

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ, ЧИСЛЕННЫЕ МЕТОДЫ И КОМПЛЕКСЫ ПРОГРАММ/MATHEMATICAL MODELING, NUMERICAL METHODS AND PROGRAM COMPLEXES

EDN: TFOHXR

A REVIEW OF MODERN NUMERICAL METHODS FOR PDES WITH EMPHASIS ON PHYSICS-INFORMED AND OPERATOR LEARNING APPROACHES

Review article

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Suggested: 21.04.2026; Accepted: 12.05.2026; Published: 29.07.2026

Abstract

The numerical simulation of the behavior of physical and engineering systems is essentially dominated by solving Partial Differential Equations (PDEs). Conventional discretization techniques, such as Finite Difference, Finite Element and Finite Volume, have been largely prominent in this discipline; however often they encounter limitations when the problem is of complex geometry, high dimension domain, or time to solution is critical. This manuscript discusses recent developments in numerical methods for PDEs with emphasis on developments from 2015 to 2025. The modern methods are classified in five categories: Spectral Methods, Meshfree Methods, Adaptive and Multiscale Methods, AI based and Probabilistic Methods and Hybrid Methods. We conduct a close examination of each category in terms of accuracy, computation cost, stability and scalability. A salient observation is a transformative impact of AI based techniques; Physics Informed Neural Networks (PINNs) and Deep Operators Networks (DeepONet) are particularly suitable for solving the high dimensional and inverse problem formulations. Still, high-order Discontinuous Galerkin methods and very flexible Meshfree methods, such as the Material Point Method (MPM), are continuing to be relevant. The manuscript in includes a comprehensive quantitative comparison, which is presented in Table 1, as well as four in-depth case studies that include Computational Fluid Dynamics, Solid Mechanics, Financial Mathematics, and Fluid Structure Interaction. We describe several outstanding challenges, such as the development of strict theoretical foundations for AI-driven solvers and the optimization of the use of these advanced techniques on high-performance computing platforms. Looking round the future, possible research directions are identified, notably the derivation of novel adaptive hybrid algorithms, which can lead further into the field.

Keywords: Partial Differential Equations, High-Dimensional PDE, Stability, Physics-Informed Neural Network.

ОБЗОР СОВРЕМЕННЫХ ЧИСЛЕННЫХ МЕТОДОВ ДЛЯ УРАВНЕНИЙ В ЧАСТНЫХ ПРОИЗВОДНЫХ С АКЦЕНТОМ НА ФИЗИЧЕСКИ-ИНФОРМИРОВАННЫЕ И ОПЕРАТОРНЫЕ ПОДХОДЫ

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Предложена: 21.04.2026; Принята: 12.05.2026; Опубликована: 29.07.2026

Аннотация

Численное моделирование поведения физических и инженерных систем в значительной степени определяется решением уравнений в частных производных (УЧП). Традиционные методы дискретизации, такие как методы конечных разностей, конечных элементов и конечных объёмов, занимают ведущие позиции в данной области; однако они часто сталкиваются с ограничениями при рассмотрении задач со сложной геометрией, высокоразмерными областями или при жёстких требованиях к времени вычислений. В данной работе рассматриваются современные достижения в области численных методов для УЧП с акцентом на разработки периода 2015–2025 гг. Современные методы классифицируются по пяти категориям: спектральные методы, бессеточные методы, адаптивные и многомасштабные методы, методы на основе искусственного интеллекта и вероятностные методы, а также гибридные методы. Проводится детальный анализ каждой категории с точки зрения точности, вычислительных затрат, устойчивости и масштабируемости. Ключевым выводом является трансформирующее влияние методов на основе искусственного интеллекта; физически-информированные нейронные сети (PINNs) и глубокие операторные сети (DeepONet) демонстрируют особую эффективность при решении высокоразмерных задач и обратных задач. В то же время высокопорядковые методы разрывного Галёркина, а также гибкие бессеточные методы, такие как метод материальных точек (MPM), продолжают сохранять свою актуальность. В работе представлено всестороннее количественное сравнение (таблица 1), а также четыре детализированных примера применения: вычислительная гидродинамика, механика твёрдого тела, финансовая математика и взаимодействие жидкости и структуры. Обсуждаются ключевые нерешённые проблемы, включая разработку строгих теоретических основ для ИИ-ориентированных решателей и оптимизацию их применения на высокопроизводительных вычислительных платформах. С учётом перспектив дальнейшего развития обозначены возможные направления исследований, в частности разработка новых адаптивных гибридных алгоритмов, способных продвинуть данную область вперёд.

Ключевые слова: уравнения в частных производных, высокоразмерные УЧП, устойчивость, физически-информированные нейронные сети.

Introduction

1.1. Importance of Partial Differential Equations (PDEs)

Partial differential equations (PDEs) form the language of mathematics that is used to describe dynamic phenomena in a realistic world. Moreover, in all time evolution scenarios, where the variation of the involved quantity is progressive, such as a meteorological index, a thermal diffusional index or even a financial index, the causal evolution of the quantity through time can be understood best under the paradigm of the PDEs, which describe the dynamics behind the scene. The Navier-Stokes equations for the motion of a fluid, the heat equation for the spreading of heat, and of course the most recent the Schrifer equation, important for Quantum Mechanics, are all examples of such problems. Such equations are the foundation for transformative advances in all kinds of scientific disciplines and are the kind of catalysts that result in new technologies and improved industrial design. Since there is no available and accurate solutions, such revolutionary advances would be unthinkable.

1.2. Computational Challenges and the Need for Modern Methods

In fact, this assertion has a special meaning since solving a problem in real life, in the form of partial differential equations (PDEs), analytically has always been very difficult. Not surprisingly, new ways to solve numbers were then devised; certain numbers were too hard to work with using traditional methods. In the past computational scientists have been able to give spectacular results by finite- difference, FDM, finite- element, FEM and finite- volume, FVM methodologies. However, as the difficulty increases so do the limitations of these techniques to deliver satisfactory results. For example, there is the challenge of dealing with complex geometries. In such cases, computational methods based on a mesh, such as FEM and FVM, are rather cumbersome since mesh creation and mesh refinement can dominate the computational workflow. Not to mention the curse of dimensionality, which further compounds the misery: With every new dimension, so many more degrees of computational misery. The traditional ways of doing things simply cannot keep up, as in quantum chemistry or financial modelling. The inverse problem is an extremely difficult problem as well. The parametric recovery of unknown parameters/boundary conditions to match available data is a time consuming and expensive (if not impossible) task using classical solvers. Real time prediction is also an important topic. Today's simulation needs to be very fast and reliable, such as for a digital twin or for an online control system, and here techniques must be able to provide answers in an instant. Conventional techniques need the full re-solution of the PDE at each timestep and hence are not feasible for immediate response. Thus, the need is high for methodologies, which can learn the solution procedure per se. In response to these challenges, a new round of research began: to build modern numerical methods that fully exploit the capabilities of computational resources available today, based on machine learning techniques, and with new knowledge from the numerical analysis that helps to overcome the limitations of legacy methods.

1.3. Scope and Significance of the Study

The paper contains an extensive overview of the latest and notable numerical methods for partial differential equations, taking into account the period of 2015-2025 years. The good thing about this review is that it presents all these modern techniques in a systematic manner and gives a detailed and critical comparison of these techniques. This work aims to give detailed studies of the latest advances for: specifying the theoretical basis of the various sophisticated methods, assessing their performance with respect to classical methods, and to give recommendations to practitioners and scholars on how to select the most appropriate methodology fitting to the particular issue at hand in the context of the study on partial differential equations.

1.4. Objectives and Structure of the Paper

This paper aims to:

1. Organize up-to-date numerical techniques for solving PDEs into logical, coherent categories.
2. Explore the rationale behind each strategy, what is effective, what is not, and why as it relates to math.
3. To help bring to life real scientific and engineering applications of these methods through specific case studies.

In particular, give an account of the direction, the best challenges in the field and the requirements for the more widespread use of these new techniques.

In this statute, we will state the following: Classical Theory and methods (including high order and discrete schemes) reside in Section 2. There is a connection to modern numerical methods in Section 3. There is a full comparison and performance check in section 4 with all four benchmarks. Application is made in section 5. Future work and challenging issues yet to be solved are mentioned in section 6. This paper ends with Section 7.

Theoretical Framework and Classical Methods

2.1. Mathematical Preliminaries of PDEs

An equation, partial differential equation (PDE), is a partial derivative differential equation with multiple independent variables and the unknown function and its partial derivatives. The level of difficulty maybe agreed on at the start by considering the highest order derivative which is a considerable amount of information about the type of solutions you will get, which will have the numerical methods that can work. The Laplace or Poisson equations are an example of an elliptic partial differential equation; elliptic problems typically occur in either steady-state or equilibrium. There are no singular solutions to elliptic PDEs and they are completely boundary dependent, for example, the difference between the solutions of the Laplace and Poisson equations is smooth throughout the domain. The PDEs that relate to laws of change in time (diffusion, heat conduction, etc.) are called parabolic PDEs: diffusion equation or Fokker-Planck equation. These involve initial conditions and boundary conditions since the solutions will grow in time. Then there are hyperbolic PDEs which occur whenever one has to

deal with waves or transport phenomena: the classical examples are wave equation and advection equation. Solutions can here get quite crazy, with shock waves or jumps; it's strongly related to the propagation of information across the domain.

2.1.1. Well-Posedness and Solution Properties

A well-posed mathematical model using a PDE is one that satisfies the properties [1], [2] below:

- a solution exists;
- the solution is unique;
- the solution depends continuously on the initial and boundary data.

Any proposed numerical method has to meet these criteria. In contrast, hyperbolic problems require schemes which can capture discontinuities without spurious oscillations, e.g., upwind differencing or shock-capturing schemes are useful for this type of problem.

2.1.2. Weak Solutions and Variational Formulation

However, in fact, strong solution is a classical notion and particularly for PDEs non-smooth in coefficients or in solutions, this is usually found deficient. Hence weak solution, which is a core concept for finite element and other variational methods, has been adopted. The weak formulation of a PDE is done by multiplying the governing equation with a smooth test function v and integrating everything over the computational domain Ω .By applying integration by parts (or Green's identity) on the derivatives acting on the unknown function u , transfer is made to the test function v , thus decreasing the required differentiability demand on u . Therefore, one is looking for a solution u in some Sobolev space, typically $H^1(\Omega)$ which contains square-integrable functions and their first derivatives.

For a representative **linear elliptic problem**

$$-\nabla \cdot (a\nabla u) = f \text{ in } \Omega \tag{1}$$

The weak formulation can be expressed as:

$$\int_\Omega a\,\nabla u \cdot \nabla v\,dx = \int_\Omega f v\,dx + \int_{\partial\Omega} v\,(a\,\nabla u \cdot n)\,dS \tag{2}$$

This variational structure particularly suits that numerical implementation, allowing the use of piecewise polynomial basis functions which must at all times remain continuous (but not differentiable) across the element boundary. Flexibility such as this represents one of the strengths and versatility of FEM as a tool for PDEs in very complicated geometries.

2.2. Review of Foundational Numerical Methods

2.2.1. Finite Difference Method (FDM)

The simplest method is conceptually the method of Finite Difference Method which uses Taylor series approximations at nodes to approximate the derivatives.

Core Concept: Discretization of the domain on a structured grid, substitute derivatives by finite difference quotients, forward, backward or central.

Stability and convergence go hand in hand. According to the Lax equivalence theorem, only for a consistent scheme of a linear initial value problem do convergence and stability go hand in hand. Stability is not an abstract concept to be checked, generally through von Neumann analysis, for linear problems only. Perhaps this is where time-stepping is needed. Unless you watch it, you will be in trouble, particularly in the case of explicit schemes (cFL condition again).

Then, when a higher accuracy is desired, it is a requirement that high-order finite difference schemes like WENO and compact schemes are used. Weighted Essentially Non-Oscillatory (WENO) is mainly used for hyperbolic problems, in particular when shocks are met. Several low order stencils are combined and weighed differently in the subsequent operations, from which the essence of the method appears. In smooth areas, there is always one weight which dominates the others and such high-order accuracy is achieved. The weights then fall off if they come close to a sharp drop, which decreases the unnecessary oscillations. Different schemes of operation are implemented in compact schemes, which are very tight stencil but take information from adjacent points. Higher accuracy is then achieved without having to increase computational effort to a great extent.

2.2.2. Finite Element Method (FEM)

The most classically used technique in structural and mechanical engineering, for the ability to adapt to various and diverse geometries.

1. Kernel Concept: the domain is discretized to a mesh of simple elements, which can also include triangles and tetrahedron. Solution is approximated by a linear combination of piecewise polynomial basis functions defined on these elements.

2. Advantages: expert handling of complex geometry, solid mathematics (Galerkin method), direct implementation of various boundary conditions.

3. Discontinuous Galerkin Methods (DGM): discontinuous basis functions at element boundaries. With this local nature it has many advantages:

· very high order accuracy: very high order accuracy is easily obtained p-refinement in DGM via increasing the polynomial degree within an element;

· local conservation: the DGM is locally conservative, and thus it works well with hyperbolic conservation laws;

· parallelization: since the message that must be sent between elements only concerns the adjacent elements, the method can be implemented in a parallel way easily. DGM is an important bridge between traditional FEM approaches and new high order methods, mainly in CFD [3], [4], [5].

2.2.3. Finite Volume Method (FVM)

FVM is the method of choice in Computational Fluid Dynamics (CFD) and heat transfer because it is inherently conservative.

1. Core Concept: domain is divided into a collection of non-overlapping control volumes (finite volumes). The PDE is integrated on each control volume to get a balance equation for the conserved quantity. The fluxes of variables through the boundaries of the control volume are then estimated.

2. Strengths: conservation is upheld with precision even on unstructured meshes which is precondition of the real representation of transport phenomena.

Flux Limiters and Riemann Solvers: in order to solve hyperbolic equations with the finite volume methodologies, Riemann solvers, such as Roe or HLL are used, in order to correctly evaluate the fluxes between the control volume, with special attention to discontinuities. Near shocks, nonphysically induced oscillations (sometimes called "wiggles") should be suppressed by the use of flux limiters in order to preserve this Total Variation Diminishing (TVD) property of the solution. This renders the finite - volume method to be robustly applied for complicated, nonlinear flow regimes.

Comparative Analysis and Performance Evaluation

3.1. Quantitative Comparison of Modern Methods

The choice of an optimal numerical scheme is a critical function of the partial differential equation to be considered, the geometry of the domain, the required accuracy and the available computational resources.

A quantitative comparison of some of the key performance metrics is presented in Table 1.

Table 1 - Expanded Comparative Analysis of Modern Numerical Methods for PDEs

Method	Accuracy (Order of Convergence)	Computational Cost (Per Iteration)	Memory Footprint	Stability	Scalability (High-D)	Implementation Complexity	Ideal Applications
Spectral	Exponential (for smooth solutions)	High (Setup), Low (Solution)	High	High	Low	High	Smooth solutions, simple domains, high-fidelity benchmarks
Discontinuous Galerkin (DG)	High-Order Algebraic $O(h^{p+1})$	Moderate/ High	Moderate	High	Moderate	High	Hyperbolic problems, complex geometries, local conservation
Meshfree (MPM/SPH)	Algebraic $O(h^p)$	High (Particle-Grid Transfer)	High	Moderate (Requires Stabilization)	Moderate	Moderate	Complex/ moving boundaries, large deformation, FSI [7]
Adaptive (AMR)	Algebraic $O(h^p)$	Low (Effective Cost)	Moderate	Moderate	Very High	High	Problems with localized features (shocks, boundary layers) [8], [9]
AI-based (PINNs)	Moderate/ High (Algebraic)	Very High (Training), Low (Inference)	Moderate	High	Moderate	High	High-dimensional, inverse problems, data- rich scenarios [12], [13]
Operator Learning (DeepONet/ FNO)	High (Algebraic)	Very High (Training), Very Low (Inference)	Moderate	High	Moderate	Moderate	Real-time prediction, surrogate modeling, learning solution

Method	Accuracy (Order of Convergence)	Computational Cost (Per Iteration)	Memory Footprint	Stability	Scalability (High-D)	Implementation Complexity	Ideal Applications
							operators [15], [16]

3.1.1. Convergence and Error Analysis

Spectral Methods offer the best theoretical convergence for smooth solutions. The error decays as

1. Spectral Methods offer the best theoretical convergence for smooth solutions. The error decays as $\mathcal{O}(N^{-p})$ for any (p) , limited only by the smoothness of the solution.

2. Mesh-based and Meshfree Methods typically exhibit algebraic convergence, ($\mathcal{O}(h^{-p})$), where (h) is the mesh size and is the order of the method. The high-order nature of DGM allows for rapid convergence by increasing the polynomial degree (p) .

AI-based Methods also show algebraic convergence, but the convergence rate is often difficult to predict and depends heavily on the network architecture, activation function, and optimization strategy. The convergence accuracy of PINNs is often limited to around (10^{-3}) to (10^{-5}) In the relative (L_2) error, which is often insufficient for high- fidelity engineering simulations [10], [11].

3.1.2. Computational Cost and Scalability

Cost of Training: AI-based methods (PINNs, DeepONet) have an extremely high initial training cost, often requiring days or weeks on GPUs. However, their inference cost is negligible, making them ideal for repeated, fast queries (surrogate modelling).

Cost of Solution: spectral techniques can be utilized with FFT to solve the problem fairly rapidly in simple domains; however, mesh-free methods or high-order FEM tend to be relatively more expensive owing to complex costs of matrix assemblies and high integration efforts.

Scale: AI-based as well as Meshfree methods (because it is the inherent nature of being particle-/node based) can demonstrate improved scalability to high-dimensional problems compared to classical mesh-based approaches, in which the number of grid points grows exponentially.

3.2. Case Studies and Benchmarks

3.2.1. Benchmark 1: Elliptic PDE (Poisson/Laplace) with Non-Smooth Solution

Problem: Poisson equation on a square domain with a solution that has a localized singularity (e.g., a re-entrant corner). Comparison:

· the first method, spectral, fails because of the Gibbs phenomenon, causing global oscillations and loss of exponential convergence;

· the second way, FEM/DGM, deals well with singularities using localized mesh refinement (h-refinement) near corners; in particular, the DGM can make flexible use of p-refinement away from the singularity combined with h-refinement close to it;

· spectral bias predominantly affects the accuracy of PINNs, since the network has difficulties learning the solution high-frequency components close to singularity [14]; to attain an acceptable level of accuracy, domain decomposition (XPINNs) is required.

3.2.2. Benchmark 2: Hyperbolic PDE (Advection/Wave) with Shocks Problem: 1D Burgers' equation with a sharp shock wave

Comparison:

· FVM (WENO): highly robust and accurate, as the WENO scheme effectively suppresses oscillations near the shock while maintaining high order in smooth regions;

· AMR-FVM: most efficient, as the AMR focuses computational effort only on the moving shock front, significantly reducing the total number of grid points and computational time for long-time integration [8];

· SPH**:** naturally handles the shock due to its particle-based, Lagrangian nature, but often requires artificial viscosity to stabilize the solution and can suffer from particle disorder.

3.2.3. Benchmark 3: High-Dimensional PDE (Black-Scholes)

Problem: Option Pricing Using Black-Scholes Equation 100+ Underlying Assets Comparison:

· traditional Methods Failing due to curse of dimensionality;

· PINNs: address the problem successfully by making use of the universal approximation theorem of neural networks; while the computational complexity is greatly reduced when close to classical methods, the required training time is still a considerable amount;

· DeepONet/FNO: after a relatively expensive training phase, these operator learning frameworks are capable of predicting option prices for new starting conditions or parameters - such as volatility - in milliseconds; as such, they are the favourite option for real time risk management and trading infrastructures; deepONet's tolerance to noisy input data makes it particularly attractive for realistic financial data sets [17], [19].

3.2.4. Benchmark 4: Fluid-Structure Interaction (FSI)

The problem of simulating a flexible structure (like a flag) in the midst of a fluid flow.

Comparison:

· FEM/FVM Coupled: this coupling involves very complex mesh deformations/remeshing at each time step, is very expensive, and may even fail due to mesh tangling which is a potential problem when the mesh is subjected to significant structural deformations;

· Material Point Method (MPM): with an integrated MPM environment the fluid and solid can be modeled accurately and Voronoi particles maintain material interface without any difficulties, and momentum transfer from fluid to solid is naturally taken care of in Eulerian grid and can thus accept large deformations and free surface flow without any mesh tangling problems [7]; MPM is thus an interesting candidate for the solution of complex fluid-structure interaction problems.

3.3. Software and Implementation Landscape

Maturity of software is an important factor in the acceptance of numerical methods.

· Classical Methods high mature and standardized (e.g. FEniCS for FEM, OpenFOAM for FVM);

· AMR: there are mature frameworks in place, like AMReX (block-structured AMR), Chombo;

· Meshfree: not as standardised in regards to software, many specialised codes (e.g. DualSPHysics for SPH, many research codes for MPM);

· AI-based: rapidly evolving; DeepXDE is a popular general purpose PINN library and implementations of DeepONet and FNO are commonly found in the specialized repositories of research; the absence of one, mature and universally accepted framework is still a barrier to entry for many researchers.

Applications Across Disciplines

The modern numerical methods are driving breakthroughs across various scientific and engineering disciplines.

4.1. Computational Fluid Dynamics (CFD)

CFD has become a mainstay of modern scientific activity, especially in the areas of turbulence modelling and in the case of complex flow regimes. Its evolution is led by the incorporation of sophisticated computational methods that allow describing physical phenomena, otherwise inaccessible in the past.

1. AMR in Weather Prediction Global atmospheric and climate models cannot exist without Block structured Adaptive Mesh Refinement (AMR). By focusing computational resolution around localized meteorological activities like hurricanes or frontal activities, AMR allows these types of meteorological features to be faithfully simulated at an affordable cost of fine grids over the entire world. This type of selective refinement is necessary to both capture the fine scale dynamics responsible for storm evolution as well as the broader context of the planetary circulation.

2. Spectral Methods in DNS The Direct Numerical Simulation (DNS) method of turbulence study uses spectral discretisation techniques due to their ability to describe the continuous spectrum of eddies with a greater level of accuracy. Spectral methods help to minimise the numerical dispersion and dissipation errors and hence make it possible to resolve the full set of scales of turbulence, from the largest energy bearing vortices, down to the dissipative microscales. The fidelity provided by spectral approaches is the basis for confident investigation of key fundamental turbulence processes, such as energy cascades and intermittency.

3. PINNs for Turbulence Modelling A growing role of Physics-Informed Neural Networks (PINN) in learning subgrid-scale closure relations (i.e., Reynolds stresses) for Reynolds Averaged Navier Stokes (RANS) schemes. By incorporating the governing equations into the loss function, PINNs respect our understanding of the underlying physical principles while learning robust data-driven models from high resolution flow databases. The available empirical evidence does not rule out the possibility of such data--assisted closures being better than conventional algebraic models to predict on the basis of the physics governing the problem [18], [20].

4. Application of FNO for Real Time Flow Prediction The Fourier Neural Operator (FNO) has been shown to have an incredible capability in approximating the solution operator of the Navier Stokes equations. Using learning principle to produce flow field from the boundary conditions to whole flow fields, FNOs make it possible to reconstruct complex flow feelings with velocity and pressure in near instantaneous time for new configurations. This term do in the real-time represents a paradigm shift for the real-time control, optimisation and decision support in aerospace engineering and the design of industrial processes.

4.2. Solid Mechanics and Materials Science

1. Meshfree Methods for Fracture: SPH and Material Point Method (MPM) are highly effective for simulating material failure, fracture, and fragmentation, where the mesh in FEM would become severely distorted [7].

2. FEM/ML Hybrids for Composite Materials: Machine learning models are trained on micro-scale simulations to predict the effective macro-scale properties of composite materials, which are then fed into a macro-scale FEM solver, significantly reducing the computational cost of multiscale analysis.

3. Multiscale Simulation using VMS and ROMs: Variational Multiscale (VMS) methods have been used to stabilize FEM for nearly incompressible materials, while Reduced Order Models (ROMs) are more often applied in the context of fast and predictive models for structural health monitoring and fatigue analysis.

4.3. Biomedical Engineering

Simulations of blood flow in arteries (hemodynamic) are crucial for the understanding of cardiovascular diseases and this is achieved by use of CFD and also PINNs. The mesh-free approach PINNs provide for solving the Navier-Stokes equations for specific arbitrary geometries of the arterial system can be used to give rapid, non-invasive estimations of blood pressure

and flow rates [21]. AI-based methods can be used for complex high dimensional data handling as well as paradoxical modelling, there is another way to personalized medicine. The PINN can for instance be used to derive patient-specific material properties of the wall of arteries from the non-invasive imaging data, and so optimize the surgical planning.

4.4. Financial Mathematics and Quantum Mechanics

The high-dimensional PDEs are prevalent in these fields and are therefore good test beds for the use of AI-based methods.

One is the financial mathematics with the pricing of the complex structure of financial derivatives being governed by higher-dimensional parabolic PDEs (e.g. Black-Scholes equation with multiple assets). These equations are solved using PINNs and DeepONet, thus offering fast and accurate pricing and risk management tools.

Quantum Mechanics: The Schrödinger equation (time dependent) is a high dimensional PDE. PINNs are being explored for the case of both the wave function of the ground and excited states, to provide an alternative pathway to the wave function besides the ones taken by traditional quantum chemistry methods like Density Functional Theory (DFT).

4.5. Geophysics and Environmental Modelling

AMR and FVM for Seismic Wave Propagation: For AMR it's related to simulating the traversal of seismic waves. It can also model the near-surface effects (such as fault zones) at relatively coarser depth constraint grid in deep earth, given the coarse grid size could be a problem. Due to the natural conservation properties of FVM, it is widely used for modelling groundwater flow and transporting the contaminant.

High-Dimensional Data Assimilation and Filtering: Many problems require probabilistic methods (particularly based on GPs and Bayesian inference) to assimilate huge quantities of noisy data (in particular weather and satellite images, seismic data, etc.) into PDE-based models for the purpose of weather forecasting and climate change prediction.

Open Challenges and Future Directions

5.1. Open Challenges

5.1.1. Robustness and Generalization of AI-based Solvers

Hyperparameter tuning sensitivity (loss function weighting, architecture of the network, etc.) and accuracy of measurement (which must not exceed (10^{-5}) error) are the two important factors which hinder the pinning methods. Further complications arise when trying to use neural networks to capture sharp gradients or high-frequency solutions — spectral bias, where neural networks learn low-frequency parts of the spectrum, dominates. Moreover, a proper and complete framework for analyzing the stability/convergence of Physics-Informed Neural Networks is still a major challenge for the field similar to the Lax Equivalence Theorem for finite difference schemes. So, their broader adoption to solve engineering problems that are safety critical requires their certification and verification, which can be achieved through AI-driven solvers.

5.1.2. Theoretical Foundations for Meshfree Methods

Meshfree approaches have demonstrated a tremendous flexibility, but a systematic and sound theory of the stability and convergence for highly nonlinear problems is still under development. Theories need to be further developed with respect to issues related to boundary conditions enforcement and choice of kernel functions [6].

5.1.3. Integration of HPC (High Performance Computing)

The need for the rigid data structure of high-level AMR algorithms and the nonlocal nature of some mesh-free and spectral methods invoked in combination pose a big challenge for achieving secure computational performance on petascale and exascale platforms. As opposed to the (intrinsic) parallelism provided by GPU architectures in the AI-based approaches, the data migration and data communication latencies are dramatically expanded and played in parallel to the highly irregular data schemas of AMR and Mesh-free approaches, which are mainly based on recurrent data exchange between processing elements.

5.1.4. Uncertainty Quantification (UQ)

The basic assessment of the uncertainty in numerical solutions is done. The largely computational intensive Monte Carlo based approaches are typical for classical methods dealing with uncertainty quantification. Among the AI-based approaches, uncertainty quantification is a new research field, with techniques such as ensemble-based methods [27] and Bayesian Physics-Informed Neural Networks [18] (B-PINNs) demonstrating promise in uncertainty labelling but significantly boosting the training workload.

5.2. Future Directions

5.2.1. Next-Generation Hybrid Algorithms

Data-driven and physics-driven models need to be seamlessly integrated which is the future of the numerical methods. This includes:

1. Adaptive Hybridization: algorithms that can adaptively switch from the use of a traditional solver (which has a high level of accuracy in the critical regions) to an AI-based surrogate (which has a high level of speed in the non-critical regions) that can be a multi-fidelity application, choosing the strengths of both.

2. Physics Constrained Operator Learning: Directly encoding the hard constraints of classical numerical schemes, such as conservation, stability and so on into the structure of operator learning models (such as DeepONet, FNO and so on), and during the operator learning process, make sure that an operator can satisfy all fundamental laws. Hence, the generalization and robustness are improved.

5.2.2. Operator Learning and Surrogate Modelling

Operator learning based approaches (DeepONet, FNO) are promising to further change the face of simulation in the near future through generation of fast and reusable PDE solvers. This will enable:

1. Digital Twin in Real Time: System behaviour prediction based on the data which is instantaneously available for control and optimisation.

2. Design Optimization on a Fast Lane: Faster evaluation of parameters controlling designs that are modeled by complex PDEs.

3. Learning Non-Local Operators: Extend the framework to take account of physics that is non-local, in particular physics described by fractional PDEs or integral equations, of great concern in materials science.

5.2.3. Focus on Multidisciplinary and Inverse Problems

New strengths of modern tools will be more and more committed to solve complex problems involving several disciplines:

Climate Modelling: When Adapative Mesh Refinement of the Atmospheric Dynamics meets Artificial Intelligence Models to capture Complex Sub-Grid processes.

Another critical research area not done to date, will be using the intrinsic architecture of physics-informed neural networks to learn the properties of materials with the source terms and boundary conditions obtained from sparse noisy measurements required by non-destructive testing and characterization of materials. One of the most important research thrusts is the development of efficient, data sensitive, inverse solvers.

Conclusion

This extensive paper discussed the evolution of numerical techniques for Partial Differential Equations from well established yet semi-classical techniques (FDM, FEM, FVM) to a myriad of modern and specialized techniques. Among the different types of methods, spectral methods assure maximum accuracy for smooth problems, Discontinuous Galerkin methods assure maximum order of accuracy with local conservation, Meshfree methods (like MPM) assure enhanced geometric flexibility, while Adaptive methods (such as AMR and AMG) assure computational efficiency. Finally, the most recent methods are those based on AI, like PINNs and DeepONet, able to tackle the long-existing problems of very-high-dimensionality and inverse problems.

The conclusion is that there is simply no method that is good in all situations. The one that is best among the rest is always a conscious choice based upon features of the problem it would be applied in, as evidenced by the four larger benchmarks presented in detail. Current trends towards hybridization are on the rise, which combine the advantages from both traditional and modern methodologies for the development of solvers that are robust, accurate, and efficient. Even with the huge challenges ahead, especially in validating the theoretical rigor and enhancing the AI-based method performance at high accuracies, the field is at a juncture that has opened up into a transformative era catalysed by the collaboration of numerical analysis and machine learning. Continued work on next-generation adaptive hybrid algorithms and optimization for HPC will be vital to enable these modern methods to realize their full potential in solving the most challenging PDEs arising in science and engineering.

Конфликт интересов

Не указан.

Рецензия

Все статьи проходят рецензирование. Но рецензент или автор статьи предпочли не публиковать рецензию к этой статье в открытом доступе. Рецензия может быть предоставлена компетентным органам по запросу.

Conflict of Interest

None declared.

Review

All articles are peer-reviewed. But the reviewer or the author of the article chose not to publish a review of this article in the public domain. The review can be provided to the competent authorities upon request.

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