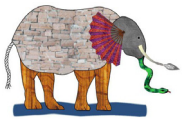

PEST – J Doherty & Friends

PUB-IAHS Workshop
Uncertainty Analysis in Environmental Modelling
6th – 8th July 2004

a) Introduction:

PEST is a software package for model-independent parameter estimation. Its model-independence is an outcome of the fact that it communicates with a model through the model's own input and output files. Its parameter estimation methodology is based on the Gauss-Marquardt-Levenberg (GML) method. Where model outputs are continuous with respect to parameters, this method finds an objective function minimum in fewer model runs than any other method. PEST is supported by a plethora of utility software to expedite its usage in the calibration of complex ground and surface water models. These facilitate the use of multi-component objective functions comprised of different types of data, and/or the same data processed in different ways for "distillation" of the information content of that data with respect to certain parameters or parameter types. PEST has 3 modes of operation, these being:-

•Parameter Estimation

•Regularisation

•Predictive analysis

Predictive Analysis can be carried out in variety of methods within the package briefly:

•Constrained Optimisation – The prediction is maximised and/or minimised by selecting a set of model parameters from those that have an overall calibration fit (using a predefined measure) within a specified range of the optimal parameter set (in terms of the measure).

•Stochastic Field Warping – Assess the effect of spatial hydraulic detail, un-captured in the calibration data, on the predictive uncertainty through stochastic realisations of the hydraulic detail which are then "warped" to the minimum level needed to calibrate the model. Repeated evaluation using different initial stochastic fields yields a posterior predictive probability distribution.

•Predictive Calibration - The idea behind "predictive calibration" is to incorporate an extra "observation" in the calibration dataset, this observation actually being a "prediction". If the model can be "calibrated" against both historical observations, and against this prediction, in a manner that results in reasonable parameter values, then the prediction is possible.

•MCMC – Implemented within the MICA package. Allows the production of post-calibration predictive probabilities in a full Bayesian framework. A variety of likelihood measures and proposal distributions are available within the package.

•Composite Linear Predictive Uncertainty Analysis - Formulae for calculation of parameter and predictive uncertainty, exact for linear models, but only approximate for nonlinear models, have been available in the literature for years. These formulae are based on statistics arising from model-to-measurement misfit. Recently I have extended these formulae to the context of under-determined parameter estimation, using regularization theory. A second term has been added to the traditional equations to accommodate the contribution to predictive uncertainty arising from "uncaptured heterogeneity". In many modelling contexts this is a far bigger contributor to predictive uncertainty than model-to-measurement misfit.

b) Advantages

- Many techniques from the unashamedly pragmatic to the fully Bayesian
- Some techniques are numerically fast and stable
- Usable with arbitrary models due to interaction through the model input file
- Ready available code

c) Disadvantages

- Some techniques are numerically intensive (Parallel Processor version available)
- Some techniques are inefficient when parameters are highly correlated

d) Assumptions

Various dependant upon method

e) Most appropriate application areas

Any model. Widely used in Groundwater modelling.

f) Reading list

Doherty, John, and John M. Johnston, 2003. Methodologies for calibration and predictive analysis of a watershed model, J. American Water Resources Association, 39(2):251-265.

Gallagher, M. and Doherty, J., 2004. Predictive uncertainty analysis for a watershed model. Submitted for publication to Journal of Hydrology.

g) Software availability

PEST is in the public domain. PEST and all of its utility software can be downloaded from the referenced website

h) Web links or other information

http://www.sspa.com/pest

i) Figures – None given

j) Delegates Comments (please add !!)