Scuola Superiore Meridionale

MERC PhD Project Proposal 2023/2024

Title of the research project:

Uncertainty Quantification of Physics-informed machine learning for the Solution of the Inverse and Forward Problems in Complex/Stochastic Systems

Keywords (up to five)

Physics-Informed Machine Learning, Complex Systems, Differential Equations, Uncertainty Quantification

Supervisors (at least two from two different areas):

Supervisor 1 (Constantinos Siettos, MERC board member, Complex Systems, Physics-Informed Machine Learning, Numerical Analysis
Supervisor 2 (Athanassios Yannakopoulos, Department of Statistics and Stochastic Modelling and Applications Research Laboratory, Athens University of Economics and Business, Athens, Greece (Stochastic and Applied Analysis)
ept. of Chemical and Biological Engineering, Dept. of Mathematics and Statistics, Johns Hopkins, Algorithms, Equation-Free computations, Dynamical Systems, Data Mining, Complex Systems Modelling)
Supervisor 3 (Lucia Russo, STEMS, CNR, Agent-based modelling, Bifurcation theory, Spatio-Temporal Dynamics)

Project description (max 5000 characters)

Solving the inverse problem for complex systems with machine learning involves the tasks of determining parameters, variables and more generally forms of differential equations in the form of ODEs, PDES and/or Integral-PDEs from data [1,2,3,4]. All in all. the construction of reduced-order surrogate models (ROMs) for complex systems, in order to parsimoniously perform useful numerical tasks (simulations, bifurcation calculations, controller design and obtain additional physical insight. The forward problem refers to the solution of these equations bases on machine learning [1,5].

Uncertainty quantification (UQ) in the above tasks arises due to various factors such as measurement errors and noise, assumptions of the form of the model and inherent multiscales that underpin complex systems. In particular uncertainty can be categorized into two main categories (that are in a dialectic relationship): aleatoric UQ referring to inherent randomness and epistemic UQ referring to model uncertainty.

Uncertainty Quantification of ML models is increasingly important in solving complex problems as it aids in constructing robust/resilient models for numerical analysis, forecasting and control purposes. This is an open and challenging problem in many areas ranging from the design of materials, and control systems to financial forecasting, and from crowd dynamics and epidemiology to neuroscience to name just a few.

State of the art

Surrogate ML models in the form of ordinary, stochastic or partial differential equations via machine learning, can be constructed with approaches include, to name a few, sparse identification of nonlinear dynamical systems (SINDy) [6], Gaussian process regression (GPR) [2], Feedforward neural networks (FNN)[2], random projection neural networks (RPNN) [7], recursive neural networks (RvNN) [8], and Physics-informed neural networks and Deep-o-Net [1].

UQ of such surrogate machine learning models include, Gaussian Process Regression (GPR), Bayesian Neural Networks (BNNs), Physics-informed and Neural Network and Deep Ensembles. For a review of UQ in scientific machine learning see in [9].

Objectives

(a) Development of UQ methods leveraging machine learning for the solution of differential equations and inverse problems involving both finite and infinite-dimensional function spaces.
(b) Integrate Bayesian methods in PINNs for the epistemic UQ of models and their closures from spatio-temporal data
(c) Developing ML methods for propagating uncertainty across different scales in multi-scale models, and complex systems considering both spatial and temporal dimensions.

Relevance to the MERC PhD Program (max 2000 characters)

Briefly describe how this project fits within the scope of the MERC PhD program describing its interdisciplinary aspects, relevance in application and beneficiaries.

The proposed research is highly interdisciplinary at the junction between contemporary Scientific Machine Learning, Numerical Analysis, UQ multiscale complex systems modelling and analysis. Through the integration, the proposed approach holds the promise for making a step change to our ability of understanding and analyzing the emergent dynamics of complex systems from spatio-temporal data.
The research will also have a far-reaching educational significance through the fundamentally new results that aims to introduce. In the short term, the research will have immediate educational impact on the graduate students and post-doctoral scholars who will be involved in the research.

Key references

[1] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics, 378, 686-707.
[2] S Lee, M. Kooshkbaghi, K. Spiliotis, CI Siettos, I.G. Kevrekidis, 2020, Coarse-scale PDEs from Fine-scale Observations via Machine Learning, Chaos, 30, 013141.
[3] Fabiani, G., Evangelou, N., Cui, T., Bello-Rivas, J. M., Martin-Linares, C. P., Siettos, C., & Kevrekidis, I. G. (2023). Tasks Makyth Models: Machine Learning Assisted Surrogates for Tipping Points. arXiv preprint arXiv:2309.14334.
[4] G. E. Karniadakis, I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, and L. Yang, 2021, Physics informed machine learning, Nature Reviews Physics, 3 (2021), pp. 422–440

[5] F. Gianluca, F. Calabrò, L. Russo, C. Siettos, 2021, A Numerical Solution and Bifurcation Analysis ofNonlinear Partial Differential Equations with Extreme Learning Machines, Journal of Scientific Computing, 89, 44.
[6] Kaheman, K., Kutz, J. N., & Brunton, S. L. (2020). SINDy-PI: a robust algorithm for parallel implicit sparse identification of nonlinear dynamics. *Proceedings of the Royal Society A*, *476*(2242), 20200279.
[7] Galaris, E., Fabiani, G., Gallos, I., Kevrekidis, I., & Siettos, C. (2022). Numerical bifurcation analysis of pdes from lattice Boltzmann model simulations: a parsimonious machine learning approach. *Journal of Scientific Computing*, *92*(2), 34.
[8] Vlachas, P. R., Arampatzis, G., Uhler, C., & Koumoutsakos, P. (2022). Multiscale simulations of complex systems by learning their effective dynamics. *Nature Machine Intelligence*, *4*(4), 359-366.
[9] Psaros, A. F., Meng, X., Zou, Z., Guo, L., & Karniadakis, G. E. (2023). Uncertainty quantification in scientific machine learning: Methods, metrics, and comparisons. Journal of Computational Physics, 477, 111902.

Joint supervision arrangements

Describe joint supervision arrangements, e.g. weekly/monthly meetings with one or both supervisors, how will the joint supervision be split etc.

The supervisors are world-wide experts in the various fields of the project, they are collaborating along the research lines of the project since many years, they share common vision and enthusiasm to transfer knowledge and motivation and educate students. They will work closely with the PhD student for the successful completion of the Thesis. The student will meet and discuss on a daily basis with the principal supervisor while there will be other regular meetings on a weekly basis with all supervisors, including the period abroad when such meetings will be held remotely.

Location and length of the study period abroad (min 12 months)

The PhD student will spend a period of 12 months: (1) at the group of Professor Yannakopoulos, AUEB and will also shorts visits at world-expert research groups and in particular at the groups of Professor Geroge Karniadakis, Brown University and Professor Yannis Kevrekidis, Johns Hopkins University.

Any other useful information

The student will also benefit with the interactions with these groups through short visits during the while period of the PhD Thesis.