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MACHINE LEARNING-DRIVEN ENGINEERING: DESIGN OPTIMIZATION AND FLUID MECHANICS PERSPECTIVES

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ABSTRACT

Machine learning and artificial intelligence have profoundly transformed the landscape of modern engineering, providing powerful tools to model, analyse, and optimise complex systems. Its applicability extends across diverse domains, including engineering design optimisation and fluid mechanics, where traditional approaches often struggle with high computational costs or limited interpretability. Importantly, machine learning does not replace established methods but synergises with engineering disciplines, creating new opportunities to integrate data-driven models with physical understanding. This progress is inherently interdisciplinary, drawing on advances in mathematics, statistics, and computational science to build models that are both predictive and explainable. Several applications will be demonstrated. Physics-Informed Neural Networks (PINNs) have been employed to predict flow behaviour in porous media, while explainable machine learning has been applied to support the design optimisation of auxetic materials and aircraft, revealing how data-driven insights can complement physical intuition and knowledge. These case studies demonstrate the potential of machine learning to transform engineering practice. The talk concludes with a perspective on how machine learning techniques, when combined with engineering know-how and strengthened by interdisciplinary approaches, can drive future innovation in design optimization and fluid mechanics.

KEYWORD

Machine learning, design optimization, fluid mechanics

INTRODUCTION

It can be assured that at least one of these expressions has been heard repeatedly: *data-driven decision making, data-driven policy, data-driven design*, or *data-driven discovery*. Perhaps *data-driven science* and *data-driven engineering* have also been encountered. What is so special about *data-driven*? Has data not been with us for centuries, or even millennia? After all, science and engineering have always relied on data (measurements, observations, experiments, and empirical correlations) to understand physical phenomena and to design reliable systems. From early astronomical records to wind-tunnel experiments and flight tests, data has long been a cornerstone of scientific discovery and engineering practice. The key to understanding this lies in the following paradigm shift: the role of data has evolved from *supporting* to *driving*. Data is no longer viewed merely as a byproduct of scientific and engineering practice, but increasingly as the *engine of discovery* itself.

In the present era, which is greatly transformed by artificial intelligence, with machine learning being one of its most influential subsets, data literacy has become an essential skill for scientists and engineers alike. As engineers, it is possible to go further. It is possible to move beyond being merely data literate toward truly mastering data. The key to this is to understand and master the technology of machine learning.

Based on research experience, this document shares how such technologies can be leveraged to address challenging engineering problems in the field of design optimization and fluid mechanics.

DATA-DRIVEN ENGINEERING

The discussion begins by addressing the following question: What is *data-driven engineering*? Figure 1 illustrates the integration of data science and engineering as a unified framework for addressing the inherent complexity of modern engineering problems. On one side, data science, encompassing artificial intelligence and machine learning, provides tools for extracting patterns, learning representations, and constructing predictive models directly from data. On the other side, engineering contributes physical understanding, mathematical modeling, and statistical reasoning that ground these data-driven methods in real-world behavior and constraints. By combining these two domains, data is no longer treated merely as supporting evidence, but as an active driver in modeling, analysis, and decision making. This is *data-driven engineering*.

It should be noted that applying machine learning to scientific and engineering problems is not straightforward.. Many machine learning models are designed to optimize predictive accuracy, yet they may violate fundamental physical principles. In addition, engineering applications often suffer from limited, noisy, or expensive data, since high-fidelity simulations and experiments can be costly to perform. These challenges mean that blindly applying standard machine learning techniques can lead to models that appear accurate within the training set but fail to generalize or provide physically meaningful insights. As a result, successful machine learning-driven engineering requires careful integration of physical knowledge, data efficiency, and domain-specific modeling considerations.

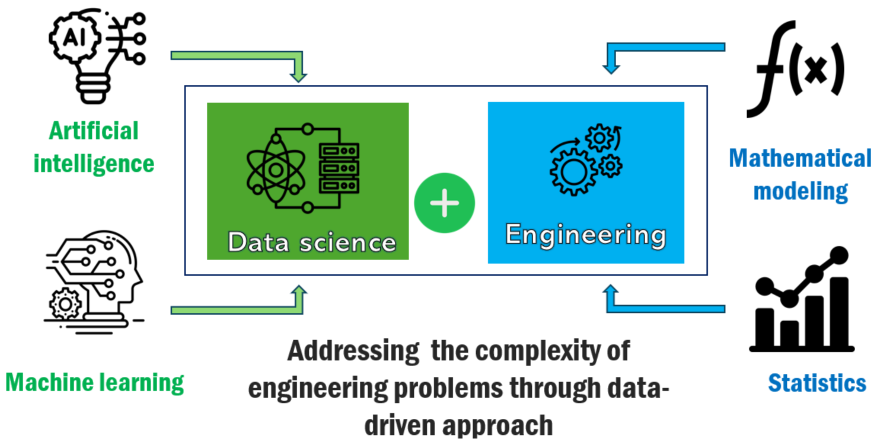

Figure 1: Data-driven engineering.

DATA-DRIVEN ENGINEERING IN DESIGN OPTIMIZATION AND FLUID MECHANICS

The most effective way to illustrate how data-driven engineering works is through concrete examples. To this end, the capabilities of these methods are demonstrated using selected studies conducted by the author, collaborators, and students in the areas of design optimization and fluid mechanics. A number of examples are available; however, only two are presented in this paper.

The first example concerns the design of auxetic materials. The author was approached by his colleagues to support their research on understanding a specific class of auxetic materials known as hexachiral structures. Auxetic materials are a class of engineered materials that exhibit a negative Poisson's ratio, meaning that they expand laterally when stretched and contract laterally when compressed. The key question then becomes how to design and optimize the configuration of such auxetic materials (Figure 2). Can the Poisson's ratio be systematically optimized? Can we uncover the relationship between geometric parameters and the resulting Poisson's ratio?

The research team proposed an alternative approach by suggesting the use of machine learning. This direction proved to be fruitful, leading to a successful joint collaboration. From this effort, two journal papers were published. The first focuses on the optimization of the Poisson's ratio, specifically on identifying designs that achieve a highly negative Poisson's ratio (Afdhal et al., 2023). The second addresses the inverse problem of discovering auxetic designs with a near-zero Poisson's ratio (Afdhal et al., 2024). We specifically leveraged a machine learning method called *Gaussian Process Regression*, which is advantageous for small data regime, typical in engineering problems. Gaussian Process models played a central role in this endeavor by identifying key relationships between design parameters and mechanical performance, while also guiding the discovery of structures with targeted properties. The training data were generated using finite element simulations, which were subsequently validated through experimental testing.

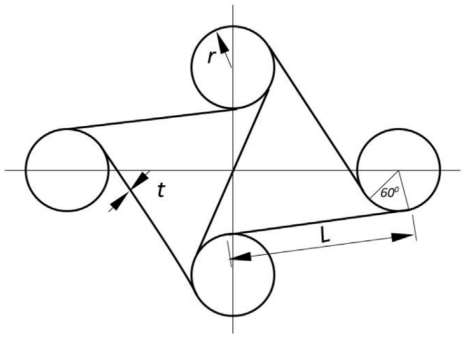

Figure 2: The schematic of hexachiral material. There are three tunable parameters: the radius (r), the thickness (t), and the length (l).

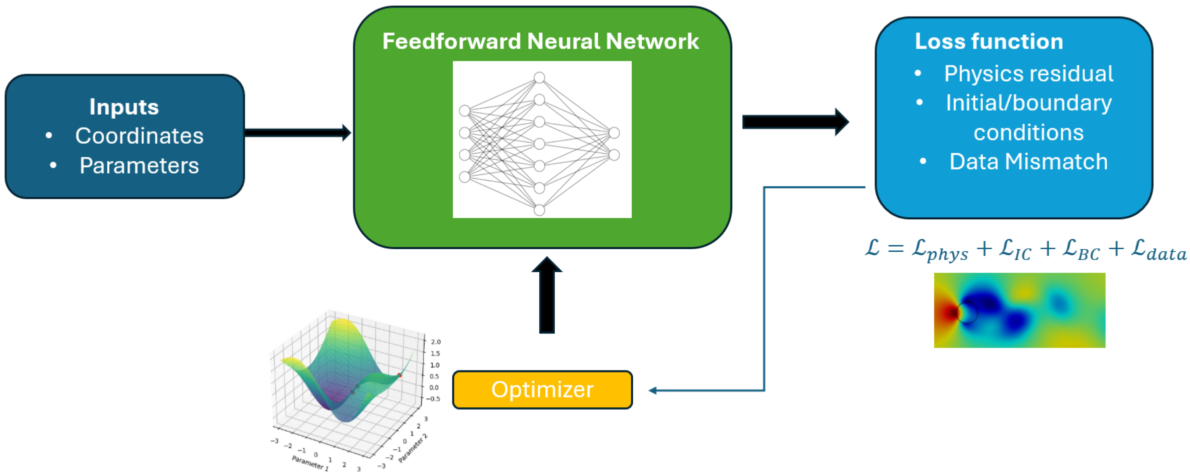

Figure 3: A simplified schematic of Physics-informed Neural Networks.

The second example comes from the field of fluid mechanics. Before presenting it, it is important to emphasize that for many problems in this field, the governing equations and physical laws are already well established. However, when machine learning is applied naively, this prior knowledge is sometimes overlooked, leading to models that may fit data but violate fundamental physical principles. Physics-informed neural networks (PINN) provide a systematic framework to address this issue by embedding the governing equations and physical laws directly into the machine learning model (Raissi et al., 2019), as can be seen in Figure 3. By doing so, PINNs ensure that the learned solutions remain physically consistent while benefiting from the flexibility of machine learning.

In our recent work, we use a PINN to study how fluid flows around a porous object (Nguyen et al., 2025). The main goal is to estimate how easily fluid can pass through the object, which is known as its permeability, using only information from the flow outside the object. Instead of relying purely on data, we teach the neural network the basic physical laws that govern fluid motion. This allows the model to learn the flow pattern and at the same time figure out hidden properties of the object, even when only limited data are available. The results closely match those from data, showing that the method can capture realistic flow behavior. This example shows how combining data with physical knowledge makes machine learning more reliable and useful for solving real engineering problems.

SOME FINAL THOUGHTS

Machine learning offers tremendous potential for advancing engineering practice, from accelerating design optimization to enabling new ways of understanding complex physical systems. However, these tools should not be applied naively or in isolation. Effective and trustworthy use of machine learning in science and engineering requires a strong fundamental, along with a clear understanding of the physical context. When combined with domain knowledge, machine learning becomes a powerful enabler rather than a black box, allowing engineers to extract meaningful insights, respect physical laws, and make informed decisions. Ultimately, the greatest impact of machine learning in engineering will come from those who understand not only the algorithms, but also the problems they are meant to solve.

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