



# Introduction to Partial Differential Equations and Machine Learning Solutions

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## ABSTRACT

Partial differential equations (PDEs) are foundational tools in modeling various physical phenomena in science and engineering. Traditional numerical methods such as finite difference, finite volume, and finite element methods have been the primary approaches for solving PDEs. However, these methods often struggle with high-dimensional and nonlinear problems. Recently, machine learning (ML) has emerged as a promising tool for enhancing the efficiency and accuracy of PDE solutions. This paper provides an overview of PDEs, traditional numerical methods for solving them, and the integration of ML techniques in these methods. We explore how ML, particularly deep learning, can address challenges such as the curse of dimensionality and computational inefficiency. The discussion includes various ML approaches, including physics-informed neural networks (PINNs) and data-driven discretizations, and their applications in fields such as fluid dynamics and medical physics.

Keywords: Partial Differential Equations, Machine Learning, Numerical Methods, Deep Learning and Physics-Informed Neural Networks

## INTRODUCTION

Partial differential equations (PDEs) are crucial mathematical models used to describe a wide range of physical phenomena, from wave propagation and heat conduction to fluid dynamics and structural analysis [1, 2]. Traditional methods for solving PDEs, such as finite difference methods (FDM), finite volume methods (FVM), and finite element methods (FEM), have been extensively developed and applied over the years. However, these methods often face significant challenges when dealing with high-dimensional spaces and strongly nonlinear systems, commonly referred to as the curse of dimensionality (CoD). In recent years, the advent of machine learning (ML) has opened new avenues for solving PDEs more efficiently and accurately [3-5]. Scientific machine learning, which combines numerical analysis and ML, is an emerging field that leverages advances in both domains to tackle complex problems. Convolutional neural networks (CNNs) and attention-based deep learning architectures, which can handle multi-scale features and translation invariance, are particularly well-suited for PDEs [6-9]. This paper reviewed the integration of ML in traditional numerical methods, focusing on how ML can overcome existing limitations and enhance the solution process.

### Introduction to Partial Differential Equations

In response to this, the PDE research community is increasingly considering machine learning (ML) as a tool for the fast and reliable solution of PDEs in multi-dimensional physical problems. Through examples in the data-driven discovery of PDEs, apparent since the 1990s, DL-based models have begun to demonstrate significant success in the learning of strongly non-linear dynamical systems. A collaboration of ML and numerical analysis, “scientific machine learning” is a rapidly evolving field that is constantly absorbing improvements in both numerical methods and statistical modeling [10-12]. Moreover, convolutional nets (CNNs), which preserve translation invariance in their inputs, and attention-based deep-learning architectures, well-suited to assimilate multi-scale features, are better optimized for PDEs within specialized operator-form networks designed to amplify their locality properties via motivated spatial discretizations without the loss of efficiency observed in full periodic [13-15]. The curse of dimensionality (CoD), a central problem in traditional FDM and FEM simulations, remains in their application to the aforementioned field. For a discretized model to develop its predictive capabilities when confronted with a variety of initial conditions and boundary specifications, a vast volume of training data

is needed, a process highlighted by diminishing returns. Although the finite element method (FEM) is formulated using Fréchet derivatives, the application of “reverse-mode” automatic differentiation has recently been reported for the solution of the time-dependent wave equation, characterized in the literature by the time-step summation [16, 17].

Partial differential equations (PDEs) are among the most widely used mathematical models to describe a variety of phenomena in science and engineering. PDEs are used to describe wave propagation phenomena and have further found a variety of applications in the context of medical physics. More precisely, the wave equation and its mathematical models have found relevance in ultrasound image reconstruction, radiation cancer therapy, and nondestructive evaluation (NDE) for quantitative data analysis [18, 19]. Despite satisfying the desired thermodynamic properties of a minimally invasive procedure, ultrasound surgery has the limitation of requiring high submillimeter precision in the target region. When the planned treatment is disrupted, the user needs to stop therapy and pose the patient for additional imaging. Work has begun in substituting standard ultrasound imagery for model predictions, an approach researchers in this field hope results in less required imaging and facilitates real-time monitoring of thermal exposure over critical structures [20, 21].

#### **Definition and Classification of PDEs**

The issue can be related to the increase in the number of dimensions or the increase in the number of degrees of freedom. For instance, a partial differential equation of the first order, which is a system of ODEs, that governs an  $n$ -dimensional system will have  $2n-1$  spatial dimensions, which will represent, in any way, the boundary surface of an  $n$ -dimensional rectangular cuboid. The PDEs are difficult to handle mathematically, particularly for large-scale problems, and often also computationally. Usually, PDEs are solved using either analytical or numerical methods [22, 23].

PDEs are usually classified based on their properties. There are several distinct classes of partial differential equations: elliptic, parabolic, and hyperbolic. Other features that help to classify PDEs include whether the PDE is linear and whether the coefficients in the PDE are constant or considered as functions of the independent variables. Key feature Physical examples of PDEs include the steady-state heat transfer, one-dimensional viscous flow in a pipe, and some inverse heat conduction problems. In general, PDEs are fundamentally more challenging to solve than ordinary differential equations. This is because PDEs model systems with infinitely many degrees of freedom whereas ordinary differential equations model systems with finitely many degrees of freedom [24, 25].

PARTIAL differential equations (PDEs) are important mathematical models, which govern a variety of physical processes and have wide applications in numerous disciplines. A partial differential equation (PDE) is an equation that relates the values of a function defined on some domain in Euclidean space and its partial derivatives over this domain. The solution of a PDE is the unknown function, or a function of this function satisfying the equation together with suitable boundary or initial conditions [26-28].

#### **Traditional Numerical Methods for Solving PDEs**

Spectral methods are based on Fourier, Chebyshev, or other basis expansions. These methods are still quite competitive for problems that don't have discontinuities in spatial scales. Finite-difference method (FDM) and finite volume method (FVM) transform the continuous PDEs into discrete forms using a regular grid. They are widely used for simple code implementation structures and can be learned quickly. Of course, there are still essential differences between these two types of methods. For example, FDM is more suitable for elliptic and hyperbolic problems, and FVM is more suitable for convection-diffusion problems. In the past few decades, the finite element method (FEM) has become extremely popular in the simulation of various PDEs with irregular geometries. Specially, for fluid and structural simulations, it is one of the most popular choices for accuracy and effectiveness. The intrinsic computational stencil of FEM is sparse which makes it also become a prevalent tool of sparse linear algebraic solving [29-32].

In many applied sciences and engineering, we characterize real-world physical processes by PDEs. Many analytical solutions based on simplified assumptions and approximations are presented for PDEs, which also leads to a great demand for numerical simulations. However, PDEs are generally difficult to solve in the simulation due to their natures of high dimensionality and nonlinearity. It's reported that the cost to solve PDEs may be super-linearly increased with time for traditional methods [33, 34]. To manage these challenging issues, a variety of traditional numerical methods have been proposed and developed. Based on the discretization strategy, traditional numerical methods can be generally classified into grid-based and mesh-based methods [35, 36].

#### **Finite Difference Methods**

The data structures are employed to store the solution variables efficiently and the arrangement of which depends upon the numerical method that is used for the PDE. In finite difference techniques, one of the common data structures used for the solutions of PDEs is matrix. Multi-dimensional (ND) data are stored

using a flat storage layout which is expressed in  $B = (Bi + j + IM)$  where  $N$  is the number of dimensions,  $k = 0, 1, 2, \dots, N$  and  $M = MI - 1 - M_0$  [37].  $M_0$  corresponds to the number of grid points used for each direction and  $i = 0, 1, 2, \dots, N-1$ . The distance and direction among the elements of the matrix are stored as subscript formulas. The number of elements of a matrix required by a numerical solver can be expressed as  $(M_0 - 1)MN - 1$  ND. For an  $m_0 = 4$  aluminum matrix with an additional integer, 64 states can be given to fit into about 4 GB RAM [38].

Partial differential equations (PDEs) govern varieties of physical, biological, and societal phenomena. Their analytical solution is difficult to obtain and it leads to the development of numerical solution of PDEs (PDE solvers). The finite difference techniques provide initial and boundary conditions in a discrete form, so they discretize the spatial dimensions in general, to approximate the continuity and/or differentiability of the solutions. The goal is to approximate the solutions in such a way that they result in very small errors concerning the actual problems. Consequently, a collection of algebraic equations (system of linear or non-linear) is obtained from PDEs, which can be solved on a digital computer to obtain a fully discrete approximated solution, thereby serving as the foundation for advanced algorithms of PDEs [39-41].

### Finite Element Methods

A more advanced strategy that couples FEM with a DNN, the so-called “physics-informed” neural network, uses prior knowledge of the PDEs to guide the training of the DNN. In the works available in the literature, the formulation of this prior information is problem-dependent (i.e., for the heat conduction the DNN, must satisfy the source term in the PDE definition, i.e.,  $\nabla u(x) = f(x)$  on  $\Omega$ , with  $u(x)$  being the neural network and  $f(x)$  the source term) [42-44]. To achieve this purpose, a new class of numerical methods was proposed, the so-called meshless methods, including Smooth Particle Hydrodynamics (SPH). Recently, some works have proposed the idea to couple FEM and ML techniques. A DNN is used to approximate the solution at a set of input parameters, without the necessity of solving the PDE at these locations. This “strategy” in the numerical calculus community is known as a “response surface”, and it is widely used in the design of experiments to understand high-dimensional spaces/processes [45, 46]. Finite element methods (FEM) are widely used numerical methods for approximating partial differential equations (PDEs). The basic idea of FEM is to replace the exact solution of a PDE with a discrete solution so that the continuous problem is transformed into a system of algebraic equations. The FEM equation error is characterized by the mesh spacing ( $h$ ) and solution regularity. With mesh refinement and a smooth solution at the same time, the solution converges to the exact solution at a minimal rate. 2D and 3D problems containing adaptive meshes, curved domains, and other geometric complications are hard to solve using classical FEMs [47, 48].

### Integration of Machine Learning in Numerical Methods

An important precursor to solving differential equations using ML is to solve the related problem of designing efficient and practical interconnections between ML models and classical, rule-based techniques. The overarching objective here is to harness each approach in its domain of excellence. The pioneering related ideas of learning coefficients in Navier—Stokes simulations using historical databases of complex simulations have led to a cluster of activity, under various names. Alongside these developments, the systematic integration of ML models with traditional simulations has also grown rapidly. This can range from using sophisticated ML in a post-processing role to recover detail in statistical simulations to hybrid methods that switch between ML and traditional techniques based on some learning-based decision mechanism [49-51]. Traditionally, differential equations are solved using specialized methods exemplified by the finite difference method and the finite element method. These are versatile and well-understood techniques that offer good accuracy and often work well in practice. Nevertheless, they face challenges when applied to complex physical systems and/or when high-fidelity simulations are required. One response to these challenges has been to devise new schemes specifically tailored to the particular problems, however, this is often a delicate process that requires significant expertise. As an alternative, an integrating Machine Learning (ML) — a more general-purpose approach for estimation and prediction across processes involving unknown dynamics [52-54]. ML is a valuable tool for estimating even complex, non-smooth, or chaotic phenomena that can evade the classical methods. ML-empowered methods can also exploit in-sample data to create reduced models which, while they have no well-defined basis functions, are readily employed. That is, the ML serves as an engine for a different numerical method [55-57].

### Overview of Machine Learning Techniques

Recently, unsupervised learning was advocated and used to capture the solution map. The approach consisted of placing warm start data points and proposed that these would facilitate the discovery of low-dimensional structure. Unsupervised learning allows such an approach but it does not necessarily follow

that fully unsupervised learning automatically leads to the discovery of the low-dimensional structure. More general unsupervised learning approaches that only require sampling instances of the high-dimensional input parameter space were also explored [58, 59].

One of the popular classical ML paradigms that have been used is supervised learning where a neural network is trained with pairs of inputs and the corresponding solutions for a fixed PDE. However, the supervised approach to learning high-dimensional PDE solution maps is intractable. To alleviate this difficulty, iterative learning where new samples are generated based on the solution surrogate is explored. Alternatively, one could attempt to learn models that allow for fast and flexible calculation of solutions to always-new instances of PDEs [60, 61].

Machine learning (ML) has recently gained significant interest in scientific computing due to its ability to accelerate the solution process of partial differential equations (PDEs), the differences herein are referred to as 'classical AI disciplines'. By integrating ML with numerical methods for PDEs, solutions can be approximated with cost-effective computational inference by replacing time-consuming numerical steps that would be required in traditional PDE-solvers. These approaches typically split in the proposed methodology of directly training a surrogate that emulates the full map from the parametric PDE problem to its solution, which is fully described by a high-dimensional input-output map and the approaches that alternate between physics-motivated iterative updates and ML-based surrogates [62-64].

#### **Hybrid Approaches Combining ML and Traditional Methods**

One of the most classical ways to merge supervised ML models and DE solvers consists of data augmentation, that is, leveraging data-driven models to provide numerous approximations of certain operations, that are explicitly present in the targeted DE solvers. For instance, when targeting wave-equation solvers, using as an additional input the lossless wavelet transform of some inputs aggregates to help the ML model prevent information loss; while in the case of reversible neural networks, aiming at the natural computation of the adjoint operator and then resorting to optimization backward using the adjoint approach. A natural way to keep the training simpler while exploiting DEs-based priors is to enforce explicitly these DEs during the training of the ML model. In that respect, the most standardized perspective relies on PINNs; being nothing else but an energy method for collecting the scattered residual computations [65-67]. The past decade has witnessed a rapid growth of interest in hybrid approaches combining deep neural networks and traditional differential equations (DEs) solvers. Consequently, many promising directions have emerged, like designing efficient neural network architectures that respect the functional properties of the nonlinear operators present in the DEs, like devising PINNs (physics-informed neural networks) that exploit the governing DEs during the supervised training or employing neural networks as components of specific numerical methods to this end, which makes it feasible to raise eigensolvers or Gaussian process-based solvers. Notwithstanding these recent breakthroughs, the quest for a more reliable and less black-box scientific machine learning approach revives the close relationships between DEs and ML models. One should be able to search efficiently the deployment of a supervised ML model to solve a specific DE, by taking into account the specifics of the source DE, without making the training harder, or the achieved accuracy poorer [68-70].

#### **Data-Driven Discretization**

There has been a growing literature over the last few years that applies machine learning (ML) to the study of partial differential equations. Applying ML methods to PDEs is an efficient way to define physical constraints implicitly, but these approaches are generally difficult to implement and rarely satisfy constraints exactly, due to their direct modeling of the dynamics [71, 72]. Recent studies have proposed data-driven methods that optimize PDE models to encode the dynamics directly and model to ensure that the learned models satisfy physical constraints. Another recent approach to moving past the difficulties that come with direct modeling of FG dynamics is to encode the FG CG boundary statistics directly rather than trying to memorize the full dynamical maps, with method PT as a representative example.

Discretization is an important step when solving partial differential equations (PDEs) numerically. Classically, this work has been informed by linear theory only. This article studies learning data-driven discretizations by encoding higher-level components that are captured with simplifying assumptions and verifies a substantial computational advantage [73, 74]. Specifically, this work is based on a data-driven partial dynamics learning (DPL) method, which models only the coarse-grained (CG) variables and requires a fixed PDE whose form is already known from theoretical or empirical grounds in conjunction with the coarse-graining process. That approach is contrasted with the present methodology, in which 'full dynamical learning' is employed in which the ML model additionally requires direct access to the fine-grained (FG) variables. DPL learns only the basis features used to express the true dynamics co-domain [75, 76].

### Applications and Case Studies

Following the growing interest in the area, various models and approaches have been proposed for the high-dimensional classical PDEs as time-space dependent: using regression models and feed-forward neural networks, adaptive resolution training of neural networks using stacked Boussinesq equations and KdV systems, learning compact representation from time series for solvers of evolution equations (such as Burgers', Fisher-KPP, Kuramoto-Sivashinsky, code-equation, normalized-LAP, KS) by minimizing the cost function in the temporal domain, computation resource-efficient overturning solutions for PDEs, physics-informed machine learning techniques using numerical time arrival information and convolutional neural networks on wave field, using reinforcement learning frameworks with observation action reward (OAR) scheme and travel time, PDEs with bulk reading in physics-informed real embeddings [77, 78].

The ability of machine learning (ML) to learn from historical data to make decisions has made it a very powerful and popular tool in various domains [79]. In recent years, the research community has witnessed the emergence of a powerful combination of classical numerical solvers and ML, where ML models are used to accelerate existing numerical solvers, train reduced-order models and surrogate models to approximate the solutions of high-dimensional PDEs with a much smaller number of parameters, or even optimize the numerical solvers. In addition, the ability of the ML algorithms to learn and approximate the complex relationships in input and output data has been exploited to identify the appropriate discretizations of the continuous PDEs and even control them; this way, they have been used to solve high-dimensional PDEs directly without any discretization step. Efforts have been made to apply modern machine-learning techniques in the aforementioned area in various domains [80, 81].

### Fluid Dynamics Problems

Besides developing the proper ML-based sub-solvers, the other challenge to solving large classes of problems with the described approach is to develop a suitable ML-based method to construct the sub-systems responsible for generating the discrete weak solutions arising from the separation of the time scales. Moreover, the numerical integration from one light system of the reduced basis to the next one must ensure that the reduction strategy explicitly accounts for the presence of external forces with unknown forms. Here, an ML-enhanced strategy, called unsupervised proper generalized decomposition, to approach deep-learning-based MorRom built on a recursive neural network will be successfully applied to general, convection-dominated problems with strong boundary layer behavior. In this paper, this approach is applied to 1D test problems over thermo-fluid-dynamics benchmark domains; in 2D, various geometries will be analyzed under different initial or boundary conditions [82, 83]. Machine learning (ML) and artificial intelligence (AI) have found good acceptance in computational fluid dynamics (CFD) to predict, accelerate, and improve the results of flow simulations [84]. Typically, machine learning algorithms are used to predict the properties of the fluid, its behavior, and its characteristics. Reports have also shown that machine learning and deep learning algorithms have been integrated within CFD solvers to bypass various sub-models and reduce computational costs. However, most of these studies applied machine learning, deep learning, and AI to bypass various hydrodynamics, turbulence, and heat transfer models present in CFD solvers, Model Order Reductions (MORs), and Reduced Order Models (ROMs) based on machine learning and AI. Proper handling of singularities, discontinuities, and boundary layers, particularly in the context of highly complex conservation law problems [85].

### CONCLUSION

The integration of machine learning with traditional numerical methods for solving partial differential equations represents a significant advancement in computational science. By leveraging the strengths of both fields, it is possible to overcome many of the challenges associated with high-dimensional and nonlinear PDEs. Techniques such as physics-informed neural networks and data-driven discretizations demonstrate the potential for ML to enhance the accuracy and efficiency of PDE solutions. As the field of scientific machine learning continues to evolve, it promises to deliver more robust and versatile tools for tackling complex physical phenomena in various domains, from fluid dynamics to medical physics. Future research will likely focus on refining these hybrid approaches, improving their computational efficiency, and expanding their applicability to a broader range of problems.

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