# ETICS 2023 École Thématique sur les Incertitudes en Calcul Scientifique Research School on Uncertainty in Scientific Computing https://www.gdr-mascotnum.fr/etics.html

October, 8-13, VVF Lège Cap Ferret, France



Source : <u>https://www.lege-capferret.com</u>

#### **Objectives**

The goal of this school is to develop the skills of researchers and engineers in the domain of uncertainty management of computer codes and machine learning techniques in support to engineering studies. Lectures will be followed by practical computer works. Discussions and poster sessions will promote exchanges between participants. The prerequisites to possess are the mathematical bases of the uncertainty quantification science.

#### Lecturers

Prof. Pierre Barbillon (AgroParisTech): Calibration of deterministic and stochastic computer models

Prof. Sébastien Le Digabel (Polyetchnique Montréal): Black-box optimization

Prof. <u>Mathilde Mougeot</u> (ENSIIE and ENS Paris Saclay): Leveraging knowledge to design machine learning despite the lack of data using Transfer Learning and PINNS models

Warning: The language of this ETICS edition will be in French

# Organization



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<u>Registration</u>: <u>https://www.gdr-mascotnum.fr/eticsregister23.html.</u> Registration fees (935 $\in$ , taxes included, 850 $\in$  without taxe) include accommodation, meals and transport by bus from and to Bordeaux train station.

### Schedule

Sunday, October, 8th: Bus (~1h) from Bordeaux Saint Jean (train station) to VVF at 17:30

#### Monday, October, 9th:

09:00 - 9:15	Opening and Welcome speech	Bertrand Iooss & Claire Cannamela
09:15 - 12:30	Calibration of deterministic and stochastic computer models	Pierre Barbillon
14:00 - 17:30	Blackbox optimization (Part 1)	Sébastien Le Digabel
18:30-20:00	Apéritif	All

## Tuesday, October, 10th:

09:00 - 12:30	Blackbox optimization (Part 2)	Sébastien Le Digabel
14:00 - 17 :30	Calibration of deterministic and stochastic computer models	Pierre Barbillon

### Wednesday, October, 11th:

09:00 - 12:30	PINNS	Mathilde Mougeot Khoa Nguyen Thi Nguyen
14:00 - 20 :00	Social event or free afternoon	

#### Thursday, October, 12th:

09:00 - 12:30	Talks PhD students	O. Baldé (30') M. Il Idrissi (30') T. Appriou (25')
		A. Van Biesbroeck (25') B. Ketema (20') N. Polette (20') R. Carpintero Perez (20')
14:00 - 17:30	Transfer learning	Mathilde Mougeot

# Friday, October, 13th:

10:00 - 12:15	Talks PhD students	G. Chennetier (30') B. Kratz (25') E. Jaber (20') A. Barry (25')
14:00 - ~15:00	Bus to Bordeaux Saint Jean (train station)	

## Coffee breaks of 30mn every day at 10:30 and 15:30

#### ABSTRACTS

# • Prof. <u>Pierre Barbillon</u> (AgroParisTech): Calibration of deterministic and stochastic computer models

We propose an overview of calibration methods for deterministic computer models. The choice of the design of experiments and the validation of computer models will be dealt with. The extension to stochastic simulators will be discussed.

#### • Prof. <u>Sébastien Le Digabel</u> (Polyetchnique Montréal): Black-box optimization

Derivative-Free Optimization typically occurs in engineering applications, when the function to be optimized, as well as the constraints of the problem, are given by the outputs of a computer simulation seen as a blackbox, possibly expensive to execute and contaminated by noise. In such a context, the derivatives are neither accessible nor calculable, which prevents the application of classical gradient-based methods. This course adopts a practical approach to solve such problems, by going around the different families of methods, as well as the different software available. Specific subjects will also be covered, such as handling of constraints, use of surrogates, discrete variables, multiobjective optimization, etc. The practical course includes manipulation of a solver as well as the modeling of a problem in the blackbox optimization setting.

# • Prof. <u>Mathilde Mougeot</u> (ENSIIE and ENS Paris Saclay): Leveraging knowledge to design machine learning despite the lack of data using Transfer Learning and PINNS models

In recent years, considerable progresses have been made in the implementation of decision support procedures based on machine learning methods through the exploitation of very large databases and the use of learning algorithms. In many research or production environments, the available databases are rarely so voluminous and the question arises as to whether in this context it is reasonable to use machine learning methods. The ETICS lessons will introduce transfer learning and hybrid models that use knowledge from related application or from physics to implement efficient models with an economy of data. Several achievements will be presented that successfully use these learning approaches to design machine learning for industrial small data regimes and to develop powerful decision support tools even in cases where the initial data volume is limited. Practical sessions will help to handle such models in python environments. References: -de Mathelin, A., Deheeger, F., Mougeot, M., Vayatis, N. From Theoretical to Practical Transfer Learning: the ADAPT library, Federated and Transfer Learning Springer book. 2023. -Weiss K., Khoshgoftaar, T Wang, D. A survey of transfer learning, Journal of Big data, 2016. -Nguyen, Khoa.T.N, Dairay, T., Meunier, R., Mougeot, M. (2022) Physics-informed neural networks for non-Newtonian fluid thermo-mechanical problems: an application to rubber calendering process, Engineering Applications of Artificial Intelligence, vol. 141. -Raissi, M., Perdikaris, P. Karniadakis, G.E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 2019.

#### Lectures from PhD students'

Tanguy Appriou, 2<sup>nd</sup> year: Combination of Optimization-free Kriging Models for High-Dimensional problems

Oumar Baldé, 3<sup>rd</sup> year, Bayesian calibration for the quantification of conditional uncertainty of input parameters in chained numerical models

Adama Barry, 2<sup>nd</sup> year, Plans d'expériences pour la calibration de codes de calcul

Raphaël Carpintero Perez, 1st year: Gaussian process regression for high dimensional graph inputs

Guillaume Chennetier, 3<sup>rd</sup> year: Simulation d'événements rares pour des marches aléatoires sur des graphes finis

Marouane II Idrissi, 3<sup>rd</sup> year: Hoeffding-ANOVA decomposition of functions with dependent random inputs

Edgar Jaber, 1st year: Conformal Prediction for surrogate modelling in the UQ framework

Baalu Ketema, 1st year: Optimization on Riemannian Manifolds for Uncertainty Quantification

Boris Kratz, 2<sup>nd</sup> year: Calibrating a 3D Finite Element Model of Tunnel Boring Machine Excavation Using Monitoring Data Through Bayesian Approaches

Nadège Polette, 1st year: Field uncertainties estimation through [hyper]parameters sampling using Bayesian inference

Antoine Van Biesbroeck, 2<sup>nd</sup> year: Reference prior construction for Bayesian inference applied to seismic fragility curve estimation