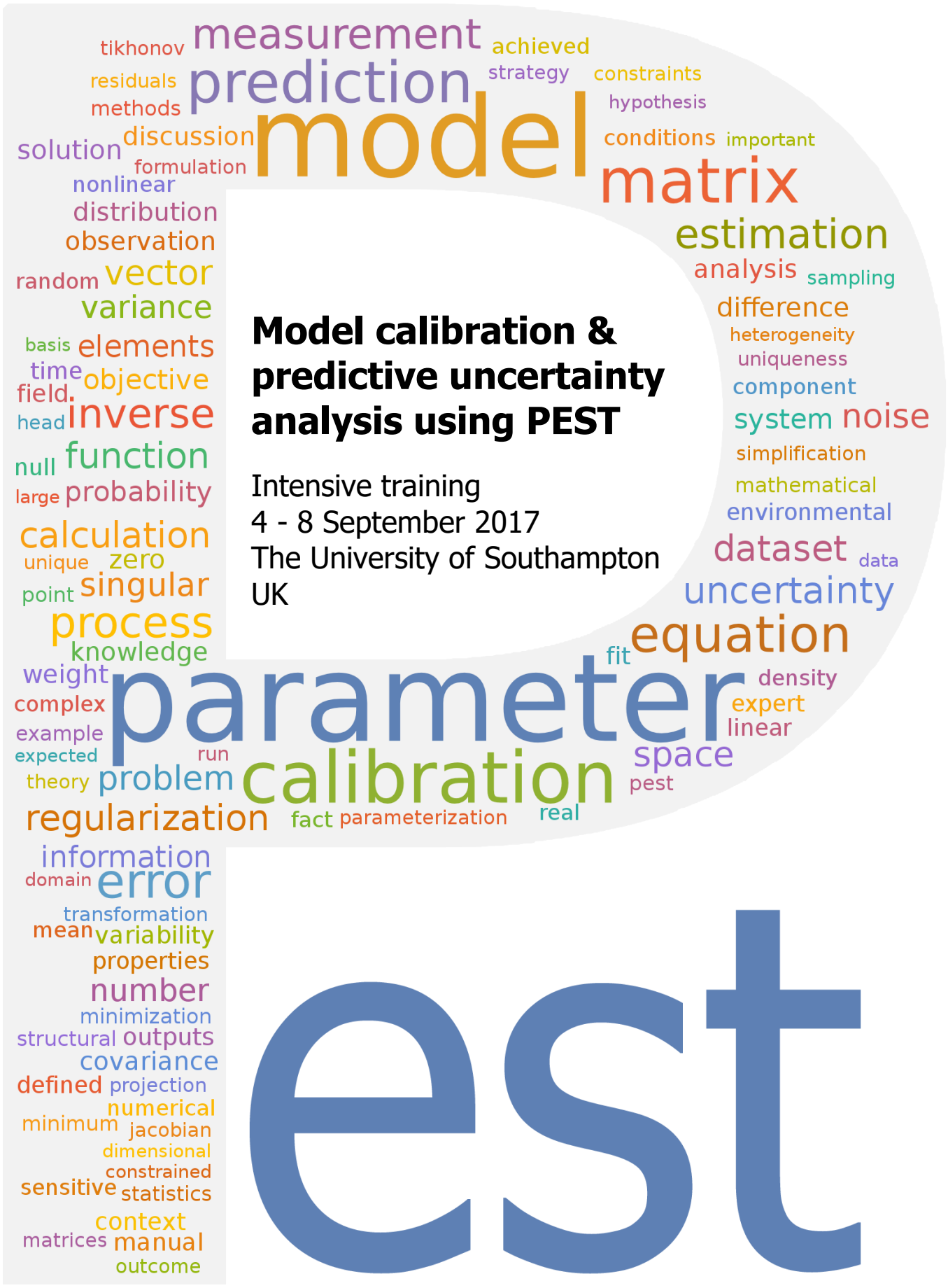
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Model calibration & predictive uncertainty analysis using PEST
Intensive training
4 - 8 September 2017
The University of Southampton
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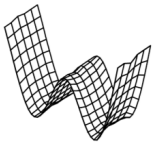


Watermark Numerical Computing

PEST
Model-Independent Parameter Estimation & Uncertainty Analysis

Course programme

Course aim

The course provides comprehensive theoretical and practical background for parameter estimation and uncertainty analysis in groundwater modelling, through the use of PEST (Parameter ESTimation)

PEST

Open-source software suite with extensive documentation, downloadable at www.pesthomepage.org

Knowledge prerequisites

Basic knowledge of groundwater numerical modelling, statistics, geostatistics can help a better understanding of the course topics. However, this is not essential.

Training mode

Each training day is divided into four sessions of 2 hours duration devoted to workshops and practical sessions. The course will be as informal as possible, with plenty of time provided for discussions on topics of interest (including participants' own models). In addition, after the course optional on-line sessions can be organised (without extra fee).

Laptop requirement

All attendees should bring their own laptop computer. However, if it is not possible the University of Southampton provides a laptop lending service (£25 GBP for laptop hire for the length of the training course). This can be ordered during the online registration.

PEST training certificate

Course participants will obtain a course certificate upon successful completion of the full five-day course "Model calibration and predictive uncertainty analysis using PEST". This includes full course attendance and active participation in workshops.

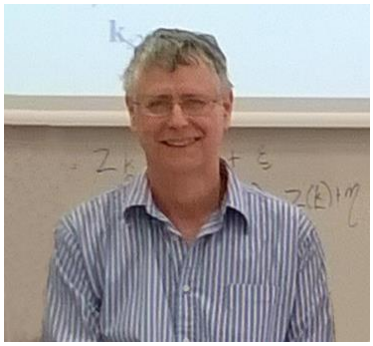
Provided materials

Each participant will be provided with a memory stick. This will contain:

- Reading material (mainly peer-reviewed papers which document theory and use of PEST)
- Copies of slides shown at the course
- The latest version of PEST
- The latest version of all PEST utilities
- A suite of PEST workshops that can be done after the course if desired.

Necessary printed materials will also be provided.

Instructors



Dr. John Doherty is the author of PEST and its supporting utility software suites. He is a self-employed consultant, but has also held positions with the National Centre for Groundwater Research and Training, Flinders University, Australia, and with University of Queensland, where he has undertaken research and supervised PhD students. He started his career as an exploration geophysicist, but then moved to environmental modelling. He has since worked in the government, private and tertiary sectors. His research interests include the continued development of software and methodologies for solution of inverse problems using environmental models, quantification of model predictive uncertainty, and appropriate use of models in the decision-making context.

Dr. Francesca Lotti is a consultant hydrogeologist and partner at Kataclima (Italy). She has 15 years of experience in field investigations and numerical modelling of contaminated sites, mines, geothermal systems, etc. She is adjunct professor at the University of Camerino, supervisor of many students/PhD/interns, trainer at professional courses and lecturer at II level Masters.

Dr. Alastair Black is a hydrogeologist and computer code developer specialising in numerical groundwater modelling. He has over 10 years' experience in technical modelling and code development for the mining, nuclear and water resource industries. His primary interests include: groundwater flow modelling, coupling of surface water processes to groundwater models, parameter estimation/uncertainty analysis, contaminant fate modelling, code development and model review.

Supporting organisations:

Watermark Numerical Computing

Groundwater Science

kataclima
CATALYZING ENERGIES

UNIVERSITY OF Southampton

Daily course schedule:

Dates:	4 - 8 September 2017*
Duration:	5 full days
First day introductions	8:40 – 9:00
Morning - Session 1	9:00 – 10:45
Tea/Coffee & light snacks (ground floor foyer)	
Morning - Session 2	11:15 – 13:15
Lunch	
Afternoon - Session 3	14:30 – 16:15
Tea/Coffee & light snacks (ground floor foyer)	
Afternoon - Session 4	16:45 – 18:45

*For your information

A separate course is being held in Italy following the UK course. The PEST course in Italy will be held from 11th to 15th September 2017. Working language is English. For information about the course programme in Italy, please contact Dr Francesca Lotti f.lotti@kataclima.com

Venue

Room 2040 in Building 45
The University of Southampton
Highfield campus,
Southampton, UK
Campus map:
https://maps.southampton.ac.uk/#17/50.93734/-1.39408

Venue details:
http://data.southampton.ac.uk/building/45.html

Parking

Parking is free of charge.
Available parking places are in walking distance from the course venue: Glen Eyre (for the University halls residents) or Avenue Campus for non-residents. Delegates must display a valid parking permit, which we will provide to you.

Accommodation

We offer an opportunity to book the University of Southampton halls of residence
at price 49.50 GBP per person per night
This accommodation can be booked during the online registration
Details:
Ensuite type
Bed & breakfast
Full English & Continental breakfast
http://www.southampton.ac.uk/uni-life/accommodation/halls/glen-eyre.page
Available number of rooms is limited
The reception for the University halls accommodation works 24/7
Check-in after 3 pm (there might be a possibility to check-in earlier upon request)
Check-out before 9:30 am
Note: Room keys need to be returned. If room keys are not returned or lost the fee of £25 GBP per key should be paid.

Other accommodation options near Highfield campus could be:
Highfield House Hotel www.highfieldhousehotel.co.uk
Elizabeth House Hotel www.elizabethhousehotel.com
Airbnb

Catering

Tea/coffee and light snacks will be provided twice per day during training.
Lunch can be purchased (it is not included in the course fee) from the nearby retail outlets on campus. Hot lunches can be purchased from the nearby Terrace Restaurant or Arlott Bar in the Staff Social Centre.
There will be an option for a social dinner on the 4th Day of the course.

Link to online registration form

Participants are invited to register online with this Google registration form

https://docs.google.com/forms/d/e/1FAIpQLScDkAyFvkFJel9T_zaP-XAffoSh4QYjldOZOPKa93qM5Tmamg/viewform

Early-bird Training fee for the whole 5-day course

Standard fee	857 GBP
Student fee (including PhD students)	657 GBP

Places are limited.

Early-bird registration closes on 26th June 2017

Note: The training fees starting from 27th June 2017 will be:

Standard fee	957 GBP
Student fee (including PhD students)	757 GBP

Registration closes on 14th August 2017

Cancellation policy

The cancellation is free of charge if cancellation is requested before 26th May 2017 (GMT). From the start of 26th May 2017 (GMT) the cancellation fee is £100 GBP.

Payment method

Note to students: In case you selected the student registration fee, please send your student enrolment confirmation to oop1g10@soton.ac.uk, before the payment.

Your registration will be valid only after the payment of the registration fee is made.

You will receive the confirmation of your registration and payment within 5 working days after the payment of your registration fee is received.

The fee is to be paid as follows:

Please write your Payment identifier as PEST_***Your Surname*** (for example: *PEST_**Johnson***)

Bank Transfer to:

Acc: 10191339
sort code: 16-31-23
SWIFT: RBOSGB2L
IBAN:GB26RBOS16312310191339

Contacts

For administrative enquiries please contact Oleksandra Pedchenko oop1g10@soton.ac.uk

Course instructors:
johndoherty@ozemail.com.au
f.lotti@kataclima.com
a.black@GWScience.co.uk

Training contents

DAY 1

4 September 2017

Day 1 sessions start 8:40 am

Day 1 sessions finish 6:45 pm

Session 1: Overview of calibration and uncertainty analysis using PEST

Presenter: John Doherty

- What is calibration?
- Metrics of a "good model"
- What should be expected of a model and what should not be expected
- Bayes equation
- Overview of PEST capabilities;
    - highly parameterized inversion
    - linear uncertainty analysis
    - nonlinear uncertainty analysis
    - direct hypothesis testing

Session 2: Some Basic Theory

Presenter: John Doherty

- Quick review of matrices and vectors
- Quick review of some statistical principles
- Random vectors and propagation of covariance
- Traditional parameter estimation – the well-posed inverse problem
- Parameter and predictive uncertainty where parameters can be uniquely estimated

Session 3: Traditional Parameter Estimation

Presenter: John Doherty

- Residuals as measures of misfit
- Definition of the objective function
- Use of observation weights
- Prior information
- Linear and nonlinear parameter estimation
- The Marquardt lambda
- Parameter bounds
- PEST and model-independence
- Template and instruction files

Session 4: Workshop

In this workshop PEST will be used to solve a well-posed inverse problem based on a simple model and a small calibration dataset. Students will work directly with PEST template, instruction and control files to inform PEST what steps it must take to calibrate the model. They will review the outcomes of the calibration process by inspecting PEST output files.

Day 2

5 September 2017

Day 2 sessions start 9:00 am

Day 2 sessions finish 6:45 pm

Session 1: PEST control variables

Presenter: John Doherty

- Termination criteria
- Calculation of finite-difference derivatives
- Parameter transformations
- Observation covariance matrices
- Examples of model types that can be used with PEST
- Serial PEST and Parallel PEST
- BEOPEST and PEST_HP
- Dealing with problematical models

Session 2: Regularization – some theory

Presenter: John Doherty

- The null space and the solution space
- Parameter non-uniqueness
- Regularization - the "cost of uniqueness"
- Optimum regularization
- Singular value decomposition
- Parameter/predictive error and parameter/predictive uncertainty
- Minimization of predictive error variance
- Linearization of Bayes equation

Session 3: Highly parameterized inversion

Presenter: John Doherty

- Tikhonov regularization
- Measurement and regularization objective functions
- Pilot points as a spatial parameterization device
- Optimal pilot point emplacement
- Pilot points and geostatistical regularization
- Covariance matrices as a regularization device
- Saving model runs with SVD-Assist
- Parameter identifiability
- The resolution matrix

Session 4: Workshop

In this practical session, course participants will solve a highly-parameterized inverse problem using Tikhonov regularization with singular value decomposition as a solution device. The same problem will then be solved using SVD-assist.

Day 3

6 September 2017

Day 3 sessions start 9:00 am

Day 3 sessions finish 6:45 pm

Session 1: Calibration of groundwater models – some practicalities

Presenter: John Doherty

- Steps to ensuring good finite-difference derivatives
- Detecting problematical finite-difference derivatives
- PEST groundwater utilities
- The PLPROC utility
- Defence against model defects
- Incorporating temporal and spatial differences into the objective function

Session 2: Some UK experiences

Presenter: Alastair Black

- Perceived philosophical problems with use of PEST
- Convincing the sceptics that PEST is OK
- Practical problems in using PEST with real-world models
    - model numerical instability
    - long run times
- Overcoming these problems

Session 3: Introduction to uncertainty analysis

Presenter: John Doherty

- Uncertainty analysis and sensitivity analysis
- Monte Carlo methods
- The RANDPAR and FIELDGEN utilities
- Basic statistics – the variogram
- Multiple point geostatistics
- Some other modern geostatistical methodologies
- Predictive uncertainty and spatial parameterization detail

Session 4: Simple calibration-constrained uncertainty analysis

Presenter: John Doherty

- Conceptualization of the problem
- Review of Bayes equation
- Constrained predictive maximization/minimization
- PEST's predictive analyzer
- Rejection sampling
- Markov chain Monte Carlo
- A pseudo-linear methodology available through PEST

Day 4

7 September 2017

Day 4 sessions start 9:00 am

Day 4 sessions finish 6:45 pm

Session 1: Highly-parameterized calibration-constrained uncertainty analysis

Presenter: John Doherty

- Examples of how calibrated models can make very wrong predictions
- Linear parameter and predictive uncertainty analysis
- Contributions to parameter and predictive uncertainty by different parameters
- Observation data worth
- Optimization of acquisition of further data
- Null-space Monte Carlo
- Examples

Session 2: Workshop

This workshop is a continuation of the workshop started on day 2. Participants will use linear analysis to:

- Compute parameter identifiability
- Calculate parameter and predictive uncertainty
- Quantify data worth
- Evaluate contributions to uncertainty by different parameter types

The same problem will then be addressed using nonlinear analysis. Participants will:

- Generate random parameter fields
- Subject these fields to calibration constraints
- Use null space Monte Carlo to evaluate parameter and predictive uncertainty

Session 3: Some Italian experiences

Presenter: Francesca Lotti

- A contaminated site in northern Italy: from conceptual model mistakes to uncertainty analysis
- How PEST can support the decision-making process

Session 4: Case Histories and other examples

Presenter: Alastair Black

- North East Anglia Chalk water resources
- London water resources
- Phosphate mine, Congo

Day 5

8 September 2017

Day 5 sessions start 9:00 am

Day 5 sessions finish 6:45 pm

Session 1: Accommodating model defects

Presenter: John Doherty

- Some examples of model defects
- Defence against model defects through formulation of a multi-component objective function
- Surrogate roles played by parameters
- Calibration-induced bias
- Implementation of the scientific method using models and inversion
- Model-based hypothesis testing; an example
- PEST's "pareto" mode

Session 2: Using PEST in surface water model calibration

Presenter: John Doherty

- Special problems that arise in surface water model calibration
- Regionalisation of parameters
- Transformation of flows
- Baseflow filtering
- Formulation of a multi-component objective function
- Simultaneous calibration of multiple models
- Suggestions for Tikhonov regularization
- The TSPROC utility
- Global optimization methods: SCE and CMAES

Session 3: Discussion and review

During this session participants can discuss issues raised in the course, ask for a review of certain topics, or examine how the lessons learned over the previous 5 days can be applied in their own modelling contexts.

Session 4: Continued discussion or workshop

Depending on the desires of course participants, we can either continue the preceding discussion, or do a workshop. The workshop allows participants to gain experience in using the PLPROC pre-processor which is designed to facilitate use of pilot points with structured and unstructured grid models. The workshop also provides experience in using the popular PARAVIEW 3D visualization package.

Post-Course On-line Sessions

(Free of charge, Optional - days and hours will be agreed with interested participants)

Online sessions will be held in the Moodle e-learning platform and will be provided after a few days of "ideas settlement". Instructions and credential for the access to the platform will be provided during the last course session. All on-line sessions will be recorded and available at a later time.

Online session 1: Q&A session

· During this session participants can ask questions about difficulties encountered in performing the exercises during the workshop sessions.
· An additional exercise (based on a simple real case-study) will be assigned to carry out as independent homework.

Online session 2: Discussion of completed homework

· During this session, participants can discuss about the ideas, solutions and results found for the exercise. Main challenges encountered will be discussed.

Online session 3: PEST suggestions and tips

· Participants will have the chance to take an individual skype meeting with the course leaders and ask suggestions about the optimal PEST use for any specific project. A preliminary email explaining the problem is recommended.