**Program AI4OAC'2023 workshop**

# Workshop on AI for Ocean, Atmosphere and Climate Dynamics

*11-13 April 2023 Brest (France)*

**Workshop venue for in-person participants**: PNBI, Brest (google map)

- Room 207 (3rd floor) for keynote and tutorial sessions
- Rooms 207, 113 and 127 for working groups (2nd and 3rd floors)
- Coffee breaks, lunch and oyster aperitive (1st floor)

**Webex links below for remote attendees:**

- **Tuesday, April 11th, 2023:** link
- **Wednesday, April 12th, 2023:** link
- **Thursday, April 13th, 2023:** link

## Tuesday, April 11th, 2023

**Video-conference link**:
https://imt-atlantique.webex.com/imt-atlantique/j.php?MTID=mec4ebf7e2cb36dbe2bfa731d5a30f432

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| 1.30pm-1.50pm | **Welcome coffee & tea** |
| 1.50pm-2.00pm | **Welcome word** (R. Fablet) |
| 2.00pm-4.00pm | **Keynote session on ML for climate model calibration**<br>*Chairs: R. Lguensat and J. Brajard*<br><br>**R. Roehrig.** Addressing the calibration bottleneck using machine learning: application to the CNRM-CM6-1 climate model (abstract)<br><br>**K. Hayes**. AI Uncertainty Quantification: An Introduction to Approaches for Creating and Evaluating Uncertainty Estimates Using Neural Networks. (abstract) |
| 4.00pm-4.30pm | **Tea & Coffee time** |
| 4.30pm-5.00pm | **2-minute poster pitches #1 (see list below)** |
| 5.00pm-5.30pm | **Presentation of the proposed working groups' themes** |
| 5.30pm-6.30pm | **Poster session #1** |
| 6.30pm-8.00pm | **Oyster pause** |

## Wednesday, April 12th, 2023

**Video-conference link**:
https://imt-atlantique.webex.com/imt-atlantique/j.php?MTID=m7d394d0bbb4752e310b4768fc526d652

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| 9.30am-10.45am | **Tutorial on Diffusion Models. (abstract)**<br>*Chair: F. Rousseau* |
| 10.45am-11.00am | **Tea & Coffee time** |
| 11.00am-12.30pm | **Working group sessions (**in parallel**)** |
| 12.30pm-2.00pm | **Lunch** |
| 2.00pm-4.00pm | **Keynote session on ML for climate data analytics**<br>*Chair: P. Naveau*<br><br>**L. Raynaud**. About Machine Learning to explore and enhance ensemble weather forecasts : an overview of current activities at CNRM. (abstract)<br><br>**M. Demangeot**. Insight into spatial extremes and Geostatistics (abstract) |
| 4.00pm-4.30pm | **Coffee break** |
| 4.30pm-5.00pm | **2-minute poster pitches #1 (see list below)** |
| 5.00pm-6.00pm | **Poster session #2** |

## Thursday, April 13th, 2023

https://imt-atlantique.webex.com/imt-atlantique/j.php?MTID=m576b5d781145559d53de22b5fc155cbd

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| 9.30am-10.45am | **Tutorial on Implicit Representations.**<br>*Chair: J.E. Johnson* |
| 10.45am-11.00am | **Tea & Coffee time** |
| 11.00am-12.30pm | **Working group sessions** |
| 12.30pm-2.00pm | **Lunch** |
| 2.00pm-4.00pm | **Keynote session on ML for model discovery**<br>*Chairs: F. Bouchet*<br><br>**T. Beucler**. AI Uncertainty Quantification: An Introduction to Approaches for Creating and Evaluating Uncertainty Estimates Using Neural Networks. (abstract)<br><br>**P. Hassanzadeh**. Learning Data-driven Subgrid-scale Parameterizations: Stability, Extrapolation, and Interpretation (abstract) |
| 4.00pm-4.30pm | **Coffee break** |
| 4.30pm-5.30pm | **Wrap-up session** |

## Workshop Keynotes

**Addressing the calibration bottleneck using machine learning: application to the CNRM-CM6-1 climate model. Romain Roehrig, CNRM, Meteo France.**

Atmospheric models, used for either weather or climate applications, encompass so-called parameterizations, which aims at summarizing and quantifying the impact on the resolved model variables of radiative, thermodynamical, or chemical processes, as well as dynamical processes that occur at scales smaller than the computational grid. Though these parameterizations are developed on a physical basis, some simplifications underlying them introduce parameters that need to be properly calibrated to achieve a skillful model. Given the number of parameters (several tens), the possible number of performance metrics used for validation or evaluation, and the computational cost of models, the modelling experts need help to better address this calibration bottleneck. In this work, we experiment the history matching with iterative refocusing framework with the CNRM-CM6-1 climate model to assess whether the model current deficiencies are related to poor model calibration, or if they critically rely on the scientific content of the model. Using a rather small physics perturbed ensemble of short simulations as a learning dataset, Gaussian processes are used to cheaply explore the full space of model parameters and identify the part of it, which provides model configurations compatible with references, given a set of usual performance metrics and the various sources of uncertainty in the whole process. The calibration framework also builds on several waves of true model simulations, to parsimoniously increase the size of the learning dataset only where the surrogate model uncertainty needs to be reduced. We show that several new configurations, in which many CNRM-CM6-1 biases are significantly reduced or even removed (e.g., precipitation over West Africa, regional biases in cloud radiative effect), can be found. Though, some CNRM-CM6-1 biases are truly structural (e.g., biases over eastern sides of tropical ocean basins), calling for further understanding and parameterization development.

**AI Uncertainty Quantification: An Introduction to Approaches for Creating and Evaluating Uncertainty Estimates Using Neural Networks. K. Hayes. CIRA, CSU.** (Joint work with Ryan Lagerquist, Marie McGrawa, Kate Musgravea, and Imme Ebert-Uphoff**)**

Due to the availability of large amounts of simulation and observation data in ocean-atmosphere-climate science, AI methods can be useful for exploring open questions in these scientific fields. Due to the increasing impacts of climate change, results from this community are vital in informing policy decisions. Given the critical nature of these applications, it is increasingly important to obtain uncertainty estimates along with the results. The computer science community has recently made significant advances in developing methods for neural networks that allow these models to provide uncertainty estimates for both prediction and classification tasks. The goal of this talk is to provide an accessible introduction to AI-based uncertainty quantification, focusing on four key questions: (1) What uncertainties are we tasking our machine-learning (ML) models to estimate? (2) What are some simple approaches that can be implemented in neural network models to create uncertainty estimates? (3) Once we obtain uncertainty estimates, how do we know whether they are any good? (4) How do we best communicate the uncertainty estimates?

This presentation discusses these topics and illustrates several common approaches and evaluation metrics using a real-world atmospheric science application. We hope that this introduction will pave the way for researchers in this community to quickly start incorporating uncertainty estimates in their applications.

**About Machine Learning to explore and enhance ensemble weather forecasts : an overview of current activities at CNRM. Laure Raynaud. CNRM, MEteo France.**

Ensemble forecasts have become a major tool to anticipe high-impact weather events and their uncertainties. However, their effective use is currently limited by two main aspects. First, their configuration, using kilometer-scale resolution and about twenty members for state-of-the-art systems, is generally not sufficient to accurately predict location, intensity and timing of events. Secondly, summarizing this ensemble information in a relevant and user-oriented way is still a challenge. In recent years, Machine Learning (ML) has been considered as a potential solution to address these two subjetcs. Several post-processing tools relying on feature extraction and dimension reduction have been developed to better explore ensembles. Going toward hybrid Physics/ML forecasts is another avenue of improvement to significantly increase ensemble size and resolution at almost no additional cost.

**Insight into spatial extremes and Geostatistics. M. Demangeot. Univ. Montpellier.**

**Physically and Causally-Informed Machine Learning for Atmospheric Convection. Tom Beucler. Univ. Lausanne.** (Joint work with Fernando Iglesias-Suarez, Veronika Eyring, Pierre Gentine, Michael Pritchard, Jakob Runge)

Data-driven algorithms, in particular neural networks, can emulate the effects of unresolved processes in coarse-resolution Earth system models (ESMs) if trained on high-resolution simulation or observational data. However, they can (1) make large generalization errors when evaluated in conditions they were not trained on; and (2) trigger instabilities when coupled back to ESMs. First, we propose to physically rescale the inputs and outputs of neural networks to help them generalize to unseen climates. Applied to the offline parameterization of subgrid-scale thermodynamics (convection and radiation) in three distinct climate models, we show that rescaled or "climate-invariant" neural networks make accurate predictions in test climates that are 8K warmer than their training climates. Second, we propose to eliminate spurious causal relations between inputs and outputs by using a recently developed causal discovery framework (PCMCI). For each output, we run PCMCI on the inputs time series to identify the reduced set of inputs that have the strongest causal relationship with the output. Preliminary results show that we can reach similar levels of accuracy by training one neural network per output with the reduced set of inputs; stability implications when coupled back to the ESM are explored. Overall, our results suggest that explicitly incorporating physical knowledge into data-driven models of Earth system processes may improve their ability to generalize across climate regimes, while quantifying causal associations to select the optimal set of inputs may improve their consistency and stability.

**Learning Data-driven Subgrid-scale Parameterizations: Stability, Extrapolation, and Interpretation P. Hassanzadeh.** Rice Univ.
The Earth system involve a variety of nonlinearly interacting physical processes spanning a broad range of spatial and temporal scales. To make simulations of the Earth system accurate while computationally tractable, processes with scales smaller than the typical grid size of general circulation models (GCMs) have to be parameterized. Recently, there has been substantial interest (and progress) in using machine learning (ML) to develop data-driven subgrid-scale (SGS) parameterizations for a number of key processes in the atmosphere, ocean, and other components of the Earth system. However, for these data-driven SGS parameterizations to be useful and reliable in practice, a number of major challenges have to be addressed. These include: 1) instabilities arising from the coupling of data-driven SGS parameterizations to coarse-resolution solvers, 2) learning in the small-data regime, 3) interpretability, and 4) extrapolation to different parameters and forcings. Using several setups of 2D turbulence, as well as two-layer quasi-geostrophic turbulence and Rayleigh-Benard convection as test cases, we introduce methods to address (1)-(4). These methods are based on combining physics and recent theoretical and applied advances in ML. For example, we will use backscattering analysis to shed light on the source of some of the instabilities and incorporate physical constraints to enable learning in the small-data regime. We will further introduce a novel framework based on spectral analysis of the neural network to interpret the learned physics and will show how transfer learning enables extrapolation to flows with very different physical characteristics. We will also briefly mention some of the advances in supervised and semi-supervised learning of the SGS models, as well as the use of equation-discovery techniques. In the end, we will discuss scaling up these methods to more complex systems and real-world applications, e.g., for SGS modeling of atmospheric gravity waves.

## Workshop Tutorials

### Introduction to diffusion models. François Rousseau. IMT Atlantique.

Diffusion models have emerged as a powerful new family of deep generative models. They have achieved remarkable performance in many applications, including image synthesis and video generation. In this presentation, we will provide an overview of the rapidly growing body of work on diffusion models, looking at key areas such as efficient sampling or likelihood estimation. Time will be devoted to a hands-on session to illustrate the use of diffusion models on toy examples and images.

### Introduction to Implicit representation learning. J. Emmanuel Johnson. CNRS/UGA.