is set to 1, PEST_HP calculates a Jacobian matrix in the “normal” way during the first iteration of the inversion process. Hence it does not employ simultaneous parameter increments for filling of this matrix unless SIMINC is set to 1. On the basis of this Jacobian matrix it calculates a blanking matrix and devises a simultaneous parameter increment strategy for use in the next iteration (or more) of the inversion process.

PEST_HP also calculates a Jacobian matrix in the normal way at intervals of FULLJCOITN iterations. Thus, for example, if FULLJCOITN is set to 2, then PEST_HP calculates a Jacobian matrix in the normal

manner during iterations 3, 5, 7, etc of the inversion process; similarly, if FULLJCOITN is set to 3, PEST_HP calculates a Jacobian matrix in the normal way during iterations 4, 7, 10, etc of the inversion process. During all other iterations of the inversion process, PEST_HP employs simultaneous increment and blanking strategies which it has calculated itself; it reads the blanking matrix and details of the simultaneous parameter increment strategy from files *case.jcz* and *case.sif* respectively, where *case* is the filename base of the PEST control file.

PEST_HP will cease execution with an error message if FULLJCOITN is set to 1 or less.

SIMINCACCEL
"SIMINCACCEL" stands for "simultaneous increment acceleration". If SIMINCACCEL is set to 1 then SIMINCCALC should also be set to 1.

If SIMINCACCEL is set to 0 and SIMINCCALC is set to 1, PEST_HP does not compute a blanking matrix or simultaneous parameter increment strategy during those iterations in which it actually uses a blanking matrix and simultaneous parameter increment strategy that it has previously calculated itself. This happens during all iterations except those for which the setting of the FULLJCOITN control variable dictates that Jacobian matrix calculation takes place in the "normal" way. However if SIMINCACCEL is set to 1, then PEST_HP updates the blanking matrix and evaluates a new simultaneous parameter increment strategy even during those iterations in which it is using a blanking matrix and simultaneous parameter increment strategy that it has previously calculated for itself. This can result in a significant reduction in the number of model runs required for filling of the Jacobian matrix during the ensuing iteration (as long as this iteration has not been decreed by FULLJCOITN to be a "normal" Jacobian iteration). Unfortunately, this reduction in model run requirements may be accompanied by some loss of integrity of the Jacobian matrix that is calculated during that iteration. Hence if SIMINCCALC is set to 1 it is good practice to set the MINSIMINC control variable (see below) to a sensible value so that the number of model runs employed for filling the Jacobian matrix does not become unworkably low.

If SIMINCACCEL is set to 1 then FULLJCOITN must be set to 3 or greater. If FULLJCOITN is not set to 3 or greater under these circumstances, then there can be no iterations to which a non-zero value of SIMINCACCEL actually pertains. This is because PEST_HP is either calculating a Jacobian matrix in the "normal" way during a particular iteration, or is employing a blanking strategy that it has devised itself on the basis of this "normally-calculated" Jacobian matrix.

MINSIMINC
If this integer variable is set to a number greater than 0, PEST_HP will never devise a parameter increment strategy which lowers the number of simultaneous parameter increments below this number.

If the value supplied for MINSIMINC is equal to or greater than the number of adjustable parameters, PEST_HP will cease execution with an error message.

MATCHAGENTS
If SIMINCCALC is set to 1, so that PEST_HP devises its own simultaneous parameter increment strategy during some iterations of the inversion process, PEST_HP will try to ensure that the number of simultaneous parameter increments that it adopts is an integral multiple of the number of agents available for carrying out model runs. First PEST_HP evaluates a simultaneous parameter increment

strategy using the FRACOBS and FRACPAR control variables described above. Then, if necessary, it raises the number of simultaneous parameter increments calculated in this way until the number of increments is equal to a multiple of the number of available agents. This ensures that no agents are idle as the Jacobian matrix is being filled. Raising the number of simultaneous increments to achieve processor-to-increment parity also raises the integrity of the thus-calculated Jacobian matrix, as less blanking of this matrix is required to forestall the assignment of changes in model outputs to the wrong parameters.

10.5 Using SVD-Assist

PEST_HP allows the use of simultaneous parameter increments when undertaking SVD-assisted parameter estimation. However because the use of super parameters already constitutes a theoretically optimal run reduction strategy, little is likely to be gained by using both methods together.

The SVDAPREP utility which prepares a super-parameter PEST control file tolerates the presence of a "simultaneous parameter increments" section in the base parameter PEST control file from which the super parameter PEST control file is derived. However it does not transfer this section to the super parameter PEST control file. It is the user's responsibility to add this section to the super parameter PEST control file him/herself.

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 minimized 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 PEST_HP agents. The first of these batch files should be run from the manager's 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 the PEST_HP manager.

```
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 the PEST_HP manager 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 until each of them calibrates the model. 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
pest_hp base_svda /h manager's_ip_address:4004
timeout /t 2
goto label1
```

Figure 11.2 A batch file used to initiate repeated runs of the PEST_HP agent.

The batch file depicted in figure 11.2 needs to be run only one; replace "*manager's_ip_address*" in this file with the IP address or hostname of the computer on which the PEST_HP manager is running. On completion of each inversion process, execution of the PEST_HP agent 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.

12. CMAES_HP

12.1 General

CMAES_HP is a "HP" version of the global optimisation utility CMAES_P supplied with the PEST suite. Differences between CMAES_HP and CMAES_P are principally that:

- CMAES_HP cannot be run in serial mode;
- When run in parallel mode (which is its only mode of operation) CMAES_HP uses the BEOPEST/PEST_HP protocol for communication between the run manager and run agents, this being based on TCP/IP communication between manager and agents.

12.2 Running CMAES_HP

The CMAES_HP manager is run using the command:

```
cmaes_hp case /r /h :nnnn
```

where:

case	is the filename base of a PEST control file;
/r	is an optional restart switch; and
/nnnn	is a user-selectable TCP/IP port number (use a high number such as 4004 to avoid conflict with other TCP/IP port users).

There is no limit to the number of agents that can be used in conjunction with a single manager. However it makes no sense to use more agents than the CMAES population size plus the optional number of trial singular value thresholds that it may optionally employ, for this is the number of model runs which comprise a single run package.

Note that there is no need to accept CMAES_HP's recommendations for population size and number of parents. CMAES_HP does not check for the number of available computing nodes before making these recommendations. If you have access to a greater number of nodes than CMAES_HP's suggested population size, inform CMAES_HP that your population size is accordingly larger. Then set the parent size to about half the population size.

See CMAES_P documentation in part I of the PEST manual for a full description of these, and other, settings.

Each agent is run using the command:

```
pest_hp case /h hostname:nnnn
```

where:

hostname	is the IP address (version 4) or hostname of the machine on which the CMAES_HP manager is running; and
nnnn	is the TCP/IP port used by the CMAES_HP run manager.

As is apparent from the above command, the CMAES_HP agent is run using the same command as the PEST_HP agent. The CMAES_HP agent is, in fact, PEST_HP acting in its capacity as a run agent.

12.3 Some CMAES_HP Details

12.3.1 Starting and Stopping

In many respects, operation of CMAES_HP is identical to that of CMAES_P. In common with its CMAES_P counterpart, the CMAES_HP run manager asks the user a series of questions on commencement of its execution. Optionally, each of these questions can be answered by simply pressing the <Enter> key to accept the CMAES_HP default response.

CMAES_HP terminates execution if any of its termination criteria are met. These are supplied by the user in response to CMAES_HP prompts. However CMAES_HP execution can also be terminated at any time by pressing <Ctl-C> while focussed on the run manager's window. Alternatively (as is the case for PEST_HP), execution of CMAES_HP can be temporarily paused and unpaused by typing the "ppause" and "punpause" commands from another command line window that is open in the CMAES_HP manager's working folder. Similarly, execution of CMAES_HP can be terminated by issuing the "pstop" or "pstopst" command from this same window; both of these stopping commands have the same effect on CMAES_HP.

If execution of CMAES_HP is terminated by the user, its execution can be resumed by starting it with the "/r" command line switch. If restarted in this way, CMAES_HP does not prompt for user-supplied information; it obtains this information from its restart file. If the CMAES_HP manager is restarted using the "/r" switch, it recommences execution at the start of the iteration in which its previous execution was terminated. It does not read the outcomes of model runs that were previously conducted during this terminated iteration.

On cessation of execution, CMAES_HP does not carry out a final model run based on optimised parameters. At any stage of the CMAES_HP optimisation process (and at the end of the CMAES_HP optimisation process), best parameters achieved up until that point can be found in file *case.par* where *case* is the filename base of the PEST control file on which its run is based. To conduct a single model run based on this optimised parameter set, do the following.

- Use the PARREP utility to write a new PEST control file based on optimised parameters;
- Run PEST with NOPTMAX set to zero using this file; or run CMAES_HP, informing it (in response to its pertinent prompt) that the maximum number of iterations is zero.

12.3.2 Extra Output Files

CMAES_HP records more files than does CMAES_P. These extra files are the same as those recorded by PEST_HP, as both of these programs share the same run manager.

Suppose that the PEST control file on which a CMAES_HP run is based is named *case.pst*. CMAES_HP records the following files:

- *case.rec*, the run record file;
- *case.ofr* which tabulates objective functions (total and group) at the end of each iteration;
- *case.par* which records best parameter values achieved to date;
- *case.per* which lists parameter values associated with failed model runs;
- *case.rme* which records run agent efficiencies;
- *case.rmr* which records the communication history between the run manger and each of its run agents.

See PEST documentation and section 6 of the present document for details of the contents of these files.

12.3.3 Other HP Functionality

Other PEST_HP functionality that is also available in CMAES_HP includes the following:

- The HARDSTOPHOURS and SOFTSTOPHOURS control variables can be used to limit the length of a CMAES_HP run. The first of these precipitates immediate cessation of CMAES_HP execution upon reaching the user-specified time limit. In contrast, CMAES_HP waits until the end of the current iteration to implement SOFTSTOPHOURS-based termination.
- CMAES_HP makes use of the RUN_ABANDON_FAC control variable. This has the same meaning for CMAES_HP as it does for PEST_HP.
- When running under Windows, CMAES_HP can instruct run agents to kill overdue runs. As for PEST_HP, the WIN_MRUN_HOURS variable which provides model timeout time in hours, is read from the PEST control file; the value of this variable is transmitted to all run agents by the CMAES_HP manager. Agents terminate model runs when the WIN_MRIN_HOURS time limit has expired. See section 7.2.4 for further details.

12.3.4 Forgiving Run Failure

One of the questions that the CMAES_HP manager asks the user on commencement of its execution is the following:

```
Forgive model run failure? [y/n]: (<Enter> if "y"):
```

If your response to this question is “n” then, should the model fail to run to completion for a particular parameter set, CMAES_HP will attempt to repeat the model run on another agent. If model run failure occurs again, CMAES_HP ceases execution with an appropriate error message. However if your response to the above prompt is “y” (or simply <Enter>), CMAES_HP does not attempt to repeat a failed model run; nor is an error condition incurred. It simply assigns a high objective function value to that run.

12.3.5 File Distribution

This aspect of PEST_HP functionality is not available for CMAES_HP.

12.3.6 Saving a Run Results File

CMAES_HP does not save a run results file. If the value of the RRFSAVE variable is set to “rrfsave” in the “control data” section of the PEST control file which CMAES_HP reads, it will cease execution with an appropriate error message. Nor can CMAES_HP be started with the “/f” switch.

12.3.7 Estimating the Cost of a CMAES_HP Run

As is discussed in section 1.9 of this document, the PCOST_HP utility can be used to estimate the cost of running PEST_HP on the cloud based on the contents of a PEST control file. However if you intend to run CMAES_HP, you should ignore the cost estimate provided by PCOST_HP and estimate the cost yourself, as its costings are inapplicable to CMAES_HP.

12.3.8 Further CMAES_HP Details

See documentation of CMAES_P in part I of the PEST manual for other CMAES_P/CMAES_HP operational details. See also section 13 of this document for a discussion of file-parameters; CMAES_HP can employ file-parameters for tasks such as optimisation under uncertainty.

13. JACTEST_HP

The role of JACTEST_HP is the same as that of the PEST JACTEST utility. That is, it undertakes a series of model runs using incrementally varied parameters. This is normally done in order to test differentiability of model outputs with respect to the varied parameter. See part 2 of the PEST manual for full details.

While the PEST JACTEST utility allows parallelization of model runs, it uses the old parallel PEST protocol for communicating between master and slaves. In contrast, JACTEST_HP uses the same parallelization protocol as that used by BEOPEST and PEST_HP. That is, communication between manager and agents is undertaken using TCP/IP. Hence there is no need to prepare a Parallel PEST run management file.

The JACTEST_HP manager is run using the command:

```
jactest_hp case param nrun outfile /h :nnnn
```

where:

case	is the filename base of a PEST control file;
param	is a parameter whose value will be incrementally varied;
nrun	is the number of parameter variations to implement (one less than the number of model runs to undertake);
outfile	is the name of the JACTEST_HP output file; and
/nnnn	is a user-selectable TCP/IP port number (use a high number such as 4004 to avoid conflict with other TCP/IP port users).

Each agent is run using the command:

```
pest_hp case /h hostname:nnnn
```

where:

hostname	is the IP address (version 4) or hostname of the machine on which the CMAES_HP manager is running; and
nnnn	is the TCP/IP port used by the JACTEST_HP run manager.

As is apparent from the above command, the JACTEST_HP agent is run using the same command as a PEST_HP agent. The JACTEST_HP agent is, in fact, PEST_HP acting in its capacity as a run agent.

Note the following:

- In the event of model run failure, JACTEST_HP does not cease execution. However the outputs of failed model runs are recorded as -1.01D300 on its output file so that they are easily recognizable.
- JACTEST_HP will accommodate the presence of secondary parameters in a PEST control file. However it will not accommodate the presence of file parameters. Secondary and file parameters are described below.

14. Special Parameters

14.1 File-Parameters

14.1.1 General

CMAES_HP can employ "file-parameters" in addition to its normal parameters. Unlike normal parameters, file parameters are not adjusted through the CMAES_HP optimisation process as it strives to lower the objective function. However random realizations of values for these parameters can be read from external files. These values are transferred, together with those of normal CMAES_HP parameters, to run agents, and then to model input files through template files. The names of file-parameters, and of the template files which feature them, must be provided in the PEST control file read by CMAES_HP, along with the names of normal parameters and the names of template files which cite them.

The purpose of file-parameters is to enable CMAES_HP to undertake optimisation under uncertainty along similar lines to that described by Bayer et al (2008) and Bayer et al (2010).

Suppose that a PEST control file names *M* file-parameters. At the beginning of every iteration of the CMAES_HP optimisation process, you can supply values for as many sets of these *M* parameters as you see fit; each set must include a value for all parameters. Suppose that you supply values for *N* such sets; these will normally constitute *N* random realizations of the set of *M* file-parameters. Then on any occasion that CMAES_HP runs the model during that iteration, it actually runs the model *N* times. For all of these *N* model runs it uses the same values for normal CMAES_HP parameters. However it uses different values for the file-parameters – a different set of values on each occasion. These values of file-parameters are read from a set of user-nominated parameter value files (hence the name "file-parameters"). Each parameter value file in the set may have been written by a program such as RANDPAR or RANDPAR1.

If you wish, *N* (the number of random file-parameter sets, and hence the number of parameter value files) can vary from iteration to iteration of the CMAES_HP optimisation process. Optionally, CMAES_HP can issue a system command through which an external program can be run in order to alter the contents of a file which informs CMAES_HP at the start of each optimisation iteration of the number of sets of file-parameters that it must employ during that iteration, and of the names of the parameter value files from which it must read their values.

14.1.2 Defining File-Parameters

The names of file-parameters must be provided in the "parameter data" section of a PEST control file. CMAES_HP must be informed of the number of file-parameters that reside in this section through a variable named NPARFILE that appears on the fourth line of the PEST control file (in the "control data" section of this file). This is illustrated in figure 14.1.

```
pcf
* control data
restart estimation
10 19 2 10 3 nparfile=9 fileparfile=fpfile.dat
2 3 single point  1 0 0
.
.
```

Figure 14.1 First part of the "control data" section of a PEST control file featuring the NPARFILE and FILEPARFILE control variables.

In the above figure, the value of NPAR (first variable on the fourth line of the PEST control file) is set to 10. Hence the "parameter data" section of the PEST control file cites 10 normal parameters; some of these must be adjustable while others may be tied or fixed. The string "nparfile=9" informs CMAES_HP that, in addition to these 10 normal parameters, the PEST control file features 9 file-parameters. (Note that spaces can surround the "=" sign in this string if desired.) The string "fileparfile=*filename*" informs CMAES_HP of the name of a "file-parameter file". CMAES_HP must read this file in order to obtain the names of the sequence of parameter value files from which the values of file-parameters are read. This file-parameter file is read at the beginning of each iteration of the CMAES_HP optimisation process; its contents can change from iteration to iteration.

If the value of NPARFILE is provided as *M*, then the names of *M* file-parameters must be provided in the "parameter data" section of the PEST control file. (Note that there is no limit on the size of *M*.) A simple example is provided in figure 14.2. Figure 14.3 provides a more complex example.

```
* parameter data
ro1   log factor 1.000000 0.1 100 ro 1 0 1
ro2   log factor 1.000000 0.1 100 ro 1 0 1
ro3   log factor 1.000000 0.1 100 ro 1 0 1
ro4   log factor 1.000000 0.1 100 ro 1 0 1
ro5   log factor 1.000000 0.1 100 ro 1 0 1
ro6   log factor 1.000000 0.1 100 ro 1 0 1
ro7   log factor 1.000000 0.1 100 ro 1 0 1
ro8   log factor 1.000000 0.1 100 ro 1 0 1
ro9   log factor 1.000000 0.1 100 ro 1 0 1
ro10 log factor 1.000000 0.1 100 ro 1 0 1
h1    file_parameter
h2    file_parameter
h3    file_parameter
h4    file_parameter
h5    file_parameter
h6    file_parameter
h7    file_parameter
h8    file_parameter
h9    file_parameter
```

Figure 14.2 The "parameter data" section of a PEST control file which cites 9 file-parameters.

```
* parameter data
ro1  log factor 1.000000 0.1 100 ro 1 0 1
ro2  log factor 1.000000 0.1 100 ro 1 0 1
ro3  log factor 1.000000 0.1 100 ro 1 0 1
ro4  log factor 1.000000 0.1 100 ro 1 0 1
ro5  log factor 1.000000 0.1 100 ro 1 0 1
ro6  log factor 1.000000 0.1 100 ro 1 0 1
ro7  log factor 1.000000 0.1 100 ro 1 0 1
ro8  log factor 1.000000 0.1 100 ro 1 0 1
ro9  log factor 1.000000 0.1 100 ro 1 0 1
ro10 log factor 1.000000 0.1 100 ro 1 0 1
h1   log factor  0.25  0.05 100 hhh 1 0 1
h2   tied factor  0.50 0.05 100 hhh 1 0 1
h3   tied factor  1.00 0.05 100 hhh 1 0 1
h4   tied factor  2.00 0.05 100 hhh 1 0 1
h5   tied factor  4.00 0.05 100 hhh 1 0 1
h6   tied factor  8.00 0.05 100 hhh 1 0 1
ff1  file_parameter
h7   tied factor  16.0 0.05 100 hhh 1 0 1
h8   tied factor  32.0 0.05 100 hhh 1 0 1
h9   tied factor  64.0 0.05 100 hhh 1 0 1
h2 h1
h3 h1
ff2  file_parameter
h4 h1
h5 h1
h6 h1
h7 h1
ff3  file parameter
h8 h1
h9 h1
```

Figure 14.3 The "parameter data" section of a PEST control file which cites 3 file-parameters.

Each line in the "parameter data" section of a PEST control file that defines a file-parameter must begin with the name of the actual parameter. The string "file_parameter" must follow that. No value is supplied for any file-parameter, as the values of file-parameters are provided in other files.

As is the case for a normal parameter, the name of a file-parameter must be 12 characters or less in length. It must also be unique. Hence it must not have the same name as a normal parameter or a secondary parameter (see the next subsection).

The two-word line which defines a file-parameter can be placed anywhere within the "parameter data" section of a PEST control file. Where this section is divided into two parts because of the presence of tied parameters, file-parameters can be defined in either, or both, of the first and/or second parts of this section.

It is important to note that the variable NPAR defined in the "control data" section of the PEST control file must not account for the presence of file-parameters; it must account only for the number of normal parameters. CMAES_HP is informed of the number of file-parameters through the NPARFILE keyword.

All file-parameters defined in the "parameter data" section of a PEST control file must appear in at least one template file that is cited in the "model input/output" section of the same PEST control file.

Prior information equations appearing in a PEST control file cannot feature file-parameters.

14.1.3 Supplying Values for File-Parameters

If NPARFILE is set to a value that is greater than zero on the fourth line of a PEST control file, then this same line must provide the name of a file-parameter file. This is supplied as the value of the FILEPARFILE variable. Figure 14.4 illustrates the contents of such a file.

```
5 0
11    h11.par
12    h12.par
13    h13.par
14    h14.par
15    h15.par
```

Figure 14.4 A file-parameter file.

The first line of a file-parameter file must contain two integers. The second integer must be 0 or 1. If the second integer is 0, then the first integer is the number of lines to follow. If the second integer is 1, then the number of lines which follow the header line must be equal to the value of the first integer plus 1. The second integer informs CMAES_HP whether an optional system command is provided on the last line of the file-parameter file. If it is set to 0 then a system command is not provided; if it is set to 1 then a system command is provided.

Suppose that the value of the first integer is *N*. Then each of the following *N* lines of the file-parameter file must contain two items. The first item must be an integer, this being an arbitrary (but unique) identifier for a file-parameter set. The second item must be the name of a parameter value file which contains values for that particular set of file-parameters.

Note the following.

- The integer identifiers which you ascribe to file-parameter sets can be supplied in any order. Their values do not matter. They are used for identification purposes only.
- A parameter value file cited in a file-parameter file must contain values for file parameters only. Furthermore, each such file must contain values for all of the file parameters which feature in a PEST control file.

Because the file-parameter file is read at the beginning of every iteration of the CMAES_HP optimisation process, it can change from iteration to iteration. The number and names of parameter value files provided during any one iteration of the optimisation process may differ from those provided in any other iteration. Dynamic alteration of the contents of a file-parameter file enables construction of dynamic stacks of file-parameter sets in the manner described by Bayer et al (2008; 2010). An external program can be used to determine the composition of a file-parameter file, and write this file at the beginning of each CMAES_HP iteration. This program can be run by CMAES_HP using a system command. As stated above, the name of this command can be supplied on the last line of the file-parameter file. This is exemplified in figure 14.5.

```
5 1
11    h11.par
12    h12.par
13    h13.par
14    h14.par
15    h15.par
"process_cmaes_outputs.exe"
```

Figure 14.5 A file-parameter file which includes a system command as its final line.

Single or double quotes are optional when supplying the system command. If they are omitted, then all characters provided on the last line of the file-parameter file comprises the command which CMAES_HP will issue to the operating system at the beginning of each iteration. If they are included, then a single or double quote must comprise the leading character on the final line of the file-parameter file; the system command then comprises all characters between the leading quote and a subsequent quote of the same type on that line.

The optional system command is further discussed below.

14.1.4 Calculating the Objective Function

During each iteration of its optimisation process, CMAES_HP calculates an objective function for each member of a population of parameter values (i.e. the values of normal PEST parameters that are included in the NPAR count). The size of the population employed by CMAES_HP can be user-specified. Alternatively, the CMAES_HP default can be accepted. Let us designate the population size as *P*.

Where file-parameters are introduced to the optimisation process, the number of parallel model runs that CMAES_HP undertakes during any iteration of the inversion process is equal to the population size times the number of sets of file parameters that it employs during that iteration; thus the number of model runs is equal to $N \times P$. If no file-parameters are defined, then each model run is based on a single set of normal PEST parameters. Where file-parameters are employed, each run is repeated *N* times, with a different set of file-parameters used on each occasion. The values of normal PEST parameters do not vary between these *N* model runs; however the values of file-parameters are different from run to run, these having been obtained from pertinent parameter value files in the manner described above.

The objective function associated with any particular set of normal PEST parameters (which generally comprise the decision-variables of an optimisation process) is set to the maximum objective function calculated over all file-parameter set realizations. CMAES_HP's task therefore is to adjust the values of its normal parameters (i.e. decision variables) in order to minimize an objective function which, for each set of decision variables, is the maximum over all realizations of file-parameters. This is the basis for optimisation under uncertainty.

14.1.5 CMAES_HP Output

CMAES_HP output when using file-parameters is very similar to its usual output. The run record file has the same format; however the fact that file-parameters are being deployed is recorded in the first section of this file. Likewise, CMAES_HP's screen output with file-parameters is similar to that without file-parameters. However a noticeable difference to its screen output when using file-parameters results from the fact that the number of model runs required per iteration is larger. Hence the record of model run completions that is written to the screen differs from that which would be the case if no file-parameters were employed.

In accordance with its normal protocol, CMAES_HP records optimised parameter values in a parameter value file named *case.par*, were *case* is the filename base of the PEST control file. This file makes no mention of file-parameters. This is because file-parameters are not optimised; they simply express uncertainties associated with certain aspects of a model.

CMAES_HP records one extra output file when using file-parameters. This is a "file-parameter objective function file". It is named *case.fpo*, where *case* is the filename base of the PEST control file. Part of a file-parameter objective function file is shown in figure 14.6. For this particular example only five realizations of file-parameters are used per iteration.

```
 Iteration number:      0
     1        1         11     545.0286
     1        2         12     646.0687
     1        3         13     845.1376
     1        4         14     515.2966
     1        5         15     543.8536

 Iteration number:      1
     1        1         11     502.3958
     1        2         12     492.6022
     1        3         13     481.7879
     1        4         14     483.4754
     1        5         15     502.3958
     2        1         11     650.2811
     2        2         12     651.8538
     2        3         13     658.0548
     2        4         14     663.1965
     2        5         15     650.2811
     3        1         11     528.5220
     3        2         12     534.6340
     3        3         13     537.7239
     3        4         14     539.2051
     3        5         15     528.5220
     4        1         11     620.1152
etc
```

Figure 14.6 The first part of a file-parameter objective function file.

The file-parameter objective function file records the objective function calculated for all model runs that CMAES_HP commissions during the optimisation process. Apart from section headers which proclaim the iteration number, each line of the file-parameter objective function file has four entries. These entries are as follows.

1. The index of the normal CMAES parameter set on which the model run is based. This ranges from 1 to *P*, where *P* is the population size. Numbering is sequential, starting at 1.
2. The index of the file-parameter set used for the model run. These are also numbered sequentially starting at 1. The highest value recorded for this index during any iteration of the CMAES_HP inversion process is equal to *N,* where *N* is the number of parameter value files cited in the file-parameter file that CMAES_HP reads at the start of each iteration.
3. The user-supplied integer which is used to identify each parameter value file cited in the file-parameter file.
4. The objective function calculated using the specified normal parameter set in combination with the specified file-parameter set.

The file-parameter objective function file is available for processing at any time. It is flushed from cached storage at the end of each iteration of the CMAES_HP optimisation process. Hence its latest contents are available for processing by an external program that may be run using the system command that is issued by CMAES_HP at the beginning of the next iteration.

14.1.6 The Optional System Command

As was discussed above, CMAES_HP can optionally read a system command from the last line of the file-parameter file. Through this command, the contents of the file-parameter file can be altered from iteration to iteration. Hence the number of file-parameters used during any iteration of the optimisation-under-uncertainty process can be increased or decreased as appropriate for efficiency and/or reliability of that process. See Bayer et al (2008; 2010) for details. The external program which is run through the system command will presumably obtain the information on which it bases file-parameter set alteration from the file-parameter objective function file written by CMAES_HP. Note that this system command is issued by the CMAES_HP run manager, but not by any run agents. Processing is thus local to the computer (and working folder) of the run manager.

It is important to understand the sequence of events that occurs during each iteration of a CMAES_HP optimisation process in which CMAES_HP reads a file-parameter file (together with parameter value files cited therein) and implements a system command. CMAES_HP actually issues the system command before it reads the file-parameter file. The system command which it issues is that which was obtained from the file-parameter file which it read during the previous iteration. During the zeroth iteration of the CMAES_HP optimisation process (when it runs the model on the basis of parameter values supplied in the PEST control file), CMAES_HP does not issue a system command at all. The same applies during the first iteration of the optimisation process if CMAES_HP had been asked not to undertake an initial model run based on parameters cited in the PEST control file.

Because CMAES_HP issues the system command prior to reading the file-parameter file, the user-supplied program which is run using this command has the opportunity to re-write the file-parameter file on the basis of results achieved during previous iterations.

14.1.7 Some Other Implementation Details

Under normal circumstances, PEST_HP and CMAES_HP save parameters that instigate model run failure in a parameter error file. This file has the same filename base as the PEST control file; its extension is "*.per*". CMAES_HP does not record this file when using file-parameters.

As when operating without file parameters, a terminated CMAES_HP run can be re-started using the "/r" switch. When re-started in this way, it re-commences the optimisation process at the beginning of the iteration in which its execution was previously halted. However a re-started CMAES_HP has no recollection of the system command that it may have read from the file-parameter file during the previous iteration. You must therefore ensure that the file-parameter file which CMAES_HP reads during the first iteration of its re-initiated optimisation process is correct for that iteration.

14.2 Secondary Parameters

14.2.1 General

The use of secondary parameters in a PEST control file replaces the need to use PAR2PAR in a model batch or script file that is run by PEST_HP or CMAES_HP.

Secondary parameters are not optimised. Their values are simply calculated, through user-supplied equations, from primary (i.e. normal) parameters. These equations can feature the primary parameters that are cited in a PEST control file (including fixed and tied parameters), file-parameters, and other secondary parameters whose values were previously calculated.

14.2.2 Defining Secondary Parameters

Like file-parameters, a secondary parameter can be defined in a PEST control file anywhere within the "parameter data" section of this file. Figure 14.7 shows an example of the "parameter data" section of a PEST control file in which secondary parameters are defined. If desired, their definitions can be mixed with those of file-parameters within this section.

```
* parameter data
ro1  log factor 1.000000 0.1 100 ro 1 0 1
ro2  log factor 1.000000 0.1 100 ro 1 0 1
ro3  log factor 1.000000 0.1 100 ro 1 0 1
ro4  log factor 1.000000 0.1 100 ro 1 0 1
ro5  log factor 1.000000 0.1 100 ro 1 0 1
ro6  log factor 1.000000 0.1 100 ro 1 0 1
ro7  log factor 1.000000 0.1 100 ro 1 0 1
ro8  log factor 1.000000 0.1 100 ro 1 0 1
ro9  log factor 1.000000 0.1 100 ro 1 0 1
ro10 log factor 1.000000 0.1 100 ro 1 0 1
h1   log factor  0.25  0.05 100 hhh 1 0 1
h2   tied factor  0.50 0.05 100 hhh 1 0 1
h3   tied factor  1.00 0.05 100 hhh 1 0 1
h4   tied factor  2.00 0.05 100 hhh 1 0 1
h5   tied factor  4.00 0.05 100 hhh 1 0 1
h6   tied factor  8.00 0.05 100 hhh 1 0 1
ep1 = ro1+ro2
ep2 = ep1+ep1
h7   tied factor  16.0 0.05 100 hhh 1 0 1
h8   tied factor  32.0 0.05 100 hhh 1 0 1
h9   tied factor  64.0 0.05 100 hhh 1 0 1
h2 h1
h3 h1
ep2 = 2*ep2
h4 h1
h5 h1
h6 h1
h7 h1
h8 h1
h9 h1
```

Figure 14.7 The "parameter data" section of a PEST control file wherein secondary parameters are defined.

Secondary parameters are defined by an equation. Their presence on any line of the "parameter data" section of a PEST control file is recognized by the fact that an "=" symbol follows their name. An equation must follow the "=" symbol. This equation can be of arbitrary complexity; see documentation of PAR2PAR and PLPROC (both of which feature parameter equations) for examples. The right hand side of the equation can feature any primary PEST parameter, file parameter, or previously-defined secondary parameter. As in any programming language, a secondary parameter can appear on both sides of an equation, provided a value has already been calculated for it; its value can thus be updated by the equation.

If desired, the equation through which a secondary parameter is given a value can have a logical outcome and involve logical operators; see "selection equations" in PLPROC. If the outcome of an equation is logical, then a calculated value of TRUE endows the secondary parameter with a value of 1.0, while a calculated value of FALSE endows the secondary parameter with a value of 0.0.

The values calculated for secondary parameters are transferred from the PEST_HP or CMAES_HP manager to its agents at the same time, and in the same manner, as are the values of primary parameters. These values are then transferred to model input files using template files. Hence

template files which are listed in the "model input/output" section of a PEST control file in which secondary parameters are defined should also feature secondary parameters. Note that it is not necessary for all secondary parameters featured in a PEST control file to appear in a template file. Some secondary parameters may thus be used only for intermediate calculations whose ultimate goal is the assignment of a value to another secondary parameter whose value is then written to a model input file.

14.2.3 Number of Secondary Parameters and Equations

PEST_HP and CMAES_HP must be informed of the existence of secondary parameters, and of equations which define them, in the "control data" section of the PEST control file which they read. This information is used to dimension arrays which hold data pertaining to these entities. See figure 14.8.

```
pcf
* control data
restart estimation
10 19 2 10 3 nparsec=2 nequation=3
3 3 single point  1 0 0
etc
```

Figure 14.8 First part of the "control data" section of a PEST control file which features secondary parameters.

On the fourth line of the PEST control file depicted in figure 14.8, the string "nparsec=2" informs PEST_HP or CMAES_HP that there are 2 secondary parameters. The string "nequations=3" informs PEST_HP or CMAES_HP that there are 3 equations. (A space can precede or follow the "=" symbol in each case.) As is obvious from the above discussion, the existence of secondary parameters implies the existence of equations, and vice versa. Also, the number of equations must equal or exceed the number of secondary parameters. It is important to note that (as for file-parameters) the NPAR variable (first variable featured on the fourth line of the PEST control file) must refer only to the number of primary PEST parameters. Note also that, as well as featuring the NPARSEC and NEQUATION control variables, the fourth line of a PEST control file may also feature the NPARFILE and FILEPARFILE variables. However, at the time of writing, only CMAES_HP (and not PEST_HP) can employ file-parameters.

The following should also be noted.

- PEST_HP will cease execution with an appropriate error message if secondary parameters are defined in a PEST control file that asks it to undertake SVD-assisted inversion.
- Prior information equations cannot cite secondary parameters.
- The values of secondary parameters are not listed in parameter value files recorded by PEST_HP in which progressively optimised values of primary parameters are recorded. As secondary parameters are not optimised, but are functions of primary parameters, there is no need to record their values in these files.
- The values of secondary parameters associated with optimised primary parameters are listed at the end of the PEST_HP and CMAES_HP run record files. However CMAES_HP does not record their values if any file-parameters are also defined in the PEST control file on which it operates. Omission of the values of secondary parameters under these circumstances makes allowance for the fact that the value of a secondary parameter may depend on that of a file-parameter; if this is the case, then it can have no optimised value.

(For efficiency reasons, CMAES_HP does not keep track of whether a secondary parameter does, indeed, depend on a file-parameter; it just assumes the worst.)

- A primary parameter cannot appear on the left side of an equation.

14.2.4 Operation of PEST_HP and CMAES_HP with Secondary Parameters

Outwardly, the operation of PEST_HP and CMAES_HP when using secondary parameters is no different from its operation without them. The values of secondary parameters are calculated by the run manager prior to these values being transferred to run agents for transfer to model input files. If any problems are encountered in parsing the equation through which a secondary parameter is assigned its value, or with calculating the value of a secondary parameter, an error message is recorded and PEST_HP/CMAES_HP ceases execution.

The following features of PEST_HP/CMAES_HP operations when using secondary parameters should be noted, however.

- If PEST_HP is run with the "/f" switch, it will accept secondary parameters in the PEST control file. However it does not record the values of secondary parameters in the run results file. (As stated above, even though these are featured in the PEST control file, they are not adjustable; hence they can be considered to be the outcome of intermediate calculations undertaken by the model.)
- Only PEST_HP, but not PEST, can parse and evaluate equations. Therefore PEST cannot be used to write a hp starter file for the use of PEST_HP if a PEST control file features secondary parameters.

15. Compatibility Issues

15.1 General

As has already been discussed, a control file for PEST_HP can cite a number of control variables that are not useable by standard versions of PEST. These are:

- RUN_ABANDON_FAC,
- WIN_MRUN_HOURS,
- SOFTSTOPHOURS and HARDSTOPHOURS,
- RRFSAVE,
- ZEROSENVAL,
- alternative LSQR control settings,
- UPTESTMIN and UPTESTLIM,
- ORR_NOT_FIRST,
- REG2MEASRAT,
- JCOWARNTHRESH and JCOZEROTHRESH.

A PEST_HP control file can also site secondary parameters and file parameters.

The free version of PEST is accompanied by a suite of utility programs that implement pre- and post-processing functionality of various types. Many of them read a PEST control file. At the time of writing, not all of these utility programs have been altered to recognize new variables and parameter types that are supported by PEST_HP and CMAES_HP. Hence, if some of them are asked to read a PEST control file that contains variables and parameter types that are specific to PEST_HP, they may complain that the PEST control file contains an error, and/or that it should be checked with PESTCHEK. Some may offer a more obscure error message.

Eventually, all PEST-support programs will be altered to accommodate the presence of HP-specific variables and parameter types in a PEST control file. For the moment, however, use of utilities which do not accept these variables and parameter types requires that these variables and parameter types be removed from the PEST control file before these utilities are run. This can be accomplished automatically using the PSTCLEAN utility that is supplied with the PEST suite.

PEST-support utilities that have, at the time of writing, been modified to recognize HP-specific variables, and take appropriate action, include the following.

- Linear analysis utilities such as IDENTPAR and members of the PREDVAR* and PREDUNC* suites can happily read a PEST_HP control file. Where file-parameters and/or secondary parameters appear in a PEST control file that is read by these programs, they are ignored. Calculation of parameter and predictive error and uncertainty variance is based only on normal PEST parameters and the sensitivities of model outputs to these parameters as recorded in a JCO file.
- The GENLINPRED program that runs many of these uncertainty and error analysis utilities can also accommodate a PEST_HP control file.

- PARREP reads a parameter value file and a PEST_HP control file. It creates a new PEST_HP control file in which the initial values of parameters are replaced by those recorded in the parameter value file. Lines in an existing PEST_HP control file which define secondary parameters and file-parameters are transferred directly to the new PEST_HP control file which PARREP writes.
- SVDAPREP will transfer the values of HP-specific control variables to the super parameter PEST_HP control file which it creates. However it will not write a super parameter PEST_HP control file if the base parameter PEST_HP control file features secondary parameters or file-parameters. Instead, it will cease execution with an appropriate error message. (It would make no sense to base secondary parameters on super parameters in a PEST_HP control file. At the time of writing, file-parameters can only be used with CMAES_HP, and are therefore of limited use in a super-parameter PEST_HP control file.)
- The RANDPAR and RANDPAR1 utilities can read a PEST_HP control file that contains any of the HP-specific functionality discussed above. They can write a sequence of parameter value files which contain random values of primary (i.e. normal) PEST parameters that are featured in the control file. These utilities do not generate random values for secondary parameters or file-parameters; hence neither of these parameter types are included in parameter value files that are written by RANDPAR and RANDPAR1.
- JCO2JCO reads a PEST_HP control file and corresponding Jacobian matrix file. It can record a JCO file corresponding to another PEST_HP control file, notwithstanding the fact that either or both of these PEST_HP control files may contain HP-specific control variables and/or file/secondary parameters. Of course, a JCO file does not record sensitivities of model outputs to file/secondary parameters.
- JCOCHEK can check for compatibility between a PEST_HP control file and a JCO file, notwithstanding the presence of HP-specific control variables and/or file/secondary parameters in the PEST_HP control file.
- RRFCALCPSI can evaluate objective functions from parameter and model output values recorded in a run results file, regardless of the presence or otherwise of file/secondary parameters in the PEST_HP control file which it reads.
- ADDREG1 and SUBREG1 can add/subtract regularisation to/from a PEST control file containing HP-specific control variables and/or file/secondary parameters.
- WTFACTOR can also accommodate the new PEST control file protocol.
- PESTCHEK can read and check the contents of a PEST_HP input dataset. This dataset can include HP-specific control variables, secondary parameters and file-parameters. PESTCHEK issues a warning message where it encounters functionality which is specific only to PEST_HP.
- PEST and BEOPEST can read a PEST control file which features variables and parameters that are specific to PEST_HP. They will then cease execution with an appropriate error message, drawing the user's attention to functionality that they are incapable of supporting. If PEST is started with the "/hpstart" switch, however, it will not complain about the presence of HP-specific control variables in a PEST control file; instead it will undertake a single model run and record a hp starter file. It will not do this, however, if a PEST control file features secondary parameters or file-parameters, for it has not been programmed to process these types of parameters. Instead it ceases execution with an appropriate message.

15.2 The PSTCLEAN Utility

The PSTCLEAN utility is a member of the PEST suite. Hence it is downloadable with the free version of PEST. It reads a PEST control file which can serve as a suitable input file for PEST_HP. It writes a new PEST control file from which all PEST_HP-specific variables have been removed. The new PEST control file is readable by all PEST utility software.

As is explained in Part II of the PEST manual, PSTCLEAN also removes variables which are specific to PEST++, as well as comments, from a PEST control file. PEST++ variables are placed on lines that begin with the "++" string. Comments can be placed on any line of a PEST control file, following a "#" character. PEST_HP tolerates both of these; hence there is no need to remove "++" lines or comments from a PEST control file before using PEST_HP.

16. References

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Appendix 1: New Control Variables Illustrated

Figure A1.1 shows the "control data" section of a PEST control file wherein values are specified for the UPTESTMIN, UPTESTLIM, RUN_SLOW_FAC, RUN_ABANDON_FAC, WIN_MRUN_HOURS, SOFTSTOPHOURS, ZEROSENVAL, JCOWARNTHRESH and JCOZEROTHRESH variables. All of these variables are optional; hence they can be omitted from a PEST_HP control file if desired. As has been discussed, a value cannot be supplied for both of SOFTSTOPHOURS and HARDSTOPHOURS in the same PEST control file. The protocol for supplying a value for HARDSTOPHOURS is identical to that for SOFTSTOPHOURS; simply replace the "softstophours" string with "hardstophours" in the example below.

Use of the OBSREREF, ORR_NOT_FIRST and RRFSAVE variables is also demonstrated in figure A1.1.

```
* control data
restart regularisation
19 19 2 10 3
2 3 single point 1 0 0 obsreref orr_not_first
.1 2 0.3 0.03 3 3 uptestmin=10 uptestlim=50 derforgive run_slow_fac=2.5 run_abandon_fac=5.0 win_mrun_hours=0.5
2 3 0.001 0
0.5  zerosenval=-1.11E29 jcowarnthresh=1.0e20 jcozerothresh=1.0e30
30 0.01 3 3 0.01 3 softstophours=24.0
1 1 1 rrfsave
```

Figure A1.1 Example of the "control data" section of a PEST_HP control file.