PROPOSITION DE POST-DOCTORAT

Title: Physics-Informed artificial Neural Network (PINN) approximation of hyperbolic systems of conservation laws

Référence : **PDOC-DAAA-2023-01**
(à rappeler dans toute correspondance)

Start of contract: January 2023	**Application deadline:** December 2023

Duration: 12 months, possibly extendable to 18 or 24 months (Net salary about 25 k€, medical insurance included)

Keywords: hyperbolic conservation laws, compressible gas dynamics, machine learning, artificial neural networks, data-driven techniques, high-performance computing

Profile and required skills: Ph. D. degree in applied mathematics or a related discipline. Skills in Machine learning, computational mechanics (numerical analysis of PDE) and Python programming language. Strong motivation to learn and good level of spoken and written (scientific) English are required.

About the research team: ONERA is a public establishment with industrial and commercial operations. ONERA carries out application-oriented research to support enhanced innovation and competitiveness in the aerospace and defense sectors. The DAAA department specifically focuses on scientific research for concrete applications on aircraft, the design of launchers and new defense technologies. The NFLU (numerical methods for fluid mechanics) group has a leading expertize in the theoretical analysis of advanced numerical methods for the approximation of complex fluid flows and the development of the next generation of flow solvers and provide cutting-edge solution algorithms and their customization for optimal efficiency on HPC clusters.

Context and objective: We here focus on *physics-informed artificial neural networks* (PINN) [1] introduced for the resolution of problems based on non-linear partial differential equations (PDE) by means of a deep artificial neural network (DNN) which easily assimilates knowledge of the underlying physics. In this way, the PINN gets rid of the prohibitive cost of data acquisition encountered in traditional machine learning techniques and is less sensitive to robustness and convergence issues. PINN may also be easily implemented in popular machine learning libraries.

Hyperbolic conservation laws are first-order PDE in space and time that describe the propagation of wave-like structures at finite speed and whose solutions may develop discontinuities, which imposes to consider weak solutions of the PDE in the sense of distributions. Weak solutions are not necessarily unique and admissibility criteria are necessary to select the physically relevant weak solution.

PINN use a supervised deep DNN representation of the solution in the classical sense. The inputs of the DNN are the space and time coordinates on a randomly sampled grid and the output is the solution field at these coordinates. The back-propagation mechanism is used to compute the space and time derivatives of the solution field in order to evaluate a discrete residual of the PDE, which is then used together with initial and boundary data to train the DNN. Using a strong form of the solution derivatives makes however difficult the capture of discontinuous solutions and recent works propose to impose further constraints to the DNN to make it conservative and to satisfy admissibility criteria [2,3].

Post-doctoral project: The main objective of this work focuses on improving the robustness and convergence properties of PINN approximation of hyperbolic PDE, in particular of the compressible Euler equations for gas dynamics. The strategy will rely on the introduction of local regularization through relaxation of the hyperbolic system [4]. The relaxation approximation consists in considering solutions to an enlarged linear system with stiff relaxation source terms. Under some conditions, solutions to the relaxation system admit smooth monotone shock profiles, but remain consistent with the original system in the limit of instantaneous relaxation. Specific and efficient relaxation techniques exist for the compressible Euler equations [5]. Convergence of such regularized PINN solutions to the physically admissible weak solution of the original PDE is however not guaranteed and additional constraints need to be imposed [3]. Likewise, the learning process is usually formalized through a minimization problem of a least-squares functional whose well-posedness is difficult to establish and whose convergence is difficult to achieve in practice.

The research activities to be conducted include:

- Bibliography/Practice on Machine learning based techniques for solving PDE (PINN, deep Ritz, ResNet, ReLU networks, EDNN, etc.) and traditional discretization methods on hyperbolic systems of conservation laws;
- Consideration of PINN-based resolution of nonlinear hyperbolic scalar equations and of the compressible Euler equations for gas dynamics in one space dimension;
- Comparison with other DNN-based solvers from the literature in terms of convergence, efficiency, robustness, etc.
- Implementation of an DNN-based solver in Python using the relaxation approximation and the imposition of constraints through the definition of a suitable minimization functional: consistency with the original PDE, the satisfaction of inequalities on convex entropies of the original PDE, conservation, minimum and/or maximum principles on some quantities, Riemann solution, etc.;
- Characterize solutions (existence and uniqueness) to the resulting minimization problem;
- Analyze the properties of the solver in terms of consistency, convergence and robustness. In particular, it will be useful to derive analogies of the solver with existing discretization techniques;
- Evaluation of the performances of the solver on HPC architectures; Identification of opportunities of efficiency improvement and analysis of the effects of the hyper-parameters on its performances;
- Evaluation of the PINN solver for other applications such as linear reciptivity-sensistivity-stability analysis, inverse and optimization problems;
- Interaction with other partners and students working on related projects about the use of DNN techniques in CFD (including internships, PhD thesis and the internal research project DIAANE 2022-2025, see below);

Bibliography:

[1] M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, J. Comput. Phys., 378 (2019), 686–707, https://doi.org/10.1016/j.jcp.2018.10.045.

[2] A. D. Jagtap, E. Kharazmi, G. E. Karniadakis, Conservative physics-informed neural networks on discrete domains for conservation laws: Applications to forward and inverse problems, Comput. Methods Appl. Mech. Engrg., 365 (2020), 113028, https://doi.org/10.1016/j.cma.2020.113028.

[3] R. G. Patel, I. Manickam, N. A. Trask, M. A. Wood, M. Lee, I. Tomas, E. C. Cyr, Thermodynamically consistent physics-informed neural networks for hyperbolic systems, J. Comput. Phys., 449 (2022), 110754, https://doi.org/10.1016/j.jcp.2021.110754.

[4] S. Jin, Z. Xin, The relaxation schemes for systems of conservation laws in arbitrary space dimension, Comm. Pure Appl. Math., 48 (1995), 235–276, https://doi.org/10.1002/cpa.3160480303.

[5] C. Chalons, J.-F. Coulombel, Relaxation approximation of the Euler equations, J. Math. Anal. Appl., 348 (2008), 872–893, https://doi.org/10.1016/j.jmaa.2008.07.034.

Collaborations

The ONERA project DIAANE (French acronym of Machine Learning techniques for the numerical analysis of PDE) will involve ONERA departments and academic partners form France and Germany.

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