Preliminary program for course on

Model optimisation and quantification of predictive uncertainty

The course is taught over five days. The program for each day is a combination of lectures and practical sessions (hands on exercises). The preliminary plan for the lectures is found below. With regard to the practical sessions the content of these will at least to some extent be defined by the individual student. These sessions are also briefly described below. However, we welcome that the student bring with her/him a model and a data set of particular relevance that she/he can work on during the practical sessions. If you wish to do this, do not hesitate to contact us if you need help on what to prepare and what to bring with you to the course.

DAY 1 (September, 15th)

Time: 9:00 – 17:30

Course introduction

Short presentation of students

Lecture: Introduction to models (Andres Alcolea, 1.5 hours)

- what is a model,
- historical view,
- type of models: conceptual, scale models, analogical models, mathematical models.
- on the use of models: philosophy: understand the past, know present day, forecast future; in practice: management of water resources, tool for knowledge integration, tool for learning.
- difficulties inherent to modelling
- the modelling process: a few examples (ground water hydrology)

Lecture: Geological modeling (Philippe Renard, 1.5 hours)

- motivation
- definition and needs for a geological model
- types of geological models
- interpolation techniques
- geometrical deterministic models (implicit and explicit approaches)
- process based simulations
- stochastic models
- testing and validating

Practical session

Afternoon: Use of basic tools for facies delineation (GSLIB, SGeMS) ???.

DAY 2 (September, 16th). John Doherty

Time: 9:00 – 17:30

Lecture: Introduction to nonlinear parameter estimation.

- mathematics of nonlinear parameter estimation (summary only),
- stochastic interpretation of nonlinear parameter estimation theory,
- explanation of covariance matrix, correlation coefficients, eigenvectors/eigenvalues etc
- linear parameter uncertainty analysis,
- use of measurement weights,
- prior information,
- parameter nonuniqueness,
- use of parameter bounds,
- the Marquardt lambda,
- analysis of residuals.

Practical session

Late morning until mid-afternoon: basic PEST practice using a simple storage model. This covers most aspects of PEST usage with a very simple model.

Lecture: 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.

DAY 3 (September, 17th). John Doherty

Time: 8:30 – 17:30

Lecture: Parameter Estimation and Groundwater Modeling

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

Practical session

Continuing with the previous workshop if it is not finished, or starting a new one.

Lecture: 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
- SVD-Assist,
- the resolution matrix
- "structural noise" and why it shows spatial correlation
- examples

DAY 4 (September, 18th). John Doherty

Time: 8:30 – 17:30

Lecture: Introduction to Predictive Uncertainty Analysis

- sensitivity analysis,
- linear propagation of parameter uncertainty to predictive uncertainty,
- the difference between "uncertainty" and "potential error"
- 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.

Practical session

Exercise of your choice.

Lecture: Regression based modeling of groundwater flow in heterogeneous media

- Theoretical background,
- Bias in estimates, residual, and predictions,
- More on nonlinearity,
- Correction of confidence and prediction intervals.

DAY 5 (September, 19th). John Doherty

Time: 8:30 – 16:00

Lecture: Advanced Linear Predictive Uncertainty Analysis

This lecture would take about 2 hours. Students may need a break in the middle.

- the mathematics of zone-based regularization
- the mathematics of subspace regularization
- derivation of equations for linear uncertainty analysis
- contribution by different parameter types to total predictive uncertainty
- optimization of data acquisition
- field examples of applications of these methods.

Practical session

Exercise of your choice.

Lecture: Advanced Nonlinear Predictive Uncertainty Analysis

This lecture would take about 1 hour.

- constrained predictive maximization/minimization with application of regularization constraints
- markov chain monte carlo
- null space Monte Carlo
- application to surface water quality modeling
- field examples

Now this may leave a couple of hours at the end of the day. Maybe students could ask questions, or we could have a "group therapy session", or students could present some problem to the class and we could discuss how best to approach it, given what has been learned so far.

Practical Sessions

During course practical sessions, participants are welcome to 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 and Parallel 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.

Use of PEST with MODFLOW – IV

This demonstrates the latest features of PEST and its uncertainty analysis utilities. Calibration of a simple one layer model is undertaken using pilot points together with a number of regularization methodologies including Tikhonov, SVD and SVD-assist. Linear analysis is then undertaken to analyze the uncertainty of a particle travel time prediction, taking into account the "null space term". Contributions to this uncertainty by different parameter groups are analyzed. Optimization of data acquisition to reduce this uncertainty is also analyzed. Finally nonlinear predictive error analysis is undertaken.

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.

Calibration of a SEAWAT Model – I

PEST's SVD-assist functionality is employed to calibrate a multilayered SEAWAT model that simulates salt water intrusion into a two-aquifer coastal system. Calibration targets include both head and concentration measurements in pumping and observation wells.

Calibration of a SEAWAT Model – II

In most instances of salt water intrusion modeling, the location of the freshwater salt water mixing zone at the start of the simulation time is only vaguely known. However errors in assessment of its location can lead to erroneous parameter estimates and erroneous model predictions. Errors in parameters and predictions from this source can be reduced (and quantified) if initial conditions are included in the parameter estimation process. This workshop addresses this issue.