Appendix 1. Basic PEST Input

Structure of the PEST Control File

This appendix supplies a short description of all PEST variables. First, a list of all of these variables is provided, with each located in its proper place within the PEST Control File (variables enclosed in brackets are optional). This listing is followed by a series of tables that describe the role of each variable.

```
pcf
* control data
RSTFLE PESTMODE
NPAR NOBS NPARGP NPRIOR NOBSGP [MAXCOMPDIM]
NTPLFLE NINSFLE PRECIS DPOINT [NUMCOM] [JACFILE] [MESSFILE]
RLAMBDA1 RLAMFAC PHIRATSUF PHIREDLAM NUMLAM [JACUPDATE]
RELPARMAX FACPARMAX FACORIG [IBOUNDSTICK UPVECBEND]
PHIREDSWH [NOPTSWITCH] [SPLITSWH] [DOAUI] [DOSENREUSE]
NOPTMAX PHIREDSTP NPHISTP NPHINORED RELPARSTP NRELPAR [PHISTOPTHRESH] [LASTRUN] [PHIABANDON]
ICOV ICOR IEIG [IRES] [JCOSAVEITN] [REISAVEITN]
* automatic user intervention
MAXAUI AUISTARTOPT NOAUIPHIRAT AUIRESTITN
AUISENSRAT AUIHOLDMAXCHG AUINUMFREE
AUIPHIRATSUF AUIPHIRATACCEPT NAUINOACCEPT
* singular value decomposition
SVDMODE
MAXSING EIGTHRESH
EIGWRITE
* lsqr
LSQRMODE
LSQR_ATOL LSQR_BTOL LSQR_CONLIM LSQR_ITNLIM
LSQRWRITE
* svd assist
BASEPESTFILE
BASEJACFILE
SVDA_MULBPA SVDA_SCALADJ SVDA_EXTSUPER SVDA_SUPDERCALC
* sensitivity reuse
SENRELTHRESH  SENMAXREUSE
SENALLCALCINT  SENPREDWEIGHT  SENPIEXCLUDE
* parameter groups
PARGPNME INCTYP DERINC DERINCLB FORCEN DERINCMUL DERMTHD [SPLITTHRESH SPLITRELDIFF SPLITACTION]
(one such line for each of NPARGP parameter groups)
* parameter data
PARNME PARTRANS PARCHGLIM PARVAL1 PARLBND PARUBND PARGP SCALE OFFSET DERCOM
(one such line for each of NPAR parameters)
PARNME PARTIED
(one such line for each tied parameter)
* observation groups
OBGNME [GTARG] [COVFLE]
(one such line for each of NOBSGP observation group)
* observation data
OBSNME OBSVAL WEIGHT OBGNME
(one such line for each of NOBS observations)
* derivatives command line
DERCOMLINE
EXTDERFLE
```

```
* model command line
COMLINE
(one such line for each of NUMCOM command lines)
* model input/output
TEMPFLE INFLE
(one such line for each of NTPLFLE template files)
INSFLE OUTFLE
(one such line for each of NINSLFE instruction files)
* prior information
PILBL PIFAC * PARNME + PIFAC * log(PARNME) ... = PIVAL WEIGHT OBGNME
(one such line for each of NPRIOR articles of prior information)
* predictive analysis
NPREDMAXMIN [PREDNOISE]
PDO PD1 PD2
ABSPREDLAM RELPREDLAM INITSCHFAC MULSCHFAC NSEARCH
ABSPREDSWH RELPREDSWH
NPREDNORED ABSPREDSTP RELPREDSTP NPREDSTP
* regularisation
PHIMLIM PHIMACCEPT [FRACPHIM] [MEMSAVE]
WFINIT  WFMIN  WFMAX  [LINREG] [REGCONTINUE]
WFFAC  WFTOL IREGADJ [NOPTREGADJ REGWEIGHTRAT [REGSINGTHRESH]]
```

Figure 1–1. Structure of the PEST Control File.

The following tables include a column labelled "usage," which contains an index whose value is between 1 and 3. An index value of 3 indicates that the variable is likely to vary in value from PEST Control File to PEST Control File, this reflecting either the different nature of different parameter estimation problems, or the fact that, as a control variable, it is one that often requires "tuning" to a particular calibration problem. On the other hand, a usage index value of 1 indicates that the variable rarely requires alteration from the value suggested in PEST documentation. A usage value of 2 indicates potential variability that is between these two extremes

Variables in the "control data" section of the PEST Control File.

Variable	Type	Values	Usage	Description
RSTFLE	text	"restart" or "norestart"	1	Instructs PEST whether to write restart data.
PESTMODE	text	"estimation," "prediction," "regularization"	3	PEST's mode of operation.
NPAR	integer	greater than 0	3	Number of parameters.
NOBS	integer	greater than 0	3	Number of observations.
NPARGP	integer	greater than 0	3	Number of parameter groups.
NPRIOR	integer	0 or greater	3	Number of prior-information equations.
NOBSGP	integer	greater than 0	3	Number of observation groups.
MAXCOMPDIM	integer	optional; 0 or greater	1	Number of elements in compressed Jacobian matrix.
NTPLFLE	integer	greater than 0	3	Number of template files.
NINSFLE	integer	greater than 0	3	Number of instruction files.
PRECIS	text	"single" or "double"	1	Format for writing parameter values to model input files.
DPOINT	text	"point" or "nopoint"	1	Omit decimal point in parameter values if possible.
NUMCOM	integer	optional; greater than 0	1	Number of command lines used to run model.
JACFILE	integer	optional; 0 or 1	1	Indicates whether model provides external derivatives file.
MESSFILE	integer	optional; 0 or 1	1	Indicates whether PEST should write PEST-to-model message file.

Variables in the "control data" section of the PEST Control File.—Continued

Variable	Type	Values	Usage	Description
RLAMBDA1	real	0 or greater	2	Initial Marquardt Lambda.
RLAMFAC	real	positive or negative, but not 0	2	Dictates Marquardt Lambda adjustment process.
PHIRATSUF	real	between 0 and 1	1	Fractional objective function sufficient for end of current iteration.
PHIREDLAM	real	between 0 and 1	1	Termination criterion for Marquardt Lambda search.
NUMLAM	integer	1 or greater	2	Maximum number of Marquardt Lambdas to test.
JACUPDATE	integer	optional; 0 or greater	2	Activation of Broyden's Jacobian update procedure.
RELPARMAX	real	greater than 0	2	Parameter relative change limit.
FACPARMAX	real	greater than 1	2	Parameter factor change limit.
IBOUNDSTICK	integer	optional; 0 or greater	1	Instructs PEST not to compute derivatives for parameter at its bounds.
UPVECBEND	integer	optional; 0 or 1	1	Instructs PEST to bend parameter upgrade vector if parameter hits its bounds.
PHIREDSWH	real	between 0 and 1	1	Sets objective function change for introduction of central derivatives.
NOPTSWITCH	integer	optional; 1 or greater	1	Iteration before which PEST will not switch to central derivatives computation.
SPLITSWH	real	optional; 0 or greater	1	The factor by which the objective function rises to invoke split slope derivatives analysis until end of run.
DOAUI	text	"aui," "auid," or "noaui"	2	Instructs PEST to implement automatic user intervention.
DOSENREUSE	text	"senreuse" or "nosenreuse"	1	Instructs PEST to reuse parameter sensitivities
NOPTMAX	integer	−2, −1, 0, or any number greater than 0	3	Number of optimization iterations.
PHIREDSTP	real	greater than 0	2	Relative objective function reduction triggering termination.
NPHISTP	integer	greater than 0	2	Number of successive iterations over which PHIREDSTP applies.
NPHINORED	integer	greater than 0	2	Number of iterations since last drop in objective function to trigger termination.
RELPARSTP	real	greater than 0	2	Maximum relative parameter change triggering termination.
NRELPAR	integer	greater than 0	2	Number of successive iterations over which RELPARSTP applies.
PHISTOPTHRESH	real	optional; 0 or greater	1	Objective function threshold triggering termination.
LASTRUN	integer	optional; 0 or 1	1	Instructs PEST to undertake (or not) final model run with best parameters.
PHIABANDON	real or text	optional	1	Objective function value at which to abandon optimization process or filename containing abandonment schedule.
ICOV	integer	0 or 1	1	Record covariance matrix in matrix file.
ICOR	integer	0 or 1	1	Record correlation-coefficient matrix in matrix file
IEIG	integer	0 or 1	1	Record eigenvectors in matrix file.
IRES	integer	0 or 1	1	Record resolution data.
JCOSAVEITN	text	"jcosaveitn" or "nojcosaveitn"	1	Write current Jacobian matrix to iteration-specific *.jco file at the end of every optimization iteration.
REISAVEITN	text	"reisaveitn" or "noreisaveitn"	1	Store best-fit residuals to iteration-specific residuals file at end of every optimization iteration.

Variables in the optional "automatic user intervention" section of the PEST Control File.

Variable	Type	Values	Usage	Description
MAXAUI	integer	0 or greater	1	Maximum number of AUI iterations per optimization iteration.
AUISTARTOPT	integer	1 or greater	1	Optimization iteration at which to begin AUI.
NOAUIPHIRAT	real	between 0 and 1	1	Relative objective function reduction threshold triggering AUI.
AUIRESTITN	integer	0 or greater, but not 1	1	AUI rest interval expressed in optimization iterations.
AUISENSRAT	real	greater than 1	1	Composite parameter sensitivity ratio triggering AUI.
AUIHOLDMAXCHG	integer	0 or 1	1	Instructs PEST to target parameters that change most when deciding which parameters to hold.
AUINUMFREE	integer	greater than 0	1	Cease AUI when only AUINUMFREE parameters are unheld.
AUIPHIRATSUF	real	between 0 and 1	1	Relative objective function improvement for termination of AUI.
AUIPHIRATACCEPT	real	between 0 and 1	1	Relative objective function reduction threshold for acceptance of AUI-calculated parameters.
NAUINOACCEPT	integer	greater than 0	1	Number of iterations since acceptance of parameter change for termination of AUI.

Variables in the optional "singular value decomposition" section of the PEST Control File.

Variable	Type	Values	Usage	Description
SVDMODE	integer	0 or 1	3	Activates truncated singular value decomposition for solution of inverse problem.
MAXSING	integer	greater than 0	3	Number of singular values at which truncation occurs.
EIGTHRESH	real	0 or greater, but less than 1	2	Eigenvalue ratio threshold for truncation.
EIGWRITE	integer	0 or 1	1	Determines content of SVD output file.

Variables in the optional "LSQR" section of the PEST Control File.

Variable	Type	Values	Usage	Description
LSQRMODE	integer	0 or 1	1	Activates LSQR solution of inverse problem.
LSQR_ATOL	real	0 or greater	1	LSQR algorithm atol variable.
LSQR_BTOL	real	0 or greater	1	LSQR algorithm btol variable.
LSQR_CONLIM	real	0 or greater	1	LSQR algorithm conlim variable.
LSQR_ITNLIM	integer	greater than 0	1	LSQR algorithm itnlim variable.
LSQR_WRITE	integer	0 or 1	1	Instructs PEST to write LSQR file.

Variables in the optional "SVD-Assist" section of the PEST Control File.

Variable	Type	Values	Usage	Description
BASEPESTFILE	text	a filename	3	Name of base PEST Control File.
BASEJACFILE	text	a filename	3	Name of base PEST Jacobian matrix file.
SVDA_MULBPA	integer	0 or 1	2	Instructs PEST to record multiple BPA files.
SVDA_SCALADJ	integer	-4 to 4	1	Sets type of parameter scaling undertaken in superparameter definition.
SVDA_EXTSUPER	integer	0, 1, 2, -2, 3	1	Sets means by which superparameters are calculated.
SVDA_SUPDERCALC	integer	0 or 1	1	Instructs PEST to compute superparameter sensitivities from base parameter sensitivities.

Variables in the optional "sensitivity reuse" section of the PEST Control File.

Variable	Type	Values	Usage	Description
SENRELTHRESH	real	0 to 1	1	Relative parameter sensitivity below which sensitivity reuse is activated for a parameter.
SENMAXREUSE	integer	integer other than 0	1	Maximum number of reused sensitivities per iteration.
SENALLCALCINT	integer	greater than 1	1	Iteration interval at which all sensitivities recalculated.
SENPREDWEIGHT	real	any number	1	Weight to assign to prediction in computation of composite parameter sensitivities to determine sensitivity reuse.
SENPIEXCLUDE	test	"yes" or "no"	1	Include or exclude prior information when computing composite parameter sensitivities to determine sensitivity re-use.

Variables required for each parameter group in the "parameter groups" section of the PEST Control File.

Variable	Type	Values	Usage	Description
PARGPNME	text	12 characters or less	3	Parameter group name
INCTYP	text	"relative," "absolute," "rel_to_max"	2	Method by which parameter increments are calculated.
DERINC	real	greater than 0	2	Absolute or relative parameter increment.
DERINCLB	real	0 or greater	3	Absolute lower bound of relative parameter increment.
FORCEN	text	"switch," "always_2," "always_3"	1	Determines whether central derivatives calculation is done.
DERINCMUL	real	greater than 0	1	Derivative increment multiplier when undertaking central derivatives calculation.
DERMTHD	text	"parabolic," "outside_pts," "best_fit"	1	Method of central derivatives calculation.
SPLITTHRESH	real	greater than 0 (or 0 to deactivate)	1	Slope threshold for split slope analysis.
SPLITRELDIFF	real	greater than 0	1	Relative slope difference threshold for action.
SPLITACTION	text	text	1	"smaller," "0" or "previous."

Variables required for each parameter in the "parameter data" section of the PEST Control File.

Variable	Type	Values	Usage	Description
PARNME	text	12 characters or less	3	Parameter name.
PARTRANS	text	"log," "none," "fixed," "tied"	3	Parameter transformation.
PARCHGLIM	text	"relative" or "factor"	3	Type of parameter change limit.
PARVAL1	real	any real number	3	Initial parameter value.
PARLBND	real	less than or equal to PARVAL1	3	Parameter lower bound.
PARUBND	real	greater than or equal to PARVAL1	3	Parameter upper bound.
PARGP	text	12 characters or less	3	Parameter group name.
SCALE	real	any number other than 0	2	Multiplication factor for parameter.
OFFSET	real	any number	2	Number to add to parameter.
DERCOM	integer	0 or greater	1	Model command line used in computing parameter increments.
PARTIED	text	12 characters or less	3	The name of the parameter to which another parameter is tied.

Variables required for each observation group in the "observation groups" section of the PEST Control File.

Variable	Type	Values	Usage	Description
OBGNME	text	12 characters or less	3	Observation group name.
GTARG	real	positive	1	Group-specific target measurement objective function.
COVFILE	text	a filename	2	Optional covariance matrix file associated with group.

Variables required for each observation in the "observation data" section of the PEST Control File.

Variable	Type	Values	Usage	Description
OBSNME	text	20 characters or less	3	Observation name.
OBSVAL	real	any number	3	Measured value of observation.
WEIGHT	real	0 or greater	3	Observation weight.
OBGNME	text	12 characters or less	3	Observation group to which observation assigned.

Variables in the optional "derivatives command line" section of the PEST Control File.

Variable	Type	Values	Usage	Description
DERCOMLINE	text	system command	1	Command to run model for derivatives calculation.
EXTDERFLE	text	a filename	1	Name of external derivatives file.

Variables in the "model command line" section of the PEST Control File.

Variable	Type	Values	Usage	Description
COMLINE	text	system command	3	Command to run model.

Variables in the "model input/output" section of the PEST Control File.

Variable	Type	Values	Usage	Description
TEMPFLE	text	a filename	3	Template file.
INFLE	text	a filename	3	Model input file.
INSFLE	text	a filename	3	Instruction file.
OUTFLE	text	a filename	3	Model output file.

Variables in the "prior information" section of the PEST Control File..

Variable	Type	Values	Usage	Description
PILBL	text	20 characters or less	3	Name of prior-information equation.
PIFAC	text	real number other than 0	3	Parameter value factor.
PARNME	text	12 characters or less	3	Parameter name.
PIVAL	real	any number	3	"Observed value" of prior information.
WEIGHT	real	0 or greater	3	Prior-information weight.
OBGNME	text	12 characters or less	3	Observation group name.

Variables in the optional "predictive analysis" section of the PEST Control File.

Variable	Type	Values	Usage	Description
NPREDMAXMIN	integer	−1 or 1	3	Maximize or minimize prediction.
PREDNOISE	integer	0 or 1	2	Instructs PEST to include predictive noise in prediction.
PD0	real	greater than 0	3	Target objective function.
PD1	real	greater than PD0	3	Acceptable objective function.
PD2	real	greater than PD1	3	Objective function at which Marquardt Lambda testing procedure is altered as prediction is maximized/minimized.
ABSPREDLAM	real	0 or greater	2	Absolute prediction change to terminate Marquardt Lambda testing.
RELPREDLAM	real	0 or greater	2	Relative prediction change to terminate Marquardt Lambda testing.
INITSCHFAC	real	greater than 0	2	Initial line search factor.
MULSCHFAC	real	greater than 1	2	Factor by which line search factors are increased along line.
NSEARCH	integer	greater than 0	2	Maximum number of model runs in line search.
ABSPREDSWH	real	0 or greater	1	Absolute prediction change at which to use central derivatives calculation.
RELPREDSWH	real	0 or greater	1	Relative prediction change at which to use central derivatives calculation.
NPREDNORED	integer	1 or greater	1	Iterations since prediction raised/lowered at which termination is triggered.
ABSPREDSTP	real	0 or greater	1	Absolute prediction change at which to trigger termination.
RELPREDSTP	real	0 or greater	1	Relative prediction change at which to trigger termination.
NPREDSTP	integer	2 or greater	1	Number of iterations over which ABSPREDSTP and RELPREDSTP apply.

Variables in the optional "regularization" section of the PEST Control File.

Variable	Type	Values	Usage	Description
PHIMLIM	real	greater than 0	3	Target measurement objective function.
PHIMACCEPT	real	greater than PHIMLIM	3	Acceptable measurement objective function.
FRACPHIM	real	optional; 0 or greater, but less than 1	2	Set target measurement objective function at this fraction of current measurement objective function.
MEMSAVE	text	"memsave" or "nomemsave"	1	Activate conservation of memory at cost of execution speed and quantity of model output.
WFINIT	real	greater than 0	1	Initial regularization weight factor.
WFMIN	real	greater than 0	1	Minimum regularization weight factor.
WFMAX	real	greater than WFMIN	1	Maximum regularization weight factor.
LINREG	text	"linreg" or "nonlinreg"	1	Informs PEST that all regularization constraints are linear.
REGCONTINUE	text	"continue" or "nocontinue"	2	Instructs PEST to continue minimizing regularization objective function even if measurement objective function less than PHIMLIM.
WFFAC	real	greater than 1	1	Regularization weight factor adjustment factor.
WFTOL	real	greater than 0	1	Convergence criterion for regularization weight factor.
IREGADJ	integer	0, 1, 2, 3, 4 or 5	2	Instructs PEST to perform interregularization group weight factor adjustment, or to compute new relative weights for regularization observations and prior-information equations.
NOPTREGADJ	integer	1 or greater	2	The optimization iteration interval for re-calculation of regularization weights if IREGADJ is 4 or 5.
REGWEIGHTRAT	real	absolute value of 1 or greater	2	The ratio of highest to lowest regularization weight; spread is logarithmic with null space projection if set negative.
REGSINGTHRESH	real	less than 1 and greater than 0	1	Singular value of $\mathbf{X}^T\mathbf{Q}\mathbf{X}$ (as factor of highest singular value) at which use of higher regularization weights begins if IREGADJ is set to 5.

Files used by PEST

The following tables list files that are read and written by PEST. Many of these possess the same filename base as the PEST Control File, this being designated as case in the tables below.

Files read by PEST.

File name	File type	Purpose
case.pst	PEST Control File	Provides problem dimensions, names of files for communication with a model, and values for all PEST control variables.
Arbitrary, commonly *.tpl	Template file	Provides means through which PEST writes current parameter values to a model input file.
Arbitrary, commonly *.ins	Instruction file	Provides means through which PEST reads outputs of interest from model output files.
case.rmf	Run management file	Provides Parallel PEST with information needed to communicate with slaves.
case.hld	Parameter hold file	Supplies details of manual intervention when holding individual parameters, or groups of parameters, at current values.

Files written by PEST.

File name	File type	Purpose
case.rec	Run record file	Contains details of progress of parameter-estimation process.
case.cnd	Condition number file	Contains continuous record of inverse-problem condition numbers.
case.mtt	Matrix file	Contains interim covariance, correlation coefficient, and eigenvector matrices.
case.sen	Parameter sensitivity file	Contains continuous record of composite parameter sensitivities.
case.seo	Observation sensitivity file	Records composite observation sensitivities.
case.res	Residuals file	Contains residuals and associated information recorded in tabular format.
case.rei	Interim residuals file	Contains residuals and associated information recorded in tabular format. This file is rewritten during every optimization iteration.
pest.mmf	Message file	Optionally recorded by PEST before every model run, contains the reason for carrying out the run and the parameter values that it employs.
case.svd	SVD file	Written only if PEST employs truncated SVD for solution of inverse problem; contains eigenvalues and, optionally, eigenvectors of $\mathbf{X}^T\mathbf{Q}\mathbf{X}$ matrix.
case.lsq	LSQR file	Records information written by LSQR solver.
case.jco	Jacobian matrix file	Binary file containing Jacobian matrix pertaining to best parameters achieved so far.
case.par	Parameter value file	Records best parameter values achieved so far in parameter-estimation process.
basecase.bpa	Best parameter file	Contains best base parameters achieved so far; the filename base is the same as that of the base PEST Control File.
case.rsd	Resolution data file	Binary file written by PEST whenever it does any kind of regularized inversion. It contains data from which the resolution and "G" matrices can be computed by the RESPROC utility.
case.rst, *case*.jac, *case*.jst	Restart files	Contain information (written in binary form) that PEST uses in restarting a previously incomplete PEST run.
case.rmr	Run management record file	Lists history of communications between Parallel PEST and its slaves.
pest.rdy, param.rdy, observ.rdy pslave.fin p###.###	Semaphore files	Used by Parallel PEST to communicate with its slaves.