PEST++ ver. 3.0.0_rc2

The PEST++ Command Line

PEST++ has a number of different command line options which are used to specify how to start a run using one of the supported run managers. Large problems (defined as having many parameters and/or observations) often require parallel computing. PEST++ relies on run mangers to complete the forward model runs and the current version provides the following four options: 1) **Y**et **A**nother Run **M**anage**R** (**YAMR**), 2) GENIE and 3) serial run manager 4) External run manager. YAMR and GENIE are sophisticated and capable of performing parallel runs on a single machine or over a TCP/IP-enabled network. YAMR duplicates the functionality of BEOPEST and is fully integrated in PEST++. Like BEOPEST, PEST++ can run as either a master or a compute node under the YAMR run manager. While PEST++ provides an interface to the GENIE run manager, this interface relies on the external GMAN and GSLAVE programs to manage and perform the actual model runs. The serial rule manager provides a simple alternative that duplicates the functionality currently in regular PEST. The external run manager was developed to terminate PEST++ execution when it comes time to make the forward model runs. It is designed to allow the user can take control over the process of making the forward model runs. The command lines required to start PEST++ are summarized in the following table where /j and /r are optional commands; /j to invokes jacobian reuse for the first iteration and /r invokes restart.

Run Manger / Mode	**Command**
Serial Run Manager / Master	pest++ control_file.pst [/j] [/r]
YAMR / Master	pest++ control_file.pst /H :port [/j] [/r]

YAMR / Compute Node	pest++ /H hostname:port
Genie / Master	pest++ control_file.pst /G hostname:port [/j] [/r]
External Run Manager	pest++ control_file.pst /E [/j] [/r]

When PEST++ is run in the serial or master mode it now supports the /j option to reuse an existing jacobian file rather than computing the jacobian for the first iteration. The functionality of this feature is identical to that in PEST. In fact PEST++ is compatible with jacobians computed by PEST as long as the PEST++ AUTONORM option is not used in the control file.

The PEST++ Control File

For ease of reference, variables within the PEST control file are listed below, and the variables used by PEST++ are highlighted. PEST++ relies on the structure of the input file to deduce the algorithmic parameters and read only those algorithmic parameters that are absolutely necessary. For example, there is no need to read the NOBS variable because each line in the "observation data" section of the control file specifies an observation; however, it is necessary to read the NPAR variable to know where specification of parameters ends and information on tied parameters begins. This list is followed by short explanation of each variable used by PEST++.

```
pcf
* control data
RSTFLE PESTMODE
NPAR NOBS NPARGP NPRIOR NOBSGP [MAXCOMPDIM]
NTPLFLE NINSFLE PRECIS DPOINT [NUMCOM JACFILE MESSFILE]
RLAMBDA1 RLAMFAC PHIRATSUF PHIREDLAM NUMLAM [JACUPDATE] [LAMFORGIVE]
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RELPARMAX FACPAR MAXFACORIG [IBOUNDSTICK UPVECBEND] [ABSPARMAX]

PHIREDSWH [NOPTSWITCH] [SPLITSWH] [DOAUI] [DOSENREUSE]

NOPTMAX PHIREDSTP NPHISTP NPHINORED RELPARSTP NRELPAR [PHISTOPTHRESH] [LASTRUN] [PHIABANDON]

ICOV ICOR IEIG [IRES] [JCOSAVE] [VERBOSEREC] [JCOSAVEITN] [REISAVEITN] [PARSAVEITN]

* 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 SVDA_PAR_EXCL

* 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]

PD0 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]]

* pareto

PARETO_OBSGROUP

PARETO_WTFAC_START PARETO_WTFAC_FIN NUM_WTFAC_INC

NUM_ITER_START NUM_ITER_GEN NUM_ITER_FIN

ALT_TERM

OBS_TERM ABOVE_OR_BELOW OBS_THRESH NUM_ITER_THRESH (*only if ALT_TERM is non-zero*)

NOBS_REPORT

OBS_REPORT_1 OBS_REPORT_2 OBS_REPORT_3..(*NOBS_REPORT items*)

++# This line is a comment as are all lines that begin with "++#"

++# PEST++ input is parsed using key words that can be specified in any order

++ MAX_N_SUPER(max_super) SUPER_EIGTHRES(eig_thres)

++ N_ITER_BASE(base_iter) N_ITER_SUPER(super_iter)

++ SVD_PACK(PROPACK)

++ AUTO_NORM(4)

MAX_SUPER_FRZ_ITER(max_frz_iter)

MAX_REG_ITER(max_reg_iter)

MAT_INV(inv_type)

SUPER_RELPARMAX(sup_relpar_max)

MAX_RUN_FAIL(max_fail)

LAMBDAS(lambda list)

ITERATION_SUMMARY(TRUE)

DER_FORGIVE(TRUE)

Variables in "control data" section of PEST control file.

Variable	Type	Values	Description
RSTFLE	Text	"restart" or "norestart"	Instructs PEST whether to write restart data.
PESTMODE	Text	"estimation", "prediction", "regularisation", "pareto"	PEST's mode of operation.
NPAR	Integer	greater than 0	Number of parameters.
NUMCOM	Integer	optional; greater than zero	Number of command lines used to run model.
RELPARMAX	Real	greater than 0	Parameter relative change limit.
FACPARMAX	Real	greater than 1	Parameter factor change limit.
FACORIG	Real	between 0 and 1	Minimum fraction of original parameter value in evaluating relative change.
PHIREDSWH	Real	between 0and 1	Sets objective function change for introduction of central derivatives.
NOPTMAX	Integer	−2, −1, 0, or any number greater than 0	Number of optimization iterations.

PHIREDSTP	Real	greater than 0	Relative objective function reduction triggering termination.
NPHISTP	Integer	greater than 0	Number of successive iterations over which PHIREDSTP applies.
NPHINORED	Integer	greater than 0	Number of iterations since last drop in objective function to trigger termination.
RELPARSTP	Real	greater than 0	Maximum relative parameter change triggering termination.
NRELPAR	Integer	greater than 0	Number of successive iterations over which RELPARSTP applies.

Variables in optional "singular value decomposition" section of PEST control file.

Variable	Type	Values	Description
MAXSING	Integer	greater than 0	Number of singular values at which truncation occurs.
EIGTHRESH	Real	0or greater, but less than 1	Eigenvalue ratio threshold for truncation.
EIGWRITE	Integer	0or 1	Determines content of SVD output file.

Variables required for each parameter group in "parameter groups" section of PEST control file.

Variable	Type	Values	Description
PARGPNME	Text	12 characters or less	Parameter group name.
INCTYP	Text	"relative", "absolute", "rel_to_max"	Method by which parameter increments are calculated.
DERINC	Real	greater than 0	Absolute or relative parameter increment.
DERINCLB	Real	0or greater	Absolute lower bound of relative parameter increment.
FORCEN	Text	"switch", "always_2", "always_3", "switch_5", "always_5"	Determines whether central derivatives calculation is undertaken and whether three points or four points are employed in central derivatives calculation.
DERINCMUL	Real	greater than 0	Derivative increment multiplier when undertaking central derivatives calculation.

DERMTHD	Text	"parabolic", "outside_pts", "best_fit", "minvar", "maxprec"	Method of central derivatives calculation.

Variables required for each parameter in "parameter data" section of PEST control file.

Variable	Type	Values	Description
PARNME	Text	12 characters or less	Parameter name.
PARTRANS	Text	"log", "none", "fixed", "tied"	Parameter transformation.
PARCHGLIM	Text	"relative", "factor", or absolute(n)	Type of parameter change limit.
PARVAL1	Real	any real number	Initial parameter value.
PARLBND	Real	less than or equal to PARVAL1	Parameter lower bound.
PARUBND	Real	greater than or equal to PARVAL1	Parameter upper bound.
PARGP	Text	12 characters or less	Parameter group name.
SCALE	Real	any number other than 0	Multiplication factor for parameter.

OFFSET	Real	any number	Number to add to parameter.
DERCOM	Integer	0or greater	Model command line used in computing parameter increments.
PARTIED	Text	12 characters or less	The name of the parameter to which another parameter is tied.

Variables required for each observation group in "observation groups" section of PEST control file.

Variable	Type	Values	Description
OBGNME	Text	12 characters or less	Observation group name.

Variables required for each observation in "observation data" section of PEST control file.

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

Variables in "model command line" section of PEST control file.

Variable	Type	Values	Description
COMLINE	Text	system command	Command to run model.

Variables in "model input/output" section of PEST control file.

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

Variables in "prior information" section of PEST control file.

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

Variables in optional "regularization" section of PEST control file.

Variable	Type	Values	Description
PHIMLIM	Real	greater than 0	Target measurement objective function.
PHIMACCEPT	Real	greater than PHIMLIM	Acceptable measurement objective function.
FRACPHIM	Real	optional; 0or greater, but less than 1	Set target measurement objective function at this fraction of current measurement objective function.
MEMSAVE	Text	"memsave" or "nomemsave"	Activate conservation of memory at cost of execution speed and quantity of model output.
WFINIT	Real	greater than 0	Initial regularization weight factor.
WFMIN	Real	greater than 0	Minimum regularization weight factor.
WFMAX	Real	greater than WFMAX	Maximum regularization weight factor.
LINREG	Text	"linreg" or "nonlinreg"	Informs PEST that all regularization constraints are linear.
REGCONTINUE	Text	"continue" or "nocontinue"	Instructs PEST to continue minimizing regularization objective function even if measurement objective function is less than PHIMLIM.

WFFAC	Real	Greater than 1	Regularization weight factor adjustment factor.
WFTOL	Real	Greater than 0	Convergence criterion for regularization weight factor.
IREGADJ	integer	0, 1, 2, 3, 4 or 5	Instructs PEST to perform interregularizationgroup weight factor adjustment, or to compute new relative weights for regularization observations and prior information equations.
NOPTREGADJ	integer	1 or greater	The optimization iteration interval for recalculation of regularization weights if IREGADJ is 4 or 5.
REGWEIGHTRAT	Real	absolute value of 1 or greater	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	Singular value of $\mathbf{x}^t\mathbf{q}\mathbf{x}$ (as factor of highest singular value) at which use of higher regularization weights commences if IREGADJ is set to 5.

PEST++ Additions to the PEST Control File

Information in the PEST control specific to PEST++ is specified on lines starting with "++". Although the previous example places all the PEST++ input in a single section at the end of the PEST control file, this is not a requirement. This information does not need to be contiguous and can reside anywhere in the PEST control file. Lines starting with "++#" are considered comments and are ignored.

Unlike the rest of the PEST control file, PEST++ uses keywords rather than location to specify variables. Lines are parsed using the space, tab, and parenthesis characters as separators. The example uses parentheses to more clearly delineate the values assigned to the variable, but these could just as well be replaced by white spaces. The following table includes a listing and explanation of the permissible PEST++ keywords.

Variable	Type	Values	Description
N_ITER_BASE	Integer	1 or greater	Number of base parameter iterations performed for each super parameter iteration.
N_ITER_SUPER	Integer	0 or greater	Number of super parameter iterations performed for each base parameter iteration.

SUPER_EIGTHRES	Real	any positive number (typically should be greater than 1.0e−7)	PEST++ will not include any super parameters whose ratio with the largest super parameter is less than this ratio.This value can as small as zero if the user wants to specify the number of super parameters solely with SUPER_NMAX. BecausePEST++uses SVD on the super parameter problem, a low value for this SUPER_EIGTHRES will not adversely impact the stability of the solution.
MAX_N_SUPER	Integer	integer between 1 and the minimum of maximum number of parameters and the maximum number of observations	Maximum number of super parameters to use in the super parameter iterations.
MAX_REG_ITER	Integer	Integer greater than 1. Default is 20.	Provides a limit on the maximum the number of iterations used to compute dynamic regularization weights when PEST++ is run in regularization mode.
MAX_SUPER_FRZ_ITER	Integer	1 or greater, Default value is 5.	Maximum number of times a super parameter iteration will try to freeze any parameters that go out of bounds andl try to recompute a jacobian. If the jacobian cannot be computed in MAX_SUPER_FRZ_ITER iterations PEST++ will switch to a base parameter iteration.
AUTO_NORM(4)	Integer	1 or greater	Automatically normalizes the parameters by assuming there are 4 standard deviations between the upper and lower parameter bounds

SVD_PACK(PROPACK)	NA		Flag to use PROPACK to compute SVD factorizations
MAT_INV	String	Q1/2J JTQJ	Flag to specify whether to solve $Q^{1/2}J$ or J^tQJ. This option is forced to "Q1/2J" when PROPACK is used
SUPER_RELPARMAX	Real	Greater than 0	Parameter relative change limit for super-parameters
MAX_RUN_FAIL	Integer		Maximum times the run manager will try to rerun a failed run
LAMBDAS	Comma separated list of real numbers		Specify the standard values of lambda to be used each iteration rather than use the default of (.01,1,10,100,1000)
ITERATION_SUMMARY	"TRUE" or "FALSE"		Setting this to "TRUE" will save a summary of each iteration to a series of comma separated files for easy plotting.
DER_FORGIVE	"TRUE" or "FALSE"		Setting this to "FALSE" will turn off derivative forgive and cause PEST++ to terminate if a run fails while computing the jacobian.

References

Doherty, J., 2011a, PEST surface water utilities: Brisbane, Australia,Watermark Numerical Computing.

Doherty, J., 2011b, Groundwater data utilities: Brisbane, Australia, Watermark Numerical Computing.

Muffels, C.T., Schreüder, W.A., Doherty, J., Karanovic, M., Tonkin, M.J., Hunt, R.J., and Welter, D.E., 2011, GENIE—A model independent TCP/IP run manager*in*MODFLOW and More 2011—Integrated Hydrologic Modeling, Proceedings of the 10th International Conference of the International Ground Water Modeling Center: Golden, Colo., Colorado School of Mines.

Muffels, C.T., Schreüder, W.A., Doherty, J., Karanovic, M., Tonkin, M.J., Hunt, R.J., and Welter, D.E., 2012,Approaches in Highly Parameterized Inversion: GENIE, A General Model Independent TCP/IP Run Manager. U.S. Geological Survey Techniques and Methods Report**.**