PhD Thesis:

Leveraging Monotone Operator Theory and Variational Principles for Physics-Informed Neural Operators

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Keywords: Physics-informed deep learning; Proximal Optimization; Complexity

Context: Recently, deep learning surrogates such as neural operators (NOs) have shown great success in efficiently approximating complex, high-dimensional dynamical systems [1]. Unlike traditional neural networks (NNs), which learn mappings between finite-dimensional spaces, NOs learn mappings between function spaces. Their design closely mirrors that of NNs, but replaces linear layers with integral operators in function space. Physics-informed NOs extend this framework by embedding physical constraints into the learning process, typically enforcing underlying physical laws such as partial differential equations (PDEs). These latter operators are trained using both data-driven techniques and physics-based regularization, where the loss function penalizes deviations from the governing PDEs [2]. They offer a promising alternative to traditional numerical PDE solvers, providing faster predictions with discretization-invariant performance.

Mission: The reasons for their success are still not fully understood. A critical aspect of this ongoing exploration is determining *how the complexity of these operators is controlled*—whether through explicit regularization techniques or implicitly via their architectural design. In the case of the latter, it's important to note that while physics-informed NOs map function spaces constrained by physical laws, their architectures remain largely unstructured, meaning agnostic to physical considerations. This highlights the need for *developing methods that can impose structure on these operators*, enabling them to more effectively capture the underlying physical phenomena, thereby reducing the amount of data required for successful training. In this thesis, we aim to adopt an ambitious approach and borrow tools from the monotone operator theory [4], an important area of nonlinear analysis, to further understand and control the complexity of (physics-informed) NOs. The objectives are as follows.

1. Establish the first framework to structure the architectural design of NOs from physical knowledge, possibly by extending the preliminary study done in [3].
2. Study how the architecture and regularized training of physics-informed NOs control the complexity of mappings they can represent.
3. Address the challenging yet rewarding task of modeling dynamics in surface engineering using structured NOs to minimize both data and physical knowledge requirements for training.

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 deep learning and numerical optimization
- Basic knowledge on partial differential equations
- High proficiency in English

Application Candidate must send the following documents to jordan.patracone@univ-st-etienne.fr.

- 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)
- 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 is expected to be funded by the *Agence nationale de la recherche* (ANR) project MONALISA, currently under review. However, other secured funding sources can be considered as alternatives. The monthly gross salary is approximately 2200€.

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`.

Host team The Inria team MALICE brings together expertise in statistical learning and laser-matter interaction at the Hubert Curien lab to advance Physics-informed Machine Learning for Surface Engineering. The team combines skills in computer science, applied mathematics, statistics, and optimization with physicists specializing in ultrashort laser-matter interaction. This synergy enables breakthroughs in both fields: tackling ML challenges such as data scarcity, theoretical guarantees, and knowledge transfer between dynamical systems, while also leveraging ML to deepen our understanding of laser/radiation-matter interactions for applications in space, nuclear, defense, energy, and health.
More information: `https://labhc-malice.github.io/`.

References

[1] Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Neural Operator: Learning Maps Between Function Spaces With Applications to PDEs". In: J. Mach. Learn. Res. (2023).

[2] Zongyi Li, Hongkai Zheng, Nikola Kovachki, David Jin, Haoxuan Chen, Burigede Liu, Kamyar Az- izzadenesheli, and Anima Anandkumar. "Physics-Informed Neural Operator for Learning Partial Differential Equations". In: ACM/IMS JDS (2024).

[3] Abdel-Rahim Mezidi, Jordan Patracone, Saverio Salzo, Amaury Habrard, Massimiliano Pontil, Remi Emonet, and Marc Sebban. "Bregman Proximal Viewpoint on Neural Operators". submitted to ICML. 2025

[4] Patrick L Combettes and Jean-Christophe Pesquet. "Deep neural network structures solving variational inequalities". In: Set-Valued Var. Anal. (2020).