

# ETICS

## École Thématique sur les Incertitudes en Calcul Scientifique

### Research School on Uncertainty in Scientific Computing

June 6-10 2016

Centre de séminaire Séolane  
<http://eost.u-strasbg.fr/seolane/>

**Barcelonnette**



### Objectives

The goal of this school is to develop the skills of researchers and engineers in the domain of uncertainty management of computer codes. Some of the lectures will be followed by practical computer works. Collaborative works, round tables and poster sessions will promote exchanges between participants. The prerequisites to possess are the mathematical bases of the uncertainty quantification science.

### Lecturers

François Bachoc (Université Paul Sabatier): Calibration of computer experiments

Sébastien Da Veiga (Safran): Advanced methods in sensitivity analysis

Stéphane Gaiffas (Ecole Polytechnique): Methods for covariance matrix estimation -

Tim Sullivan (Free University of Berlin / Zuse Institute Berlin): Optimal distributionally robust uncertainty quantification

Nicolas Vayatis (ENS Cachan): Scoring and machine learning

### Organization

CEA DAM, EDF R&D, CMLA - ENS Cachan



**François Bachoc (Université Paul Sabatier)** – <http://www.math.univ-toulouse.fr/~fbachoc/>  
Calibration of computer experiments

Two questions of frequent interest in uncertainty quantification for computer models are: ‘what is the optimal or true tuning parameters of the computer model?’ and ‘Is there a residual error between the computer model and the underlying physical system’. We will present a probabilistic model, based on a Gaussian process modeling of the error process between the computer model and the physical system. This probabilistic model provides an explicit and convenient-to-implement answer to the two aforementioned questions, at the price of a linear approximation of the computer model, with respect to its tuning parameters. Depending on available time, two extensions can be considered: considering a Gaussian process model of the computer code to remove the linear approximation and iterative design of experiments for calibration.

**Sébastien da Veiga (Safran)**

Advanced methods in sensitivity analysis

Recently several authors proposed new viewpoints for sensitivity analysis in order to go further than Sobol indices, ranging from derivative-based indices to goal-oriented measures and density-based approaches. The objective of this course is threefold. First, we will draw a comparative picture of these methods by illustrating their strengths and weaknesses. We will also discuss screening methods and emphasize how state-of-the-art feature selection techniques from machine learning can efficiently address this problematic for computer experiments. Finally, we will introduce new density-based indices which rely on kernel embeddings of probability distributions. This framework not only makes it possible to link feature selection and standard sensitivity analysis, but also generalizes Sobol indices with a similar orthogonal decomposition. Under some assumptions on the considered kernels, main and interaction effects can be separated while much more complex inputs/outputs such as curves, images or even probability distributions can be accounted for.

Practical sessions in R will also be proposed to investigate these techniques on a large range of analytical examples.

**Stéphane Gaiffas (Ecole Polytechnique)** <http://www.cmap.polytechnique.fr/~gaiffas/index.html>

Methods for covariance matrix estimation

In this lecture we will describe techniques for matrix estimation, in particular covariance matrices, in a high-dimensional context. The focus will be on giving the fundamental tools from random matrix theory and convex optimization to both derive mathematical guarantees and efficient algorithms. We will in particular consider sparsity-inducing techniques based on the convex relaxation principle, for covariances in Gaussian and graphical Gaussian models.

**Tim Sullivan (Free University of Berlin / Zuse Institute Berlin)**

<http://userpage.fu-berlin.de/sullivan/>

Optimal distributionally robust uncertainty quantification

On top of probabilistic and modelling uncertainties, many uncertainty quantification problems have an added layer of complexity: we do not know exactly which probability model to use, or is "correct". In frequentist/aleatoric contexts, this may arise due to lack of knowledge about the random processes being modelled; in Bayesian/subjectivist contexts, this is the problem of prior elicitation. Naturally, it is desirable that scientific inferences remain robust to this kind of uncertainty. These lectures will outline some underlying mathematical theory and numerical methods for exploring parametric and non-parametric classes of probability models, and giving optimal bounds on quantities of interest with respect to those classes.

**Nicolas Vayatis (ENS Cachan)** - <http://nvayatis.perso.math.cnrs.fr/>

Scoring and machine learning

Machine Learning algorithms have become very popular in the last decade or so due to their spectacular efficiency in modern applications such as digital marketing, computer vision, fraud detection, ... However, their contribution to engineering sciences which heavily rely on domain-related modeling are less clear. The talk will provide an overview of machine learning techniques, with a specific focus on the problem of scoring which consists in recovering an order relationship over a high dimensional space, and will present some applications to model assessment for uncertainty quantification and experimental design for computer experiments and system design

## Program

### Sunday, June, 5th:

Shuttle from Marseille airport 17:00 and Aix TGV 17:30 to Barcelonnette (arrival 20:00pm)

### Monday, June, 6th:

9:00 - 9:30	Opening and Welcome speech	
9:30 – 12:30	Calibration of computer experiments	François Bachoc
14:00 – 17:30	Advanced methods in sensitivity analysis	Sébastien da Veiga

### Tuesday, June, 7th:

9:00 – 12:30	Methods for covariance matrix estimation	Stéphane Gaiffas
14:00 – 17:30	Calibration of computer experiments	François Bachoc

### Wednesday, June, 8th:

9:00 – 12:30	Optimal distributionally robust uncertainty quantification	Tim Sullivan
14:00 – 18:30	Social event	
18:30- 20:00	To define	

### Thursday, June, 9th:

9:00 – 12:30	Scoring and machine learning	Nicolas Vayatis
14:00 – 17:30	Talks to be defined	EDF, CEA

### Friday, June, 10th:

9:00 – 12:30	Advanced methods in sensitivity analysis	Sébastien da Veiga
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Shuttle from Barcelonnette 14:00 to Aix TGV 16:30 and Marseille airport 17:00