Physics-Informed Neural Networks in Materials Science: a framework for optimization, symmetry identification, and inverse design

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Recent advancements in Machine Learning (ML) are transforming how physics problems are approached, offering powerful and often more efficient solutions to complex challenges. Materials Science, in particular, is exploiting these breakthroughs in multiple ways. For instance, ML-based surrogates can replace numerical methods in costly optimization problems, significantly accelerating the optimization process. ML can also enhance the predictive capabilities of experimental data by reducing noise and improving accuracy. Another key application is inverse design, where ML provides clever solutions.

We present here several ML-based approaches in the context of Physics-Informed Neural Networks (PINNs) recently developed by our group, and with direct applications in Physics. A PINN is a neural network that can embed the governing physical laws, usually written as differential equations, directly into its training process [1]. Instead of learning from data alone, a PINN is trained to minimize a loss function that includes the residuals of the governing differential equations and related quantities (initial and/or boundary conditions), the error in observed data (if available), and, in general, any other constraint known of the solution [2].

Despite ongoing advances, PINNs still face significant challenges [3]. One major issue is their tendency to converge to trivial (null) solutions when applied to differential equations over large domains. Additionally, they can also produce results that appear reliable — because the total loss is low — yet are actually incorrect. Such difficulties are especially evident in differential equations whose solutions or governing terms exhibit multiscale features and/or strongly oscillatory behavior. Recently, we introduced the Dynamic Boundary Constraint (DBC) algorithm as a solution to those limitations [4] (see Fig. 1, as an example). The main idea behind the method lies in the incorporation of additional restrictions, interpreted as boundary conditions, which are dynamically integrated into the training process alongside the existing initial conditions, thus enabling the PINN to ensure accuracy throughout the domain.

In a broader sense, PINNs may be regarded as neural networks that incorporate physical knowledge in a general manner. This is the case for part of the work we present: the use of ML to automatically identify discrete symmetry groups in physical systems [5, 6]. Our approach consist in introducing a novel neural network architecture that, using only experimental, numerical data and/or the governing differential equations, is able to identify the full set of symmetry-related multivalued solutions together with the associated representation of the underlying symmetry transformation. Furthermore, our algorithm is generalizable to any multivalued inverse design problem, including cases in which the degenerate solutions are not connected by an intrinsic physical symmetry.

We will present several examples demonstrating how Materials Science can benefit from PINNs, an approach with considerable potential to advance applications in numerous domains of science. Among others, we will show an application of our method in (*inverse*) designing twisted multilayers of α-MoO_3, enabling tailored optical responses such as canalization of phonon polaritons [7].

References

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Figures

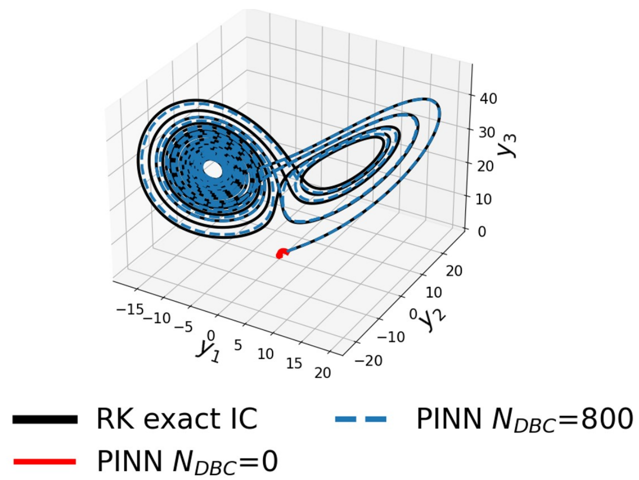

Figure 1. Lorenz attractor: RK solution (black line), PINN prediction with DBCs (blue line), and the standard PINN prediction without DBCs (red line). Notably, in the absence of DBCs, the standard PINN fails to yield a meaningful solution, as its prediction remains fixed at the initial condition for all x.