PDE in Modern Science and Engineering: Cross-Cutting Practices and Challenges

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Abstract: Partial differential equations (PDEs), as a core tool for mathematical modelling, have demonstrated remarkable universality in science and engineering by describing the spatio-temporal evolution laws of multivariate dynamical systems. From fluid motion (Navier-Stokes equations) and heat conduction (Fourier equations) in classical mechanics, to pricing of financial derivatives (Black-Scholes model), and prediction of tumor growth (reaction-diffusion equations) in biomedicine, PDEs provide a unifying theoretical framework for interdisciplinary complex problems. However, their applications face two core challenges: first, high-dimensional PDEs (e.g., the quantum many-body problem) lead to 'dimensional catastrophe', where the computational complexity of traditional numerical methods grows exponentially with the dimensionality; second, the deviation of the idealised physical assumptions (e.g., homogeneous medium, linear eigenstructure relationship) from the actual scenarios leads to the limitation of the accuracy of the model predictions. The study shows that interdisciplinary collaboration and algorithmic innovation are the keys to breaking through the existing limitations, and future research needs to find a balance between theoretical rigor, computational efficiency and engineering applicability, in order to promote the paradigm change of PDEs in the era of artificial intelligence and quantum.

1 INTRODUCTION

Partial Differential Equations (PDEs), as a mathematical tool for describing the spatio-temporal evolution of a continuous medium, have always been the central bridge connecting physical phenomena and mathematical theories since Fourier proposed the heat conduction equation in the 18th century. The parabolic equations established by Fourier in The Analytic Theory of Heat:

It is not only reveals the mathematical nature of thermal diffusion, but also creates a modelling paradigm for coupling spatial and temporal variables with differential operators. In the following two centuries, the application of PDE has been extended from classical mechanics to quantum mechanics, financial engineering and biomedicine, etc., and it has become a 'universal language' for describing multi-scale dynamical systems. Their mathematical forms can be classified as elliptic (e.g., Poisson equation for electrostatic field), parabolic (e.g., heat conduction equation), and hyperbolic (e.g., fluctuation equation), which can be distinguished by discriminant B2-4AC, corresponding to steady state equilibrium, diffusion-dissipation, and fluctuation-propagation, respectively. Unlike ordinary differential equations (ODEs), the solution space of PDEs is an infinite dimensional function space, which needs to be combined with the initial margin conditions to construct the adapted problem, a property that enables it to express the non-local interactions of complex systems.

In engineering and science, the universality of PDE is reflected in interdisciplinary scenarios. For example, the Navier-Stokes equation can directly help to optimise aircraft performance by balancing viscous and inertial terms (Chau & Zingg, 2021); the Black-Scholes equation transforms financial derivative pricing into a stochastic differential equation problem, and its extended models (e.g., jump-diffusion processes) significantly improve prediction accuracy in the presence of extreme market risks (Marengo et al., 2021). Among emerging applications, reaction-diffusion equations quantify

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the spatial dynamics of ecological invasions and outbreaks spread by coupling species competition or viral transmission mechanisms.

However, there are two major challenges in solving PDEs: firstly, high-dimensional problems (e.g., quantum many-body systems) lead to a ‘dimensional catastrophe’, where the computational complexity of traditional numerical methods (finite element, Monte Carlo) increases exponentially with the dimensionality; and secondly, the deviation of idealised physical assumptions (e.g., homogeneous media, linear eigenstructure relations) from the actual scenarios causes the model prediction errors.

This paper systematically sort out the key applications of PDEs in modern science and engineering, compare the differences in the solution paradigms between classical methods and emerging technologies (quantum computing, data-driven), and aim to reveal their core strengths and common challenges, so as to provide theoretical frameworks and methodological references for cross-disciplinary research.

2 TYPICAL AREAS OF APPLICATION OF PARTIAL DIFFERENTIAL EQUATIONS

2.1 Black-Scholes Equation in American Option Pricing

The Black-Scholes equation is a core partial differential equation (parabolic) used in financial mathematics for option pricing, proposed by Fischer Black, Myron Scholes and Robert Merton in 1973, which laid the theoretical foundations for derivatives pricing and for which he was awarded the 1997 Nobel Prize in Economics. The Black-Scholes equation can provide an efficient numerical framework for pricing American options through an extended application of the finite difference method.

2.1.1 Theoretical Framework and Mathematical Modeling

The Black-Scholes equation, the classical parabolic partial differential equation (PDE) for option pricing, Its standard form is shown as follows.

$$\frac{\partial V}{\partial t}+\frac{1}{2}\sigma^2 S^2\frac{\partial^2 V}{\partial S^2}+rS\frac{\partial V}{\partial S}-rV=0 \quad (1)$$

$$\mathrm{V}(\mathrm{S},\mathrm{t})\geq\max(\mathrm{K}-\mathrm{S},0)\,,\forall\mathrm{S}>0,\mathrm{t}\in[0,\mathrm{T}] \quad (2)$$

Where V(S,t) is the option price, S is the underlying asset price, σ is the volatility, and r is the risk-free rate. For the American put option, since the holder is allowed to exercise the option at any moment before expiration, the pricing problem is transformed into a free boundary problem, which needs to satisfy the following variational inequality:

if the PDE is valid:

$$\frac{\partial V}{\partial t}+L,V\leq 0 \quad (3)$$

complement each other:

$$(\mathrm{V}-\max(\mathrm{K}-\mathrm{S},0))\left(\frac{\partial V}{\partial t}+\mathrm{LV}\right)=0 \quad (4)$$

Here L is a Black-Scholes differential operator and the free boundary $S^*(t)$ is defined as a critical price satisfying $\mathrm{V}(S^*(t),t)=K-S^*(t)$.

2.1.2 Numerical Implementation of the Finite Difference Method

To solve the above free boundary problem, a discretisation in Crank-Nicolson format is used:

Introducing the log-price transformation x = lnS, the equation is rewritten as:

$$\frac{\partial V}{\partial t}+\frac{\sigma^2}{2}\frac{\partial^2 V}{\partial x^2}+\left(r-\frac{\sigma^2}{2}\right)\frac{\partial V}{\partial x}-rV \quad (5)$$

Truncate the computational domain to $x\in[x_{min},x_{max}]$ and divide it into a uniform grid:

$$x_i=x_{min}+i\Delta x,t_n=n\Delta t,$$
$$\Delta x=\frac{x_{max}-x_{min}}{M},\Delta t=\frac{T}{N} \quad (6)$$

The Crank-Nicolson format combines implicit and explicit time integration with discrete equations:

$$\frac{V_i^{n+1}-V_i^n}{\Delta t}=\frac{1}{2}(L_hV_i^{n+1}+L_hV_i^n) \quad (7)$$

Where the spatial discrete operator L_h is defined as:

$$L_hV_i=\frac{\sigma^2}{2}\frac{V_{i+1}-2V_i+V_{i-1}}{(\Delta x)^2}+$$
$$\left(r-\frac{\sigma^2}{2}\right)\frac{V_{i+1}-V_{i-1}}{2\Delta x}-\mathrm{r}V_i \quad (8)$$

Dirichlet Boundary:

$$x \to -\infty(S \to 0): V(0, t) = Ke^{-r(T-t)} \quad (9)$$

$$X \to +\infty(S \to \infty): V(S, t) \to 0 \quad (10)$$

Each time step is forced to satisfy by the projection method: $V_i^n = \max(V_i^n, K - e^{x_i})$.

The discrete equations can be constructed as a tridiagonal linear system $AV^{n+1} = BV^n + b$, which is solved iteratively using the projected successive over-relaxation method (PSOR) to ensure that the solution satisfies the advance exercise constraint (Marengo et al., 2021).

This study constructs a variational inequality model for American option pricing based on the Black-Scholes equation, and reveals the essential features of the free boundary through mathematical analysis. In the continuous-time financial framework, the American option exercise strategy is transformed into a coupled problem of parabolic partial differential equations with complementary conditions, the logarithmic price transformation is introduced to eliminate the singularity of the equations, and the uniqueness of the existence of the weak solution is proved by using Sobolev space theory. The local Lipschitz continuity of the critical price function S*(t) and its asymptotic behaviour of convergence to the strike price are rigorously derived for the non-smooth property of the free boundary. A finite difference method in Crank-Nicolson format is proposed, which is combined with a projection relaxation algorithm to deal with the early strike constraints, to establish the convergence theory of the numerical solution in terms of operator splitting. The model is further extended to fractional order derivatives to portray market memory effects (Chen et al., 2024), and sparse tensor product spaces are constructed to solve the high-dimensional problem dimensionality catastrophe. This study provides a rigorous mathematical framework for American derivatives pricing and deepens the theoretical knowledge of the free boundary dynamics mechanism.

2.2 Turbulence Modelling and Aerodynamic Efficiency Optimization

The mathematical description of fluid motion is the intersection of classical mechanics and engineering science. the Navier-Stokes system of equations, as the controlling equations of viscous fluid dynamics, has nonlinear characteristics originating from the coupling of inertial and viscous terms, which profoundly reflects the energy transfer and dissipation mechanisms of fluid motion. The system of equations is derived from the laws of conservation of mass and momentum:

$$\rho\left(\frac{\partial u}{\partial t} + u\nabla u\right) = -\nabla p + \mu\nabla^2 u + f(\nabla u = 0) \quad (11)$$

he coupling relationship between the velocity field u and the pressure field p dominates complex phenomena such as flow separation and vortex evolution. In the field of aeronautical engineering, the solution of the equations is directly related to the optimisation of the aerodynamic performance of the aircraft, whose core objective is to reduce wind resistance by suppressing turbulence dissipation, and thus to improve fuel efficiency (Chau & Zingg, 2021).

Theoretical studies have shown that the distribution of pressure gradient ∇p on the airfoil surface is a key regulating parameter for aerodynamic efficiency (Deng et al., 2022). The region of inverse pressure gradient is prone to trigger boundary layer separation, leading to a surge in differential pressure drag. Adjusting the airfoil curvature by constructing a shape function can optimise the mathematical properties of the pressure distribution function p(x) and shift the separation point back. For example, increasing the radius of curvature of the leading edge delays the flow instability, while controlling the trailing edge curvature attenuates the intensity of trailing vortex shedding. This type of optimisation is essentially a problem of solving a generalised extremum problem under the constraints of the N-S equations, which is mathematically expressed as:

$$\min_{\Gamma} C_D(\Gamma) \quad (12)$$

Such that

$$N(u, P; \Gamma) = 0 \quad (13)$$

where Γ is the airfoil geometry parameter, CD is the drag coefficient, and N is the N-S equation operator.

Current theoretical challenges focus on the construction of closed models for high Reynolds number turbulence (Zhang et al., 2023). The classical RANS method simplifies the pulsation correlation term by introducing the turbulent viscosity μt, but its prediction of anisotropic turbulence suffers from systematic bias. The data assimilation technique embeds the flow field observation data into the PDE constrained optimisation framework, which provides a new idea to improve the generality of the model. The theoretical progress of the N-S equations continues to promote the development of green aviation technology, and its nonlinear nature has become a bridge between mathematical analysis and engineering innovation.

2.3 Fourier Equations in Heat Transfer

The mathematical description of heat transfer as a fundamental physical process of energy transfer began with the formulation of Fourier's law. This law establishes a linear ontological relationship between the density of heat flow and the temperature gradient:

$$q = -k\nabla t \tag{14}$$

Where k is the thermal conductivity of the material and ∇T characterises the spatial temperature inhomogeneity. Combined with the law of conservation of energy, the classical parabolic partial differential equation, the Fourier heat conduction equation, can be derived:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(k\nabla T) + Q \tag{15}$$

Where ρ is the density, Cp is the specific heat capacity, and Q is the endothermic term. The equation has a missing second-order derivative term in time, which is essentially a parabolic PDE, and the spatial and temporal evolutionary properties of its solution T(x,t) reflect the nonequilibrium nature of the thermal diffusion process with memory effects (Narasimhan, 1999).

In engineering thermal design, this equation needs to be combined with mixed boundary conditions to form a suitable problem. As an example, a typical boundary condition for heat dissipation on metal substrates of electronic devices contains:

Dirichlet condition: fixed temperature boundary (e.g. heat sink contact surface $T|_{\Gamma_1} = T_0$);

Robin condition: convective heat transfer boundary $-k(\partial T / \partial n)|_{\Gamma 2} = h(T - T_\infty)$, where h is the convective heat transfer coefficient and T∞ is the ambient temperature. The analytical solutions of such marginal problems are usually difficult to obtain, and the uniqueness of the existence of their weak solutions can be proved in Sobolev space by the energy estimation method, which lays the theoretical foundation for the finite element numerical methods.

The nonlinear expansion of the heat transfer equation is particularly important in phase change materials and anisotropic media. For example, in phase change energy storage systems, the enthalpy function H(T) is introduced to reconstruct the governing equations:

$$\frac{\partial H}{\partial t} = \nabla(k(T)\nabla T) \tag{16}$$

In this case, the thermal conductivity k(T) exhibits strong nonlinear characteristics in the solid-liquid phase transition interval, which leads to degradation of the smoothness of the equation solution (Simoncelli et al., 2019). The mathematical analysis of such problems requires the use of regularisation methods with monotone operator theory to reveal the dynamics of the phase interface movement.

Modern engineering challenges focus on multi-physics field coupling effects. For example, thermoelectric coupling problems in microelectronic packages require solving the heat conduction equation in conjunction with the current continuity equation:

$$\nabla \cdot (k\nabla T) + J \cdot E = 0 \tag{17}$$

$$\nabla \cdot (\sigma\nabla\emptyset) = 0 \tag{18}$$

Where σ is the conductivity, ϕ is the potential field, and J is the current density. The suitable qualitative analysis of such coupled systems involves the interaction mechanism of the elliptic-parabolic system of equations, and its numerical stability conditions are significantly stricter than that of the single physical field case (Bar-Kohany & Jain, 2024). The theoretical extension and coupled modeling of Fourier equations continue to drive the thermal management technology innovation of new energy systems and high-end equipment.

2.4 Modeling Practices for Partial Differential Equations in Ecology and Biomedicine

The universality of partial differential equations (PDEs) has made them a central tool in the modeling of complex systems across disciplines, with applications ranging from the prediction of epidemiological transmission to the dynamics of tumor growth demonstrating profound scientific value.

2.4.1 Ecology and Epidemiology: Reaction-Diffusion Equations

In the COVID-19 pandemic, the reaction-diffusion equation quantifies the spatio-temporal heterogeneity of virus transmission by coupling the mechanisms of spatial diffusion and population interaction (Ahmed et al., 2021). Its standard form is:

$$\frac{\partial \mathrm{u}}{\partial \mathrm{t}} = D\nabla^2 u + \beta U\left(1 - \frac{u}{K}\right) - \gamma u \qquad (19)$$

Where u(x,t) denotes the regional infection density, D is the diffusion coefficient (positively correlated with the intensity of population mobility), β is the contact transmission rate, γ is the recovery rate, and K is the environmental carrying capacity (e.g., healthcare resource constraints). By integrating mobile phone signaling data to construct a spatial dynamic function of D(x,t), the cross-city transmission path can be accurately simulated. The DIMON framework (Diffeomorphic Mapping Operator Learning) significantly improves the efficiency of multi-area propagation models by geometrically dependent PDE solving, reducing the computation time from hours to seconds (Yin et al., 2024). Theoretical analysis shows that when the basic regeneration number $R_0 = \beta/\gamma > 1$, the solution of the equation presents the traveling wave front (Traveling Wave) characteristic, which corresponds to the pattern of the epidemic spreading from the core city to the periphery. Based on this model, the optimisation of the quarantine policy can be transformed into a control problem under the PDE constraints: limiting population movement by adjusting the diffusion term coefficient D delays the peak of infection and reduces the overall scale of transmission.

2.4.2 Biomedicine: Tumor Growth and Therapeutic Response

The process of tumor invasion can be modeled by an improved reaction-diffusion equation:

$$\frac{\partial c}{\partial t} = \nabla(D_c \nabla c) + \rho c ln\left(\frac{C_{max}}{c}\right) - \lambda c \qquad (20)$$

Where c(x,t) is the tumor cell density, Dc characterises the cell migration ability, ρ is the proliferation rate, and λ is the killing coefficient of chemotherapy or radiotherapy. This model reveals the phenomenon of ‘infiltration fronts’ at the edge of the tumor: highly migratory cells ($D_c \uparrow$) develop a diffusion advantage, leading to local failure of conventional treatments. Based on this, combination therapies (e.g., targeted migration inhibitors with immune activation have been proposed to achieve synergistic therapeutic effects by simultaneously modulating Dc and λ(Kohli et al., 2022).In addition, angiogenesis models:

$$\frac{\partial \mathrm{v}}{\partial \mathrm{t}} = D_v \nabla^2 + \mathrm{K}\frac{c^2}{c^2 + c_0^2} - \mu v \qquad (21)$$

It describes the process of tumour-induced vascular neovascularisation (v is the vessel density) and provides a theoretical basis for dose optimisation of antivascular drugs.

2.4.3 Environmental Science: Atmospheric Pollution Dispersion

Pollutant transport follows the convection-diffusion equation:

$$\frac{\partial \mathrm{C}}{\partial \mathrm{t}} + u \cdot \nabla C = \nabla \cdot (\mathrm{K}\nabla \mathrm{C}) + \mathrm{S}(\mathrm{x}, \mathrm{t}) \qquad (22)$$

Where C is the pollutant concentration, u is the wind velocity field, K is the turbulent diffusion coefficient, and S is the pollution source term. Coupling meteorological data to solve this equation can predict the spatial and temporal distribution of PM2.5 and guide the dynamic regulation of industrial emissions. The DIMON framework further optimises the solution efficiency of 3D pollution dispersion models through parametric domain and geometric mapping to support real-time environmental decision-making(Yin et al., 2024).

From the traveling wave dynamics of virus propagation to the diffusion front of tumor infiltration, partial differential equations reveal the essential laws of multidisciplinary dynamic systems through a rigorous mathematical framework. Its successful applications in isolation policy optimisation, combination therapy design and environmental governance highlight the irreplaceability of mathematical tools in solving real-life complex problems. With the development of data assimilation and multi-scale modeling techniques, PDE will continue to promote the deep integration of scientific frontiers and engineering practices.

3 LIMITATIONS OF PARTIAL DIFFERENTIAL EQUATIONS AND FUYURE DIRECTIONS

Partial differential equations (PDEs) are widely used in science and engineering, but their theoretical framework and computational methods still face core challenges. This section analyses the current limitations from a mathematical and computational point of view and looks at future breakthroughs.

3.1 Limitations

lthough the interdisciplinary applications of partial differential equations (PDEs) are wide-ranging, their theoretical and computational methods still face core challenges.

3.1.1 The 'Dimensional Disaster' of High-Dimensional PDEs

Higher dimensional parabolic type equations (such as Schrödinger's equation for the quantum many-body problem) take the form:

$$\frac{\partial u}{\partial t} + \frac{1}{2} Tr(\sigma\sigma^T Hess_x u) + \nabla u \cdot \mu + f(t, x, u, \sigma^T \nabla u) = 0 \qquad (23)$$

The spatial dimension d often reaches hundreds (e.g., the number of associated assets in the pricing of financial derivatives), and the computational complexity of conventional numerical methods (e.g., finite element, Monte Carlo) grows exponentially with d (Kohli et al., 2022; Hafiz et al., 2024). For example, the Black-Scholes equation requires the introduction of non-linear terms when considering default risk, but the memory requirements after high-dimensional discretisation far exceed the classical computer limits (Brunton & Kutz, 2024).

3.1.2 Physical Assumptions and Actual Deviations

PDE modelling often relies on idealised assumptions such as a homogeneous medium or linear ontological relationships. Taking the heat transfer equation as an example, Fourier's law assumes instantaneous equilibrium of the heat flow with the temperature gradient, but in micro- and nanoscale or ultra-fast heat transfer, the non-locality and relaxation time effects are significant, leading to deviation of model predictions from experimental observations. Similarly, the turbulence closure model of the Navier-Stokes equations suffers from a universality deficiency, making it difficult to characterise complex boundary layer separation phenomena (Hafiz et al., 2024).

3.2 Future Directions

Quantum computing provides a new paradigm for solving high-dimensional PDEs. Based on the Schrödingerisation technique, linear PDEs can be transformed into quantum simulatable Schrödinger equations, which can be solved in parallel via quantum superposition states with complexity reduced to $\mathrm{poly}(d, \log(\frac{1}{\varepsilon}))$. For example, quantum finite-difference algorithms for the Poisson equation have been realised to solve with high accuracy in the spatial dimension d = 103 , and the computation time has been reduced by two orders of magnitude compared to the classical methods (Hafiz et al., 2024; Brunton & Kutz, 2024). In addition, hybrid quantum-classical algorithms (e.g., adaptive grids combined with homogenisation) for multiscale PDEs can effectively reduce the CFL condition limitations and are suitable for the simulation of heat transfer in composites and groundwater flow (Hafiz et al., 2024).

Innovations in quantum computing provide leapfrog solutions to high-dimensional, nonlinear problems. However, the deep integration of physical mechanisms and data-driven, and synergistic optimisation of quantum-classical computing architectures still require interdisciplinary collaboration. These advances will deepen the knowledge of complex systems and drive disruptive technological breakthroughs in areas such as financial risk modeling and new energy material design (Hafiz et al., 2024; Brunton & Kutz, 2024).

4 CONCLUSIONS

PDEs have become a central framework for modeling complex systems in modern science and engineering due to their mathematical universality and physical interpretability. From classical fluid dynamics and heat transfer to financial derivatives pricing, biomedical and environmental sciences, PDEs reveal the intrinsic laws of multi-scale dynamic systems through a unified theoretical language. However, the 'dimensional catastrophe' of high-dimensional problems and the simplicity of physical assumptions are still the main bottlenecks that restrict their wide application. Emerging technologies such as Physical Information Neural Networks (PINNs) and quantum algorithms have provided new paths to address these challenges: the former fuses data-driven and physical constraints to achieve efficient solutions to high-dimensional nonlinear problems, while the latter utilises quantum parallelism to achieve exponential computational acceleration. Future research needs to further deepen the synergy between mathematical theory and engineering practice, and promote innovations in multi-scale modeling, uncertainty quantification and interdisciplinary algorithm design. By balancing model accuracy, computational efficiency and engineering applicability, PDEs will continue to lead the paradigm change in the cognition and regulation of complex systems in the era of artificial intelligence and quantum computing.

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