Environmental Modelling & Analysis Group

http://www.civil.uwaterloo.ca/envmodelling/

A 3-day Short Course:

Calibration and Predictive Uncertainty Analysis for Complex Environmental Models

Sponsored by the Environmental Modelling & Analysis Group,
Department of Civil and Environmental Engineering
University of Waterloo
March 24th-26th
9:00-5:00 (with breaks)
RCH 208, University of Waterloo Campus

This short course is intended to provide an intense coverage of the practical theory behind parameter estimation and uncertainty analysis for environmental modelling. The course focuses on the advanced tools provided with PEST, a software package developed by the short course instructor, Dr. John Doherty. Topics covered include traditional parameter estimation, use of pilot points as a parameterization device; advanced regularization techniques; the "SVD-assist" technique for efficient inversion of highly parameterized models; linear and nonlinear analysis of uncertainty - including the recently-developed and highly expedient null-space Monte Carlo methodology that is unique to PEST; methods for optimizing future data acquisition to reduce uncertainty, and other advanced techniques. These concepts are all taught in the context of physically-based groundwater and surface water modelling.

Dr. John Doherty, the short course instructor, is the primary developer of the PEST (Parameter ESTimation) software package and a well-respected expert in calibration and uncertainty analysis. John has worked for 30 years in the water industry, first as a groundwater exploration geophysicist, then as a modeler. 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. John has had over twelve 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.

Who is welcome:

Graduate students in Civil & Environmental Engineering or Earth Sciences programs at UW. Sufficient experience with groundwater and/or surface water models is expected. Course registration is arranged through the faculty advisor. If interested, please have your advisor contact Prof. James Craig at jrcraig@uwaterloo.ca.

Other information:

Lunches are brown bag. Coffee and limited refreshments will be provided.

Day 1

Session 1: Introduction

A broad overview of what participants can expect over the next three days. The philosophy behind the PEST approach to model calibration and uncertainty analysis based on highly-parameterized, regularized inversion will be presented, together with a suite of examples of application of the techniques and philosophy in real-world settings.

Session 2: Traditional Parameter Estimation

- Definition of inverse problem, objective function
- Minimization of the objective function
- Parameter covariance and Jacobian matrices
- Observations and weights; Prior information
- The need for parameter parsimony in traditional parameter estimation
- Composite parameter sensitivities
- Bayes Theorem

Session 3: Workshop

During this session, participants will use PEST to calibrate a simple model. Despite the simplicity of the model, and of the calibration process implemented by PEST, many features of more complex PEST usage will be demonstrated.

Session 4: PEST: Implementation Details

- Template, Instruction, PEST control files
- Calculation of model derivatives
- Observation weights and weight matrices
- Multi-component objective functions
- Special PEST utilities
- Recognizing aberrant PEST behaviour

Day 2

Session 1: Using PEST in Groundwater Model Calibration

- Using PEST with MODFLOW and MT3D
- MODFLOW dry cells
- Avoiding the effects of model structural errors on estimated parameters
- Hypothesis testing
- Formulation of a suitable multi-component objective function
- Issues related to model complexity

Session 2: Highly Parameterized Inversion - Part 1

- Problems with traditional parameter estimation
- “Over-fitting” and “under-fitting”
- What is “regularization”
- The case for highly parameterized inversion
- Pilot points as a parameterization device
- Tikhonov and subspace regularization (including singular value decomposition)

Session 3: Highly Parameterized Inversion - Part 2

- SVD-assist - a highly-efficient hybrid scheme
- “Super parameters”
- Field examples of highly parameterized inversion
- The calibration null space
- The resolution matrix
- Parameter identifiability and error
- Calibration metrics

Session 4: Open

TBA: Guest lecturer or regularized inversion application example

Day 3

Session 1: Traditional Uncertainty Analysis

- Sensitivity analysis
- The "chapter 5 syndrome"
- Concepts of post-calibration parameter and predictive uncertainty
- Measurement noise, predictive noise, structural noise
- Linear uncertainty analysis
- Nonlinear uncertainty analysis - constrained predictive maximization/minimization
- The GLUE methodology
- Markov chain Monte Carlo
- Problems with traditional uncertainty analysis
- Cooley's analysis of parsimony-induced structural noise

Session 2: Highly Parameterized Uncertainty Analysis

- How a "perfectly calibrated model" can give wrong predictions; what's missing
- Linear uncertainty analysis in the highly parameterized context
- Contribution of different parameter types to overall uncertainty
- Assessment of the worth of different existing or future observations
- Optimization of data acquisition
- Optimal level of parameterization complexity
- Highly parameterized constrained predictive maximization/minimization
- Null space Monte Carlo generation of calibration constrained parameter fields
- Heuristic but effective methods of uncertainty analysis

Session 3: Surface Water Model Calibration - Part 1

- Common problems in surface water model calibration
- Processing of observations
- Multi-component objective functions
- Flow transformations; Baseflow filtering of flows and use in calibration
- Using regularization in surface water model calibration
- Maintaining parameter ordering relationships
- The TSPROC and other PEST utilities
- Null space Monte Carlo in surface water modeling

Session 4: Surface Water Model Calibration - Part 2

- Local Optima
- Global methods - SCE
- Global methods - CMAES
- Finding local optima using the PD_MS2 utility
- Thresholds and discontinuities