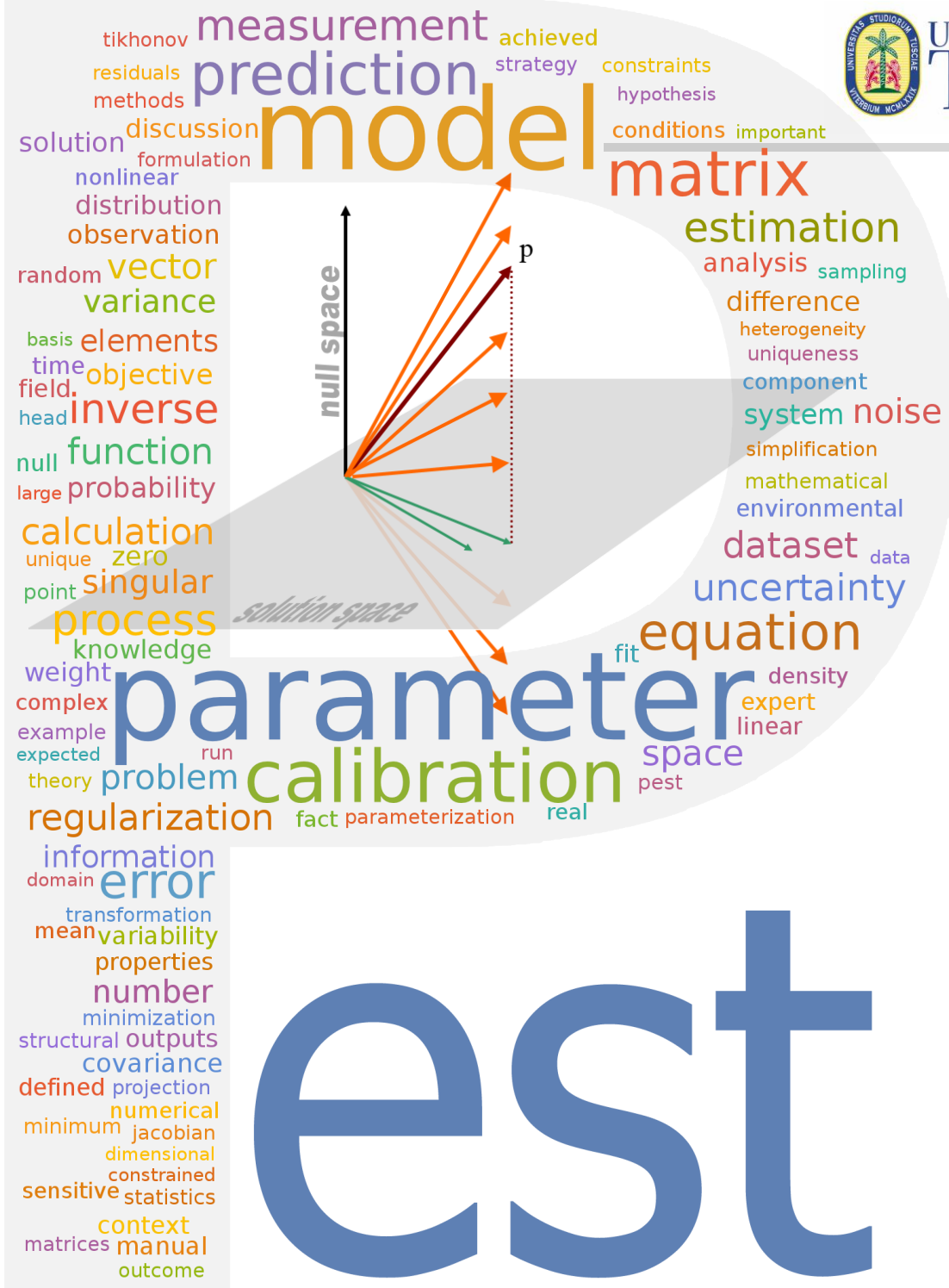




UNIVERSITÀ  
DEGLI STUDI DELLA  
Tuscia



Watermark Numerical Computing  
**kataclima**  
CATALYZING ENERGIES



## Technical Seminar

11 September 2017

# The Role of Numerical Models in Decision-Making

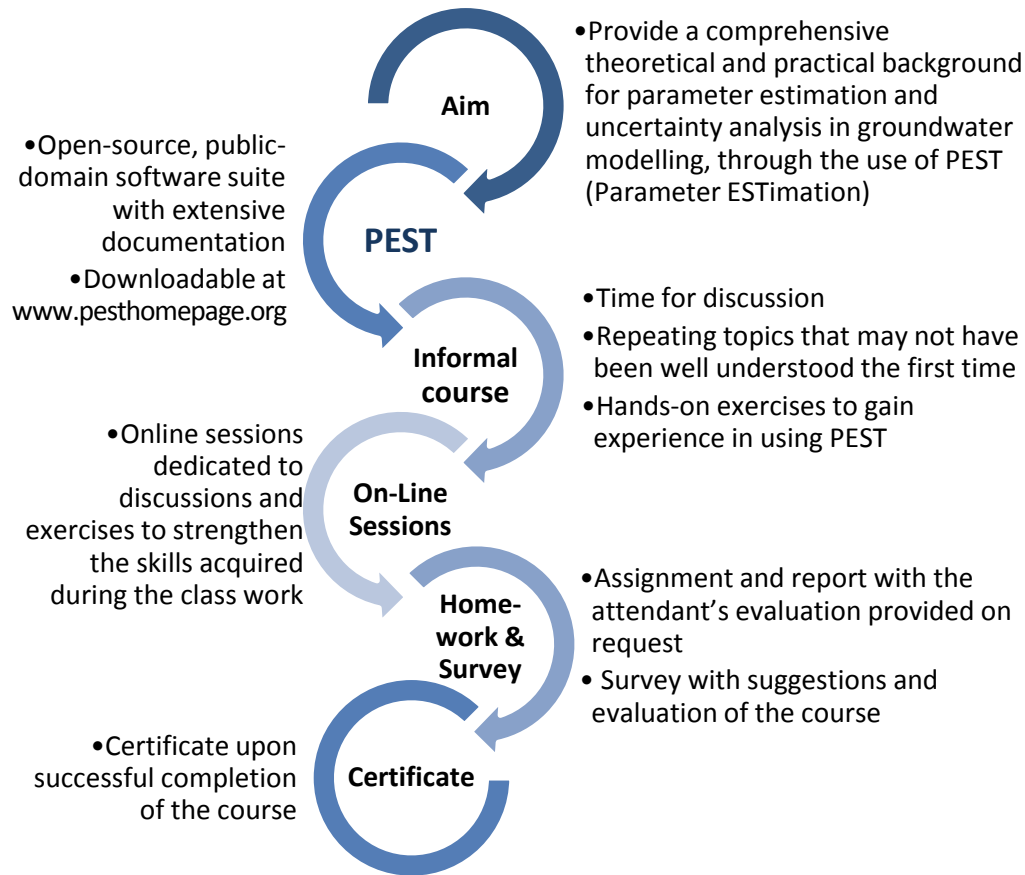
## Training Course

11-15 September 2017

# Model Calibration and Predictive Uncertainty Analysis using PEST

Dip. di Scienze Ecologiche e Biologiche (DEB)  
Università degli Studi della Tuscia  
Polo Universitario Civitavecchia  
P.zza Verdi 1, Civitavecchia

## THE COURSE



### Prerequisites

Basic knowledge of groundwater numerical modelling. Optionally, a basic understanding of matrices and vectors, statistics, geostatistics would be useful, but not essential.

### Memory Sticks content

- latest versions of PEST, BEOPEST and all PEST support utilities;
- workshop files and notes;
- published literature on PEST;
- copies of all slideshows used in the course;
- over 14 PEST workshops (with all associated documentation).

## INSTRUCTORS



**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.



**Francesca Lotti** is a consultant hydrogeologist and partner at Kataclima. She has 15 years of experience in field investigations and numerical modelling of contaminated sites, mines, geothermal systems, etc. She collaborates with research institutions and international companies. 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.

## COURSE & SEMINAR ORGANISER

Dipartimento di Scienze  
Ecologiche e Biologiche (DEB)

Università degli Studi  
della Tuscia

Course Coordinator  
Prof. **Vincenzo Piscopo**

Secretariat  
Dr. **Antonella Baiocchi**  
[baiocchi@unitus.it](mailto:baiocchi@unitus.it)

*Initiative with the recognition of the International  
Association of Hydrogeologists (IAH)*

**COURSE & SEMINAR PROGRAMME**

**DAY 1 – Sept. 11**

**Technical Seminar**

**The Role of Numerical Models  
in Decision-Making**

*(free entrance)*

- 8:30 Registration
- 9:00 Opening greetings
- 9:30 Presentation of the Workshop and of the course  
*Vincenzo Piscopo, Università della Tuscia*
- 10:00 Free and Open Source Software Tools for Water Resource Management: FREEWAT  
*Rudy Rossetto, Scuola Superiore S. Anna, Pisa*
- 12:30 Synergies among spatial databases, GIS and groundwater modelling
- 13:00 Lunch break
- 14:30 Overview of calibration and uncertainty analysis using PEST  
*John Doherty, Watermark Numerical Computing*
- 16:30 Case studies:
  - Exploring data uncertainty in the design of a hydraulic barrier  
*Giovanni Formentin, Tethys, Milano*
  - A contaminated site in northern Italy  
*Francesca Lotti, Kataclima, Viterbo*
  - Management of a thermal aquifer in central Italy  
*Vincenzo Piscopo, Università della Tuscia*
- 17:30 - Discussion and conclusions

**DAY 2 – Sept. 12**

**S1: 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

**S2: 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

**S3: Workshop**

In this practical session 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.

**S4: 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

**DAY 3 – Sept. 13****S1: Regularization – some theory**

Presenter: John Doherty

- The null space and the solution space
- Parameter nonuniqueness
- 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

**S2: 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

**S3: 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
- Defense against model defects
- Incorporating temporal and spatial differences into the objective function

**S4: Workshop**

In this 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 4 – Sept. 14****S1: Review of PEST graphical user interfaces**

Presenter: Francesca Lotti

- Available graphical user interfaces: Groundwater Vistas, Processing Modflow, GMS, FePEST, etc.
- Comparison, pros and cons
- What is not implemented yet (i.e., why it’s worth dealing with the command line)

**S2: Workshop**

This session is a continuation of the previous workshop. Alternatively (or as well) participants can discuss their own parameter estimation problems with the course leaders.

**S3: 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

**S4: 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

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**DAY 5 – Sept. 15**

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**S1: 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

**S2: 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

**S3: Workshop**

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 to:

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

**S4: Discussion and review**

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

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**Post-Course On-line sessions**

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*Optional - days and hours will be agreed with interested participants*

On-line 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.

**OL1: 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.

**OL2: Discussion of completed homework**

- During this session, participants can discuss about the ideas and solutions found for the exercise solution. Main troubles encountered will be discussed.

**OL3: PEST suggestions and tips**

- Participants will have the chance to take an individual meeting (about 2 h) with the course leaders and ask suggestions about the optimal PEST use for any specific project. A preliminary email explaining the problem is recommended.

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**General Info**

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**Laptop requirement**

All attendees should bring their own laptop computers. Software will be installed in a few minutes during the first workshop session.

**Daily course schedule**

Dates: 11 - 15 September 2017

- First day Seminar: 08:30 – 18:30
- Morning - Session 1: 09:00 – 11:00
- Morning - Session 2: 11:15 – 13:15
- Afternoon - Session 3: 14:30 – 16:30
- Afternoon - Session 4: 16:45 – 18:45

**Survey**

Participants will be welcomed to fill an on-line form about course evaluation and suggestions.

**REGISTRATION**

To register to the 1<sup>st</sup> day **Seminar** (free entrance), please write to [f.lotti@unitus.it](mailto:f.lotti@unitus.it).

To register to the **Course**, please complete the on-line form on this [link](#) or write to [f.lotti@unitus.it](mailto:f.lotti@unitus.it) to receive the link by email.

- Fees include:
- Course material
  - Memory stick
  - Coffee breaks
  - Access to live and recorded on-line sessions

**Places are limited, please register quickly!**

Participant	Early Registration	After July 15
<i>Student (Msc, PhD)</i>	600,00 + VAT 22%	750,00 + VAT 22%
<i>ECHN Member*</i>	600,00 + VAT 22%	750,00 + VAT 22%
<i>IAH Member*</i>	800,00 + VAT 22%	950,00 + VAT 22%
<i>Regular price</i>	1.200,00 + VAT 22%	1.400,0 + VAT 22%

\*If you want to take this opportunity and **join IAH**, become a member [here](#).

The fee is to be paid as Bank Transfer to:  
*Intesa Sanpaolo, via Polidori 27, Viterbo*  
 IBAN: IT76U0306914509100000300015  
 SWIFT/BIC CODE: BCITITMMXXX

Please, send the payment reference number to: [f.lotti@unitus.it](mailto:f.lotti@unitus.it)

**CONTACTS**

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 +39.338.4624787

**4 - 8 September 2017**

An equivalent **PEST** course will be held at the Southampton University, UK.

For further details, please contact:

**Oleksandra Pedchenko**  
[oop1g10@soton.ac.uk](mailto:oop1g10@soton.ac.uk)

**VENUE**

Polo Universitario Civitavecchia  
[P.zza Verdi 1](#), Civitavecchia

The Polo Universitario is at about 850 m from the Civitavecchia train station. To reach the building, walk along the Strada Statale Aurelia (Rome direction) and turn right after 850 m in Piazza Verdi.

[Train timetable](#)

[Taxi service](#) (Tel. +39.338.3661175)

