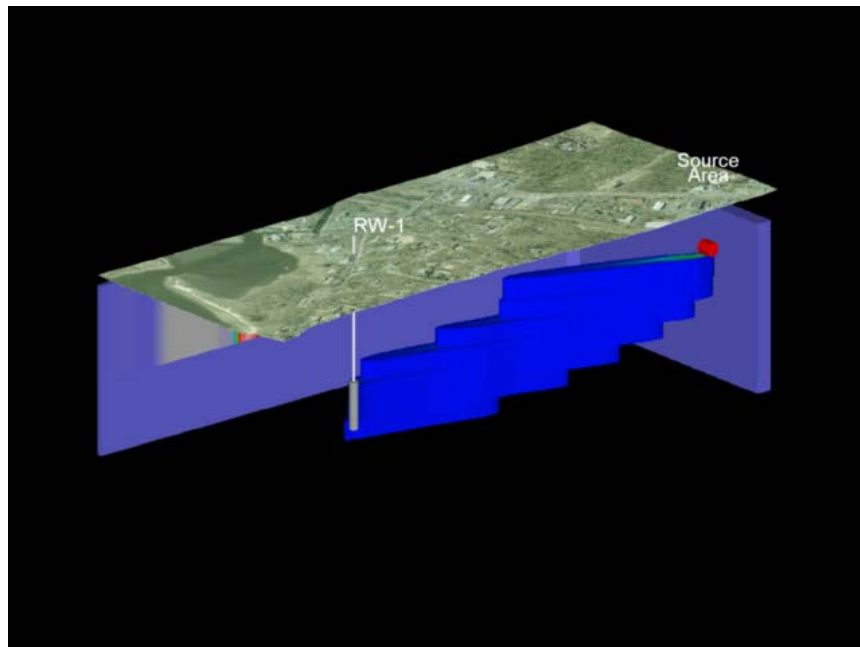


Model Calibration and Predictive Analysis using PEST Version 10



2006 Course Outline

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Introduction

This intensive short course will instruct participants on the automated calibration of environmental models, and on the analysis of the predictive uncertainty associated with such models. The principal instructor is the developer of PEST, the industry standard software package for model-independent, automated calibration and predictive uncertainty analysis.

What you will learn

While the course will include a thorough coverage of the theory and applications of nonlinear parameter estimation techniques in the calibration of different types of models, there will also be a strong practical aspect of the course. Participants will gain hands-on experience in the use of PEST, including its advanced regularization and predictive analysis features. Experience will be gained in the use of these features in the calibration of groundwater flow and transport models, surface water quality and quantity models, as well as other types of models including a vadose zone model and a biological growth model. Topics covered will include:

- theory of nonlinear parameter estimation,
- application of nonlinear parameter estimation to model calibration,
- analysis of uncertainty and nonuniqueness in calibrated parameters,
- problem regularization,
- analytical and intuitive analysis of calibration residuals,
- the effects of parameter uncertainty on model predictive uncertainty,
- simultaneous calibration of multiple models,
- use of PEST's predictive analyser,
- use of PEST in regularization mode,
- PEST's stunning new "SVD-Assist" functionality,
- use of different methods of spatial parameterisation,
- pilot points in calibration of groundwater models,
- combining stochastic field generation with nonlinear parameter estimation,
- the "calibration null space" and its contribution to model predictive error variance,
- how to choose an appropriate level of model complexity,
- how to reduce uncertainty most effectively through optimization of data acquisition.

In the practical sessions, participants gain hands-on experience in using all aspects of PEST with a number of different models, including MODFLOW, MT3DMS (popular public domain groundwater flow and transport models), SWIM (a Richard-equation-based, unsaturated zone, water-movement model), 3PG (a forest production model) and HSPF (a popular USEPA/USGS model for simulation of non-urban, non-point pollution of surface water systems). Participants will also be introduced to a suite of utility programs that automate PEST set-up for these (and similar) models, and that expedite implementation of model predictive error variance analysis.

What is Nonlinear Parameter Estimation?

In simple terms, nonlinear parameter estimation is a methodology whereby the arduous, labour-intensive and distinctly frustrating task of multi-parameter model calibration can be carried out automatically under the control of a computer. The advantages of computer-aided model calibration include the following:

- the task is accomplished more rapidly than by using manual methods;
- better parameter estimates are obtained;
- estimates of the uncertainties accompanying optimised parameters are produced as part of the calibration process;

- freed of the drudgery of undertaking countless manual model runs, the modeler is able to inject more initiative into the calibration process, thus making this process a partnership between calibration technology and the art of the modeler;
- greater understanding of the environmental processes simulated by the model can be gained by viewing model calibration as a sophisticated method of data interpretation;
- use of advanced regularization techniques to define default system conditions can allow environmental data interpretation to occur while ensuring parameter reasonableness;
- analysis of the effects of parameter uncertainty and non-uniqueness on model predictive uncertainty can be undertaken;
- use of PEST's regularization capabilities allows model predictions to be made with minimized error variance - i.e., minimized "potential wrongness" of model predictions.

What is PEST?

PEST is a model-independent nonlinear parameter estimator. Since its inception ten years ago PEST has become the industry standard in calibration of environmental models of all kinds. Three cornerstones of PEST's model-independence are:

1. PEST communicates with a model through the model's own input and output files. Hence the model does not need to be re-compiled to be linked to PEST; it can be used with PEST exactly as it is.
2. Though based on the Gauss-Marquardt-Levenberg method, the nonlinear parameter estimation algorithm used by PEST is uniquely robust and powerful, having been developed specifically for use with complex environmental models.
3. The time required for calibration of complex models with long run times can be significantly reduced through the use of PEST's powerful, operating-system-independent, parallelization capabilities.

PEST also comes with an extensive suite of utility software to automate construction of its input datasets in many common modeling contexts. This, together with the model-independent nature of PEST, allows modelers to calibrate their own tailor-made composite models, built through assimilation of one or more model executables and pre/post-processors in a single batch file. Enormous creativity can thus be exercised in the construction and calibration of these models.

PEST extends the nonlinear parameter estimation methodology to the analysis of "predictive uncertainty". This term describes the degree of nonuniqueness associated with particular model outcomes when the model is used to predict the future while simultaneously ensuring that calibration constraints are enforced, i.e. while ensuring that the model is capable of replicating historical system behavior as well. PEST also includes advanced regularization. This allows the estimation of many more parameters than would otherwise be possible in a way that is numerically stable. Furthermore, realistic values are assigned to parameters (even insensitive and highly-correlated parameters) when estimated under regularization conditions. Regularization can be particularly useful in the calibration of complex groundwater models and distributed parameter surface water models, where PEST can "find for itself" regions of high and low hydraulic property value.

Latest Developments

The latest PEST developments have introduced innovations that are destined to have a profound effect on the way environmental models are built and calibrated. These include:

- PEST's new "SVD-Assist" technology. Using the methodology, up to two thousand parameters can be estimated through a highly regularized inversion process that requires only tens of model runs per iteration, and is unconditionally stable.
- Through combining regularized inversion with predictive uncertainty analysis, new tools are now available for obtaining accurate estimates of the "potential wrongness" of any

prediction made by a calibrated model. Such estimates are far more realistic, and can be obtained with far greater efficiency, than is possible with any previous method of model predictive uncertainty analysis.

Development of PEST and its ancillary software in 2005 focused on model predictive error analysis. Attendees of the focused Predictive Error Analysis additional course component (usually offered on the morning of a fourth day) gain hands-on experience in predictive error analysis through a comprehensive 'soup-to-nuts' model calibration, regularized inversion and predictive error analysis workshop, covering such topics as:

- Sources of error in a calibrated model - the model null space and solution space
- Linear and nonlinear analysis of model predictive error
- Evaluating the contributions of various sources of model predictive error
- Optimization of data acquisition to reduce predictive error
- Predictive error analysis as an adjunct to regularized inversion
- Appropriate model complexity

Version 10 of PEST, release in November 2005 includes many additions to PEST's capabilities for use in groundwater and surface water model calibration, many new utilities, and a driver that encompasses the Shuffled Complex Evolution (SCE-UA) method - particularly suited to surface water model calibration. It also includes advanced algorithms which combine regularization and uncertainty analysis theory to provide fast and accurate appraisal of model predictive error variance in complex hydrogeological environments.

How do I find out more?

PEST has been freeware since February 2001, and is available for download together with all its accompanying utility software, from <http://www.sspa.com/PEST>. To find out more about PEST, see the PEST web pages at:

<http://www.sspa.com/pest>

or write to the dedicated PEST email account at:

pest@sspa.com

Who should attend?

Anyone interested in model calibration, parameter optimisation, or analysis of model predictive uncertainty should attend this course. Those new to PEST, as well as those with previous PEST experience, will all benefit from the course. To get the most out of the course, participants should have some modeling experience and should feel comfortable working directly with model input and output files in a command-line environment.

What you will receive

Participants will receive:

- course notes,
- a free copy of the very latest version of PEST,
- an extensive suite of ground and surface water modeling utility software,
- copies of the files and documentation for all of the practical exercises.

About the Instructors

Dr. John Doherty is the author of PEST. John has worked for over 29 years in the water industry, first as a groundwater exploration geophysicist, then as a modeler. He has worked in

the public, private and education sectors. He now directs his own company, Watermark Numerical Computing, which undertakes software development and advanced modeling for mining, environmental, agricultural, water supply and remediation applications. He also works as a senior research scientist for the University of Queensland where he supervises a number of post-graduate students who are pursuing research into issues related to model parameterization and predictive uncertainty analysis. John has had over nine years experience in presenting short courses all over the world. Course material is presented clearly and descriptively with many practical examples and illustrations. He attempts to create a learning environment that is both educational and enjoyable.

Matt Tonkin has been a hydrogeologist with S. S. Papadopoulos & Associates, Inc. since 1995, and presently resides in their Cape Cod, MA, office. Matt has worked closely with Dr. Doherty since 2001, and is presently completing his doctoral degree under the advisement of Dr. Doherty. Matt hosts the PEST web pages and is the voice at the end of the pest@sspa.com email address.

PEST Course Basic Agenda

Day 1

Day 1: Morning

Lecture - Introduction to non-linear parameter estimation: mathematical theory, development, and integration with models

Lab - Hands-on exercise: calibrating an unsaturated zone/storage model

Day 1: Afternoon

Lecture - Fundamentals of PEST - the implementation of nonlinear parameter estimation theory within PEST

Day 2

Day 2: Morning

Lecture - Use of PEST in groundwater models Flow and Transport

Lab - Hands-on exercise: choice of hands-on problems including surface and groundwater, forestry, unsaturated zone, or attendees' own studies

Day 2: Afternoon

Lecture - Sensitivity analysis, predictive uncertainty analysis, model complexity, and introduction to pilot points

Lab - Hands-on exercise: choice of hands-on problems including surface and groundwater, forestry, unsaturated zone, or attendees' own studies

Day 3

Day 3: Morning

Lecture - Use of pilot points in spatial model calibration and uncertainty analysis

Lab - Hands-on exercise: choice of hands-on problems including surface and groundwater, forestry, unsaturated zone, or attendees' own studies

Day 3: Afternoon

Lecture - The use of PEST in the surface water modeling context, focusing on HSPF and SWMM, and time-series data processing in surface water model calibration.

Lab - Hands-on exercise: choice of hands-on problems including surface and groundwater, forestry, unsaturated zone, or attendees' own studies

Optional Evening Sessions

Optional informal sessions are provided each evening. Exercises and instructor-attendee interaction are typically available until 8pm.

General Course Lecture Outline

Lecture 1: Introduction to nonlinear parameter estimation.

- mathematics of nonlinear parameter estimation (summary only),
- stochastic interpretation of nonlinear parameter estimation theory,
- linear parameter uncertainty analysis,
- use of measurement weights,
- prior information,
- parameter nonuniqueness,
- use of parameter bounds,
- the Marquardt lambda,
- analysis of residuals.

Lecture 2: Basics of PEST.

- PEST and model-independence,
- templates of model input files,
- instructions to read model output files,
- the PEST control file,
- requirements of a model,
- parameter transformation,
- calculation of derivatives,
- parameter change limits,
- composite parameter sensitivities,
- recognition of aberrant PEST behaviour,
- user intervention in the parameter estimation process,
- PEST's "automatic user intervention" functionality,
- construction of composite models,
- dual calibration and predictive analysis,
- Parallel PEST,
- Visual PEST.

Lecture 3: Parameter Estimation and Groundwater Modeling

- use of PEST with MODFLOW, MODFLOW-2000 and MT3D,
- advantages/disadvantages of MODFLOW-2000's parameter estimation process,
- advantages of using PEST for groundwater model calibration,
- MODFLOW2000-to-PEST translator,
- calibration of steady-state and transient models,
- utility software for use of PEST with MODFLOW and MT3D,
- nonlinear parameter estimation as hypothesis testing,
- multiple-re-calibration for uncertain boundary conditions,
- special steps required in multi-layer model calibration,
- coping with cell drying and re-wetting in MODFLOW,
- examples of parameter nonuniqueness.

Lecture 4: Use of Pilot Points and Regularization in Groundwater Modeling

- the need for regularization,
- brief discussion of geostatistics,
- use of pilot points as a device for spatial parameterization,

- combining pilot points and regularization,
- utility software to implement regularized inversion,
- examples of pilot points in model calibration,
- use of pilot points in multi-layer model calibration
- use of pilot points in transient model calibration.
- truncated singular value decomposition as a regularization device
- PEST's unique SVD-Assist technology,
- examples

Lecture 5: Use of PEST in Surface Water Model Calibration

- problems encountered when using nonlinear parameter estimation with surface water models,
- overcoming these problems,
- multiple objective function minima and how to handle them,
- the SCE method,
- multi-objective parameter estimation,
- simultaneous calibration of multiple models with/without inter-model regularization,
- incorporation of exceedence probabilities and other "secondary observations" into the parameter estimation process,
- digital filtering for baseflow separation and incorporation of this into the calibration process,
- description of utility software supplied with PEST,
- use of constituent and sediment data in model calibration,
- incorporation of relationships between model parameters and catchment properties into the calibration process,
- use of "super parameters" as a regularization device,
- "adaptive regularization" and surface water model calibration.

Lecture 6: Predictive Analysis and Model Complexity

- sensitivity analysis,
- linear propagation of parameter uncertainty to predictive uncertainty,
- nonlinear predictive error variance analysis,
- loss of detail in the calibration process,
- accommodating loss of detail in estimates of model predictive error variance,
- combining regularization with predictive uncertainty analysis,
- combining stochastic field generation with regularized inversion,
- "calibration constrained Monte Carlo",
- "dual calibration" as a qualitative method of predictive uncertainty analysis,
- examples of predictive analysis using PEST,
- how to choose an appropriate level of model complexity,
- predictive uncertainty analysis and optimization of data acquisition,
- predictive uncertainty analysis in surface water models.

Practical Sessions

During course practical sessions, participants can choose from the following exercises. If not completed during the course, they can be completed at a later time, for all files required for these exercises are supplied on CDs which are provided to all course participants.

Use of PEST with a Simple Storage Model

This exercise illustrates many key problems encountered in calibrating environmental models. Students will gain hands-on experience in the use of PEST, Parallel PEST and Visual PEST. PEST's predictive analysis functionality will also be explored.

Use of PEST with MODFLOW - I

MODFLOW will be used independently of any commercial graphical user interface. The utility software supplied with the course will be used to demonstrate to participants that, when the occasion demands it, they can extend the calibration functionality offered by commercial MODFLOW PEST interfaces to far more complex calibration problems.

Use of PEST with MODFLOW - II

Students will gain experience in using pilot points for calibration of a MODFLOW/MT3D model. PEST will be used in all three of its modes of operation - parameter estimation, predictive analysis, and regularization. The uncertainty associated with predictions of the efficacy of a remediation system in a geologically heterogeneous area will be explored using pilot points together with PEST's predictive analyzer.

Use of PEST with MODFLOW – III

This practical exercise is based on a real-world model in a heterogeneous geological setting. Spatial parameterization is undertaken using pilot points, and calibration of a MODFLOW model is accomplished using PEST's advanced regularization features. The use of regularized inversion is combined with stochastic field generation to explore the effects of geological heterogeneity on model predictive uncertainty.

Calibrating a Vadose Zone Model using PEST

By working through this informative practical exercise, participants will learn how to use PEST in the design of a field experiment, and in exploring the effects of parameter nonuniqueness on predictive nonuniqueness. It will be discovered that the repercussions of parameter uncertainty on predictive uncertainty are not always easy to quantify without using PEST's predictive analyser.

Surface Water Model Calibration Using PEST

Though based on the popular surface water quantity/quality model HSPF, the principals discussed in this practical session are applicable to any kind of surface water modeling. Calibration will be undertaken on the basis of observed flows, and of "processed flows", allowing volumes and exceedence times to be included in the calibration process for more robust parameter estimates. Parameter nonuniqueness will be explored, as will the effects of parameter nonuniqueness on predictive nonuniqueness. Incorporation of sediment load data into the calibration process will also be included in the practical exercise.

Parameterisation of a Forest Growth Model

Participants will learn how to prepare a PEST input dataset for calibration of a forestry production model. PEST will be used to calibrate a number of such models simultaneously, thus

making maximum use of all available data to ensure parameter consistency between calibrated models. The issue of which parameters to declare as adjustable and which parameters to fix or tie to other parameters will be explored.