

2025 USTC Future Scientist Student Exchange Program Summer Research Excellent Academic Poster Exhibition



基本信息 Basic Information

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Classical Meets Machine Learning: FDM, RFM & Physics-Informed NNs

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Background

Partial differential equations underlie virtually every physical process we seek to model—from the diffusion of heat in a metal rod and the flow of air over an aircraft wing to the propagation of seismic waves through the Earth. Unfortunately, except for a few textbook cases with simple geometries and boundary conditions, analytic solutions are out of reach: real-world domains are irregular, materials exhibit nonlinear responses, and different physical phenomena often interact. Numerical methods such as the finite-difference method (FDM) convert derivatives into difference quotients on a structured grid, while random feature methods (RFMs) approximate kernel-based solution operators by projecting inputs onto a randomized finite basis—offering mesh-free flexibility and reduced computational cost for high-dimensional problems. More recently, physics-informed neural networks (PINNs) have emerged as a learning-based alternative that embeds the governing equations directly into the network's training loss, enabling seamless incorporation of experimental data and adaptive refinement of solution accuracy. Together, these classical discretization schemes and modern randomized or machine-learning—based techniques form a complementary toolkit for conquering the most challenging PDEs in science and engineering.

Finite Difference Method (FDM)

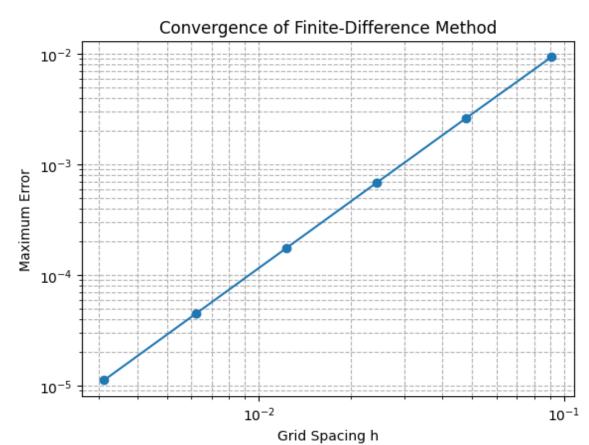
At its core, FDM replaces continuous derivatives in a PDE by finite-difference quotients on a structured grid. For example, approximating the one-dimensional heat equation:

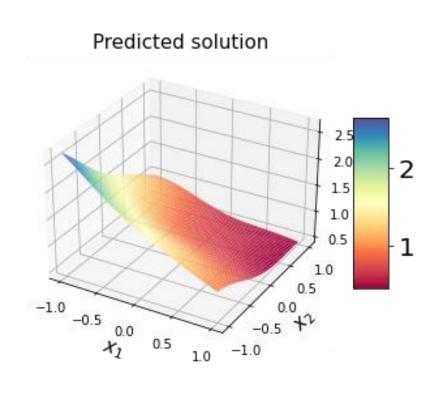
$$u_t = \alpha u_{xx}$$

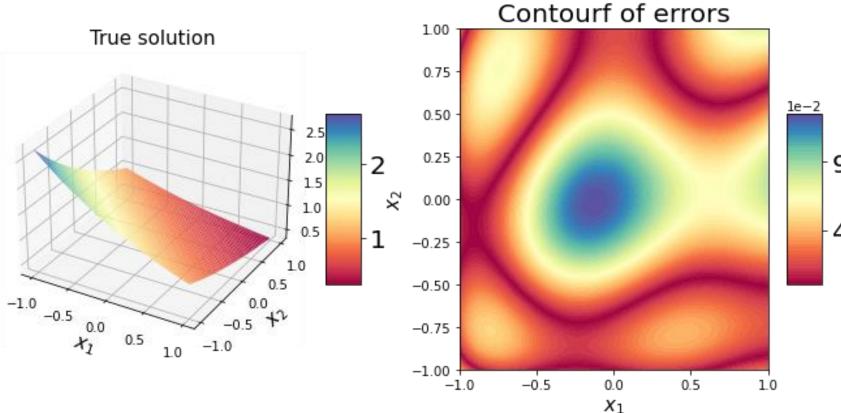
on a uniform mesh $x_i = i\Delta x$ and time-step $t^n = n\Delta t$ leads to the explicit update

 $u_i^{n+1} = u_i^n + r(u_{i+1}^n - 2u_i^n + u_{i-1}^n)$ with $r = \frac{\propto \Delta t}{(\Delta x)^2}$. This simplicity makes FDM easy to implement and very efficient for regular domains. However, stability constraints

 $(r \leq \frac{1}{2} \text{ in 1D})$ and difficulties with complex geometries or unstructured meshes limit its applicability in more intricate settings.







Random Feature Method (RFM)

The Random Feature Method (RFM) is a mesh-free approach for solving PDEs by representing the solution as a weighted sum of randomly chosen basis functions. Specifically, the solution u(x) is approximated as the formula where w_j and b_j are randomly sampled and fixed, and the coefficients c_j are optimized to minimize the PDE residual and satisfy boundary conditions. This experiment illustrates that the RFM can

Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) are a modern machine learning framework for solving differential equations by embedding the governing physical laws directly into the training process of a neural network. This unified loss enables the network to learn solutions that both satisfy the physics and match observed or simulated data.

$$\mathcal{L}_{BC/IC} = \sum_{x_i} |u_{\theta}(x_i) - u_{true}(x_i)|^2$$

Conclusion

Each method has strengths and limitations: FDM excels in speed and simplicity, RFM balances generality with interpretability, and PINNs shine in scenarios with sparse data or complicated geometries. As computational science evolves, hybrid approaches that combine the structure of classical solvers with the adaptability of machine learning are likely to shape the future of scientific computing.

effectively approximate the true solution structure, capturing smooth variations across the domain. However, accuracy depends on the number and quality of random features, with potential local deviations in regions of higher nonlinearity or complexity.

$$u(x) \approx \sum_{j=1}^{N} c_j \emptyset_j(x) \qquad \text{with} \qquad \emptyset_j(x) = \cos(w_j^T x + b_j)$$

$$\mathcal{L}_{PDE} = \sum_{x_i} |\mathcal{N}[u_{\theta}](x_i) - g(x_i)|^2$$

$$\frac{\partial u}{\partial t} - \lambda \frac{\partial^2 u}{\partial x^2} = 0 \quad \forall x \in D, \ t \in (0,T)$$

$$U(x,t) = \hat{u}(x,t) \quad \forall x \in D$$

$$u(x,t) = \hat{u}(x,t) \quad \forall x \in \partial D, \ t \in (0,T)$$

$$U_{\theta} = B(x,g(\mathbf{x})) + A(\mathbf{x})$$

$$\frac{\partial u_{\theta}}{\partial t} - \lambda \frac{\partial^2 u_{\theta}}{\partial x^2}$$

$$\frac{\partial u_{\theta}}{\partial t} - \lambda \frac{\partial u_{\theta}}{\partial x}$$

NN(x,t,eta)

Analytical differentiation