3iA Côte d'Azur
Interdisciplinary Institute
for Artificial Intelligence

Ph.D. research topic

- Title of the proposed topic: Machine Learning for Computer Simulation
- Research axis of the 3IA: Axis 1: Core elements of AI
- **Supervisor (name, affiliation, email):**
    - **Motonobu Kanagawa, EURECOM, motonobu.kanagawa@eurecom.fr**
- Potential co-supervisor (name, affiliation):
- The laboratory and/or research group: Data Science Department, EURECOM

Apply by sending an email directly to the supervisor.
The application will include:

- Letter of recommendation of the supervisor indicated above
- Curriculum vitæ.
- Motivation Letter.
- Academic transcripts of a master's degree(s) or equivalent.
- At least, one letter of recommendation.
- Internship report, if possible.

- Description of the topic:

Consequential decision-making requires a careful assessment of the resulting effects, before actually implementing that decision. For instance, for the decision of building a new facility in a city (e.g., dam, road, power plant), the policymaker must know the resulting effects on the environment beforehand. Similarly, to mitigate Climate Change, governments must assess how a candidate policy will affect the amount of CO_2 emissions and the resulting future climate. Such assessments must be done before committing the decision of interest, because the decision may be costly to implement, or may be irreversible (i.e., once the decision has been implemented, we can never recover the state before the decision).

Computer simulation is a powerful tool that enables such assessments. It has been widely used in many scientific and engineering fields for modeling time-evolving complex real-world phenomena. Examples include simulators for climate change, natural disasters (e.g., flood, tsunami), epidemics (e.g., Covid-19), transportation (e.g., traffic), and industrial manufacturing processes, to name a few. However, a key question must be addressed before using simulations for decision-making: Can we trust the results of computer simulation? A simulator is just an approximation of real-world phenomena, and its reliability totally depends on its quality of approximation. Therefore, for reliably using computer simulation in decision-making, we first need to quantify and improve the quality of approximation. These are the validation and calibration tasks that we deal with in this project.

The project aims to develop generic techniques to improve the reliability of computer simulation, based on machine learning (or AI). This topic is crucial for our society, given the widespread use of computer simulation in high-impact decision-making (e.g., policies on climate change and Covid-19). However, the literature on simulation calibration and validation is far from mature, as has been discussed for climate simulation [1]. Machine learning can play a key role here [e.g., 2,3,4], and the Ph.D. project aims to contribute in this regard.

[1] Frédéric Hourdin, Thorsten Mauritsen, Andrew Gettelman, Jean-Christophe Golaz, Venkatramani Balaji, Qingyun Duan, Doris Folini, Duoying Ji, Daniel Klocke, Yun Qian, et al. The art and science of climate model tuning. Bulletin of the American Meteorological Society, 98(3):589–602, 2017.

[2] Keiichi Kisamori, Motonobu Kanagawa, and Keisuke Yamazaki. Simulator calibration under covariate shift with kernels. In International Conference on Artificial Intelligence and Statistics (AISTATS), pages 1244–1253. PMLR, 2020.

[3] Kyle Cranmer, Johann Brehmer, and Gilles Louppe. The frontier of simulation-based inference. Proceedings of the National Academy of Sciences, 117(48):30055–30062, 2020.

[4] M. U. Gutmann and J. Corander. Bayesian optimization for likelihood-free inference of simulator-based statistical models. Journal of Machine Learning Research, 17(125):1–47, 2016.