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Physics-Informed Neural Networks

Combining machine learning and theoretical knowledge has great potential for future modeling and simulation but requires overcoming hurdles.

Systems of ordinary and partial differential equations (DEs) are ubiquitous in many fields of science and engineering, and simulating systems governed by such DEs is an essential, but computationally costly ingredient for understanding natural phenomena and for optimizing engineering processes. Machine learning, especially using neural networks, can reduce this computational cost by substituting full-scale simulations with trained surrogate models – often sacrificing consistency with the underlying physics and sometimes requiring substantial training efforts.

Physics-informed neural networks (PINNs) are a recent family of neural surrogate models that allow the direct incorporation of DEs during training. Essentially representing the solution of a system of DEs as a function of spatiotemporal coordinates, they are trained to minimize two loss components (Figure 1). The classical supervised data loss quantifies how well the learned neural function agrees with data that has been provided for training, while the physics loss quantifies how well the learned function satisfies the system of DEs. As such, PINNs can be used for solving forward problems (i.e., computing future states of the physical system from initial and boundary conditions provided as data, as in classical numerical simulation) as well as inverse problems (i.e., inferring unknown parameters of the physical system from measurements). In addition, they have been successfully used for problems between these two extremes, e.g., for inferring (unobservable) pressure fields from (easily observable) flow fields.

Especially for forward problems, PINN training is cumbersome and, ironically, often leads to physically incorrect solutions. Part of this is caused by the fact that PINN training still does not fully respect fundamental physical concepts, such as distinguishing between stable or unstable fixed points/equilibrium solutions. For example, PINNs will easily find a stationary, but potentially unstable solution to a fluid flow problem, but may not be able to find periodic solutions (which are stable for larger Reynolds numbers). This effectively limits the utility of PINNs for fluid dynamics simulations. We also discovered that the two-component loss further complicates PINN training. Indeed, during training the PINN can choose between violating the governing DEs (physics loss) or violating initial and boundary conditions (data loss). In her master's thesis, Sophie Steger (currently PhD candidate at the Signal Processing and Speech Communication Laboratory) found out that exactly this happens when using PINNs to predict the solution of a chaotic system, namely the double pendulum. The PINN violates the initial condition in such a way that the solution becomes easier to learn but still satisfies the governing equations (Figure 2). Sophie was able to trace this back to the spectral bias of neural networks. We believe that spectral bias also plays an important role in how PINNs tend to be influenced by fixed points in dynamical systems, regardless of their stability.

These insights, which we have obtained in the four-year COMET module HybTec at the Large Engines Competence Center GmbH

Differential Equation $\frac{\partial}{\partial t}u(x,t) + \mathcal{F}[u;\lambda] = 0$

Data Loss (e.g., initial condition)

$$\mathcal{L}(\theta) = \frac{1}{|D|}\sum_{(x_i,t_i,u_i)\in D}(u_\theta(x_i,t_i)-u_i)^2 + \frac{1}{|C|}\sum_{(x_i,t_i)\in C}\left(\frac{\partial}{\partial t}u_\theta(x_i,t_i) + \mathcal{F}[u_\theta(x_i,t_i);\lambda]\right)^2$$

Physics Loss (consistency)

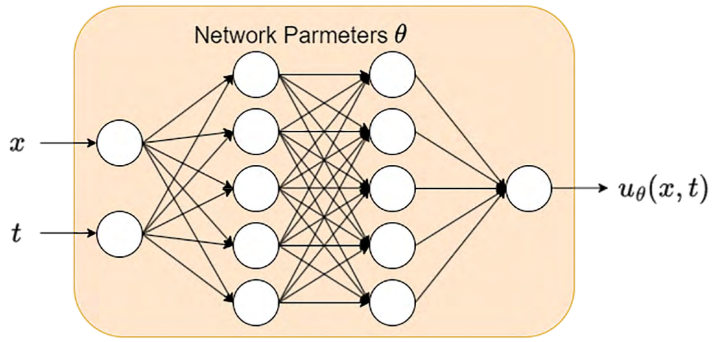


Figure 1: For a given differential equation (top left), the PINN (right) is trained by a two-component loss function (bottom left), consisting of a supervised data loss and a self-supervised physics loss.

and the Know Center Research GmbH, and which largely rested on the shoulders of our PhD candidate Franz Rohrhofer, yield important insights into why PINN training is so difficult – but our journey did not stop there. Equipped with an in-depth understanding of PINNs, we identified practically relevant application areas and developed approaches that increased the chance of successful training. Most notably, within the Horizon Europe project ENFIELD (in which the Know Center Research GmbH co-leads the task on Green AI) we adapted the physics loss and the inductive bias of the neural architecture to successfully train a PINN to solve a parametric version of the Fisher-KPP equation, a simple model for reaction-diffusion systems. The resulting surrogate model not only achieved excellent accuracy for the reaction rates on which it was trained but also generalized to a range of reaction rates spanning several orders of magnitude beyond the training data. Extending this success to more complex reaction-diffusion models can substantially speed up the simulation time required to optimize combustion processes or chemical reactors. Aside from this application-specific PINN adaptation, we also worked to address general training problems, such as a Bayesian approach ensuring that information from the initial condition successfully propagates into the interior of the computational domain, and a regularization scheme that helps avoiding unstable fixed points of ordinary DEs.

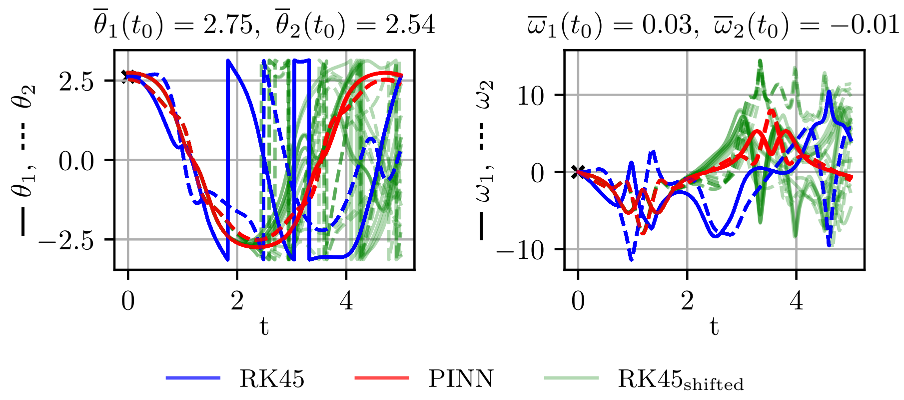
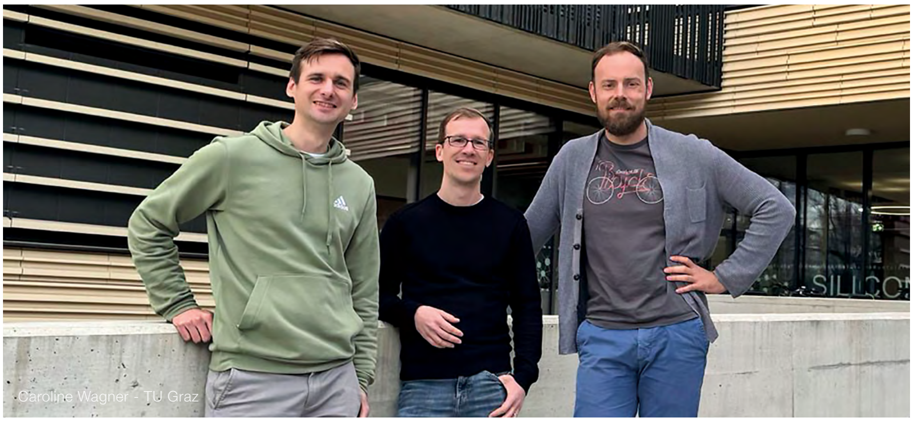


Figure 2: The solutions for a chaotic double pendulum using a Runge-Kutta 45 solver (blue) and a PINN (red), both angle (left) and angular velocities (right). The PINN yields simpler solutions by shifting the initial condition slightly. The resulting solutions are, at least initially, physically consistent, as shown by the overlap with Runge-Kutta solutions (green) obtained from the shifted initial conditions. Source: https://openreview.net/forum?id=shUbBca03f

Despite these successes, we acknowledge that applying PINNs (or, more generally, physics-informed machine learning and hybrid modelling) to practically relevant problems will require tailor-made solutions for each scenario. This, in turn, requires a team of researchers bringing machine learning expertise and substantial domain knowledge to the table. The first author's tenure track position for hybrid physics-based and data-driven modeling and simulation of complex mechanical or electrical engineering systems aims at facilitating and actively participating in such projects and can be a first point of contact in this regard.

From left to right: Franz Rohrhofer, Bernhard Geiger, Stefan Posch



Franz Rohrhofer is a senior researcher at Know Center Research GmbH, specializing in physics-informed machine learning. He holds a PhD in computer science and a Dipl.-Ing. degree in technical physics, both from Graz University of Technology. His research interests include fluid dynamics, materials science, and, more broadly, the interplay between physics and machine learning.

Bernhard Geiger is an assistant professor at the Signal Processing and Speech Communication Laboratory and holds the tenure track position for hybrid physics-based and data-driven modeling and simulation of complex mechanical or electrical engineering systems. He is also key researcher and research area manager at the Know Center Research GmbH.

Stefan Posch is a senior researcher at the Large Engines Competence Center GmbH. In his position as team leader for AI-enhanced modeling, he focuses on the integration of machine learning methods into the modeling and simulation process of sustainable energy systems.