PhD position, Paris, France

Hybrid Deep Learning and Physical approaches.

Application to energy transition: improving the sustainability of energy systems.

Contact : Patrick Gallinari, patrick.gallinari@sorbonne-universite.fr, Nicolas Thome, nicolas.thome@sorbonne-universite.fr

Location: Sorbonne Université, Pierre et Marie Curie Campus, 4 Place Jussieu, Paris, Fr

Candidate profile: Master degree in computer science or applied mathematics, Engineering school. Background and experience in machine learning. Good technical skills in programming.

How to apply: please send a cv, motivation letter, grades obtained in master, recommendation letters when possible to patrick.gallinari@sorbonne-universite.fr, nicolas.thome@sorbonne-universite.fr

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Keywords: deep learning, physics-based deep learning, energy transition systems

Context

Modeling complex physical system is a fundamental task in a wide range of scientific domains. Physics-based models are reliable, interpretable but may suffer from different drawbacks. They are slow to develop relying on an in depth understanding of the underlying phenomenon, the numerical models are often computationally intensive, requiring significant computational resources and expertise. The successes of deep-learning (DL) altogether with the increasing availability of large amounts of data, either observations or simulations, has motivated the interest of scientific communities for data intensive alternatives to the classical physical approach. On the other hand, DL predictions do not necessarily obey physical laws governing physical systems, nor do they generalize to multiple physical situations. Hence, hybrid models, exploiting both physical priors and DL ability to model data appears as a promising direction to better solve scientific problems. The objective of this PhD proposal is to explore the development of hybrid physics-machine learning models by exploring fundamental aspects and applicative ones in the context of multi-scale energy systems.

This work is part of a multi-disciplinary project aimed at developing machine learning (ML) solutions for energy transition and renewal. This PhD proposal will focus on the Machine Learning aspects with the development of methodological and theoretical contributions. In parallel another PhD will start on the same topic, at another one of the project partner site, with a focus on the application aspects in the energy domain. The two candidates will cooperate throughout the project duration.

Research directions

Hybrid physical-ML models

The primary objective is to investigate diverse modes for the cooperation of ML and physics models in order to improve the state of the art in the modeling of complex physical systems. The integration of physics priors and ML has recently motivated the interest of several communities (Willard 2020). We will focus here on the modeling of spatio-temporal dynamics that underly the evolution of physical systems in many domains such as such earth science, biology and of course energy systems which is our target application domain. The classical modeling tools for such dynamics in physics and applied mathematics rely on partial differential equations (PDE). We then consider situations where the physical prior background is provided by PDEs. A first problem corresponds to the situation where the PDEs are too complex to run a full simulation and ones wants to reduce the simulation cost. A possible strategy here is to run a simulation at a coarse precision and use ML for complementing the physical simulation and reach high fidelity prediction. This has been explored e.g. in (Um 2020, Kochkov 2021). A related problem corresponds to the case where the PDE only provides partial information about the underlying physical phenomena and this physical knowledge it is to be complemented with ML. Initial attempts to solve similar problems can be found in recent work such as (de Bezenac 2018, Harlim 2020, Yin 2021, Dona 2022). These issues (fast surrogate models, enhanced ML based physics, increased model robustness) will be further developed during the PhD project with the objective of analyzing and developing different integration frameworks.

Multi-scale modeling

A key issue for energy transition is the joint modeling of complex energy systems operating at different scales both spatially (from components to networks) and temporally (from fast dynamics to low seasons dynamics in renewable energy). On the formal ML side, this means that one should develop components that are (i) able to handle multiple scales and (ii) integrate their interactions. For the first issue, a starting point will explore how to adapt neural operators for the simultaneous modeling of multiple scales (Li 2022, Yin 2023). The second issue is largely open and has not been considered so far from a ML perspective.

Application domain

The methodological developments will be motivated and inspired by practical problems involving the modeling of energy systems in the context of energy transition challenges. Building new systems that contribute to decarbonization and sustainability make the global energy systems more complex thus requiring new tools for their modeling. In particular multi-carrier energy systems (MES) target the coupling of energy at multiple scales (for example components and distribution networks). MES modeling will serve both and an inspirational source for the formulation of physics-deep learning hybrids and for the evaluation of the hybrids in practical cases. This work will be conducted in cooperation with partners specialists of energy transition.

References

- de Bezenac, E., Pajot, A. and Gallinari, P. 2018. Deep Learning For Physical Processes: Incorporating Prior Scientific Knowledge. *ICLR* (2018).
- Dona, J., Dechelle, M., Gallinari, P., & Levy, M. (2022). Constrained Physical-Statistical Models for Dynamical System Identification and Prediction. *ICLR*.
- Harlim, J., Jiang, S.W., Liang, S. and Yang, H. 2021. Machine learning for prediction with missing dynamics. *Journal of Computational Physics*. 428, (2021), 109922.
- Kochkov, D., Smith, J. A., Alieva, A., Wang, Q., Brenner, M. P., & Hoyer, S. (2021). Machine learning accelerated computational fluid dynamics. Proceedings of the National Academy of Sciences, 118(21).
- Li, Z., Zheng, H., Kovachki, N., Jin, D., Chen, H., Liu, B., Azizzadenesheli, K., & Anandkumar, A. (2022). Physics-Informed Neural Operator for Learning Partial Differential Equations. ICML
- Um, K., Fei, Y. R., Holl, P., Brand, R., & Thuerey, N. (2020). Solver-in-the-Loop: Learning from Differentiable Physics to Interact with Iterative PDE-Solvers. Neurips.
- Willard, J.D., Jia, X., Xu, S., Steinbach, M. and Kumar, V. 2020. Integrating physics-based modeling with machine learning: A survey. *arXiv* (2020), 1–34.
- Yin, Y., Le Guen, V., Dona, J., de Bezenac, E., Ayed, I., Thome, N. and Gallinari, P. 2021. Augmenting Physical Models with Deep Networks for Complex Dynamics Forecasting. *ICLR* (2021).
- Yin, Y., Kirchmeyer, M., Franceschi, J.-Y., Rakotomamonjy, A., & Gallinari, P. (2023). Continuous PDE Dynamics Forecasting with Implicit Neural Representations. *ICLR*.