– Thesis Offer –

Unveiling and Incorporating Knowledge in Physics-Guided Machine Learning Models

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Team: Data Intelligence
Host laboratory: Hubert Curien Lab UMR CNRS 5516, Saint-Etienne, France
Application deadline: May 1st, 2023

Keywords: Physics-guided models; Neural networks; Sparsity; Transfer learning; Optimization

Context   In many physical systems, the governing partial differentiation equations (PDEs) are known with high confidence, but simulating a numerical solution can be prohibitively expensive. In other contexts, the PDEs are unknown (or partly known to some extent) and unveiling them from experimental data is the central goal since they could help in shedding some lights on the underlying physical process. Recently, physics-guided machine learning models have shown to be a promising tool in both above-mentioned scenarios. They rely on neural networks in order to simulate the physical quantities of interest at various temporal and spatial positions. Training such neural networks entails to incorporate physical constraints, usually in the form of a PDE and boundary conditions, and/or to be able to generate plausible simulated data reproducing the experimental data at hand [1].

Description   The originality of the present thesis proposal is to embrace the extreme setting encountered in surface engineering, that is limited prior physical knowledge and few experimental data [2]. In order to overcome both limitations, the thesis will develop a unified end-to-end framework from the physics modeling to the algorithms used for training physics-guided models:

1. Develop novel regularization techniques, possibly on latent representations [3], to incorporate partial physical constraints (e.g., conservation laws or decreasing lypuanov exponents along the trajectories) and incertitude about prior knowledge.

2. Promote sparse methods to circumvent the lack of data. Investigate neural network *sparse by design* preventing redundancy and over-parametrization of trivial mappings [4]. Explore optimization strategies to promote sparse weights by leveraging the properties of the compositional form of neural networks [5].

3. Discover the semantic of PDEs from few data with the dual objective of adapting to new physical environments (e.g., different surface properties or laser characteristics).

The advances that will be carried out in machine learning will allow to better understand the physics underlying the mechanisms of laser/radiation-matter interaction, enabling to address numerous societal challenges in the fields of space, nuclear, defense, energy or health.

Candidate profile

- Master in computer science, machine learning, applied mathematics or related. Outstanding applications from physicists will also be considered
- Good Python programming skills. PyTorch experience is welcomed
- Good knowledge of neural networks
- Basic knowledge on optimization and partial differential equations
- High proficiency in English

Application Candidate must send the following documents to both amaury.habrard@univ-st-etienne.fr and jordan.frecon.deloire@univ-st-etienne.fr as <u>soon as possible</u>:

- Cover letter with justification of your skills for the topic
- A complete Curriculum Vitae
- Transcript of your bachelor and master's grades (Semester 1 and 2, Semester 3 if available)
- CEFR level in English (except if university courses were taught in English)
- Any additional document: letter(s) of recommendation, publications, master thesis, etc.

Please feel free to contact us beforehand for any further pieces of information.

Funding The selected candidate will be assisted to obtain a 36 months funding from the Doctoral School ED SIS. The monthly gross salary is about 2044€.
More information: `https://edsis.universite-lyon.fr`

Host laboratory The Hubert Curien Lab combines internationally recognized experts in both machine learning and laser-matter interaction. The present thesis is in line with the Hubert Curien Lab commitment to foster the development of new joint methodological contributions at the interface between machine learning and surface engineering.
More information: `https://laboratoirehubertcurien.univ-st-etienne.fr`.

References

[1] Raissi, M. et al. (2019). Physics-Informed Neural Networks: A deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. In *Journal of Computational physics*.

[2] Brandao, E. et al (2022). Learning PDE to Model Self-Organization of Matter. In *Entropy*.

[3] Li, Z. et al. (2021). Fourier Neural Operator for Parametric Partial Differential Equations. In *International Conference on Learning Representations*.

[4] Frecon, J. et al. (2022). Bregman Neural Networks. In *International Conference on Machine Learning*.

[5] Verma S. and Pesquet J.-C. (2021). Sparsifying networks via subdifferential inclusion. In *International Conference on Machine Learning*.