Master Thesis / Internship:
Discovering the Laws of Physics Through the Bilevel Learning of Neural Operators

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Context: Recent progress in experimental physics have revealed gaps in our understanding of various phenomena. A prime example is the complex physics underpinning the interaction between ultra-fast laser pulses and surfaces, resulting in the formation of intriguing patterns with promising applications, including hydrophobic and antibacterial properties. However, the precise partial differential equation (PDE) governing these phenomena remains only partially known. In recent years, physics-informed machine learning has emerged as a powerful tool for estimating PDE solutions based on initial conditions. Unfortunately, these approaches have the drawback of requiring the PDE to be known a priori [1].

Mission: The originality of this thesis proposal lies in framing both the learning of the PDE and its solution as a bilevel optimization problem. Bilevel optimization is widely utilized in various machine learning tasks, such as neural architecture search, meta-learning, and hyperparameter optimization [2, 3]. In this context, the candidate will devise and address a bilevel problem comprising the following two nested problems. On one hand, the lower problem aims to determine the solution of a given PDE. On the other hand, the upper problem focuses on learning the PDE in a way that the solution found in the lower problem aligns with the observed data. In particular, the candidate will explore the application of physics-informed neural operators [4] for modeling the solution of the PDE and to efficiently compute its partial derivatives in the Fourier space. Expected results encompass:

- Bibliographical study on physics-based machine learning and neural operators
- Design of a PyTorch toolbox to learn the PDE governing observed data
- A publication in a leading journal or conference could be considered depending on the results

References

[1] M. Raissi et al. (2019). Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear PDE. *Journal of Computational Physics*.

[2] J. Frecon et al. (2020). Unveiling Groups of Related Tasks in Multi-Task Learning. *International Conference on Pattern Recognition* (ICPR).

[3] Z. Hao et al. (2023). Bi-level Physics-Informed Neural Networks for PDE Constrained Optimization using Broyden's Hypergradients. *International Conference on Learning Representations* (ICLR).

[4] Z. Li et al. (2021). Physics-informed neural operator for learning partial differential equations. *Preprint* (ArXiv).