21-366 FINAL PROJECT WRITEUP

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ABSTRACT. This paper explores the application of numerical methods to partial differential equations (PDEs), which model how physical systems evolve over space and time. Due to the complexity of most PDEs in real-world scenarios, analytical solutions are often infeasible, necessitating robust numerical approximations. We implemented and compared several methods: finite difference method (FDM), finite element method (FEM), spectral methods with a Fourier Transform basis, Hermite radial basis function (RBF) with differential quadratures, and the Lax-Wendroff scheme. Spectral methods excelled with smooth, periodic solutions, while finite difference and finite element approaches were reliable for time-evolution and boundary value problems. Advanced techniques like H-RBF-DQ and Lax-Wendroff offered strong performance in specific contexts but also illustrated limitations with nonlinearities and complex geometries. Our work emphasizes the trade-offs between accuracy, computational cost, flexibility, and stability inherent in different numerical schemes applied to a multitude of PDEs.

1. Project Scope

Partial differential equations (PDEs) form the foundation for modeling systems in physics, engineering, biology, and finance. However, most cannot be solved exactly due to nontrivial geometries, nonlinearities, and boundary conditions. Our project aimed to systematically explore and implement a variety of numerical methods to approximate solutions to key PDEs.

One of the most widely used approaches for numerically solving PDEs is the **finite difference method (FDM)**, a classical grid-based method that converts possibly nonlinear PDEs into a system of linear equations that can then be solved by matrix algebra techniques. [Str04] FDM replaces derivatives by finite differences, solving the derivative one point at a time in a structured grid pattern. It's straightforward to implement and extend, though is only ideal for simple geometries with simpler boundary conditions on grid domains. It's one of many variations of the weighted essentially non-oscillatory (WENO) methods, like many other high-resolution methods used today. [Gar04] While FDM is particularly effective and efficient for problems with simple geometries and boundary conditions, it struggles with PDEs with irregular domains and conditions.

This is where the **finite element method (FEM)** comes in handy. It's similar to FDM but with increased flexibility regarding more complex shapes, domains, and/or imposed boundary conditions. The idea is to divide the domain into simple pieces like polygons instead of structured grids, then approximate the solution by applying extremely simple functions on these pieces. [Str08] By utilizing a whole function rather than single points while solving, FEM cites a higher level of accuracy than FDM, though at a slightly greater computational cost. Like FDM, it's also a common variation of WENO methods, providing high resolution at (relatively) little cost. [Gar04] Originally developed by engineers to handle curved or irregularly shaped domains, FEM works remarkably well for elliptic and structural mechanics problems, supporting adaptive meshing as well. [Str08]

Spectral methods take a different approach by expanding the solution in terms of global basis functions, such as Fourier or Chebyshev polynomials. In our project, we choose a basis of Fourier Transforms, being simpler to work with Poisson equations. Spectral methods are known for their high accuracy especially when the solution is smooth and periodic, with convergence sometimes being called infinite-order accuracy (exhibiting exponential convergence for smooth solutions). [Gar04] As another WENO variation, they provide very high resolution but typically require more computational effort than the other basic methods. [Gar04] The greatest weakness is that without periodic or regular domains, solutions lose the high accuracy these methods boast.

In addition to these basic methods, several modern or specialized techniques have been developed to tackle specific challenges in PDEs. For instance, the modern **Hermite radial basis function with differential quadratures (H-RBF-DQ)** methods are mesh-free approaches that use radial basis functions and their derivatives to approximate solutions. Functions and scattered points are accurately handled, particularly in irregular domains, and extend the accuracy of RBF-DQ approximations. [Jia23] The method's Hermite interpolation coefficients are only dependent on points as time evolves and can handle both Dirichlet and Neumann boundaries particularly well, but the processes are computationally intensive. [Jia23] H-RBF-DQ can support variable-order Caputo fractional derivatives, and is capable of solving 2D advection-diffusion and fractional time PDEs.

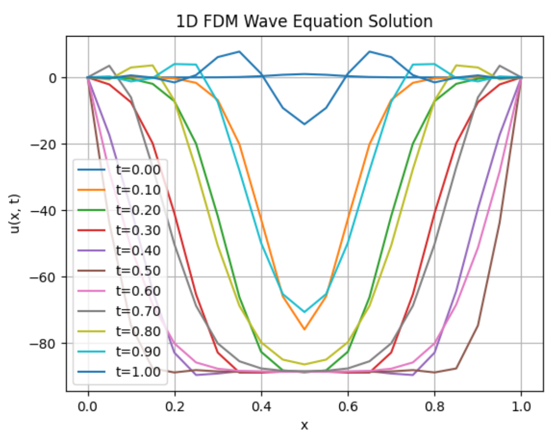
Another significant method is the classical **Lax-Wendroff scheme**, which is used for hyperbolic PDEs and provides second-order accuracy in both space and time by incorporating Taylor series expansions and flux terms. For example, in the case of the homogeneous advection equation $\frac{\partial \varphi}{\partial t} = c\frac{\partial \varphi}{\partial x}$, the second-order accurate difference scheme is: $\varphi_j^{n+1} = \varphi_j^n - \frac{c\tau}{2h}(\varphi_{j+1}^n - \varphi_{j-1}^n) + \frac{c^2\tau^2}{2h^2}(\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n)$, derived in 1960. [Ire19] Lax-Wendroff can handle both linear and nonlinear advection, capturing wave propagation with analysis tools for phase error and dispersion. This method is valuable for problems involving wave propagation or shock formation, but suffers from numerical dispersion or instability under certain conditions.

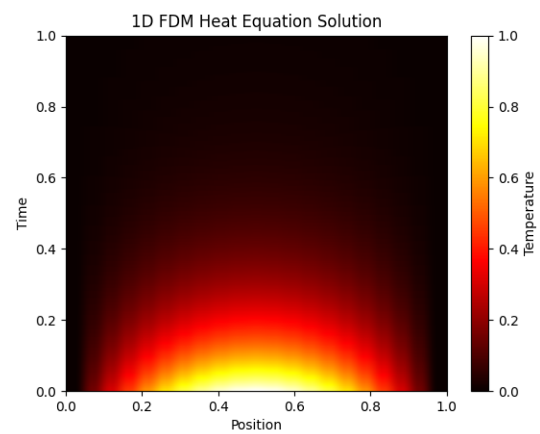
Our project seeks to implement this variety of numerical methods to apply to applicable and non-applicable PDEs to observe the trade-offs in stability, accuracy, cost, etc. that each method demonstrates.

2. Results

2.1. **FDM.** We begin by analyzing 1D wave equation $u_{tt} = c^2 u_{xx}$ with fixed endpoints, using FDM with centered differences for both terms: $\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{(\Delta t)^2} = c^2 \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}$. [Str08] We simulated the solution over time steps from 0 to 1 second in intervals of 0.1 seconds. The snapshots of each time t showed how the wave profile $u(x,t)$ changes at different moments, propagating back and forth across the domain. The numerical solution displayed the expected wave behavior, although it appeared somewhat rough—likely due to the simplicity of the discretization scheme.

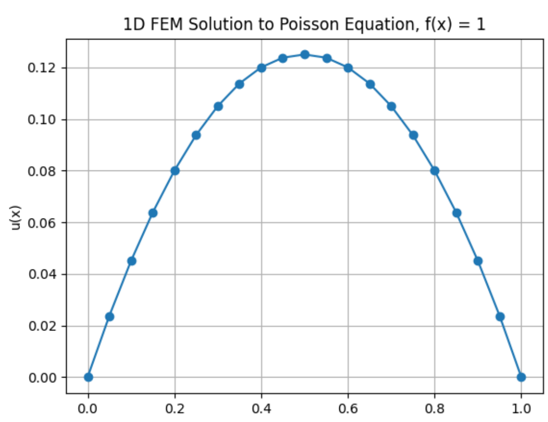
For the 1D heat equation $u_t = \alpha u_{xx}$, we used an explicit FDM approach and observed diffusion radiating outward over time, consistent with the physical behavior of heat distribution. The initial temperature profile was set as a sine wave, with diffusion flattening out the temperature to decay to zero due to heat dissipation.

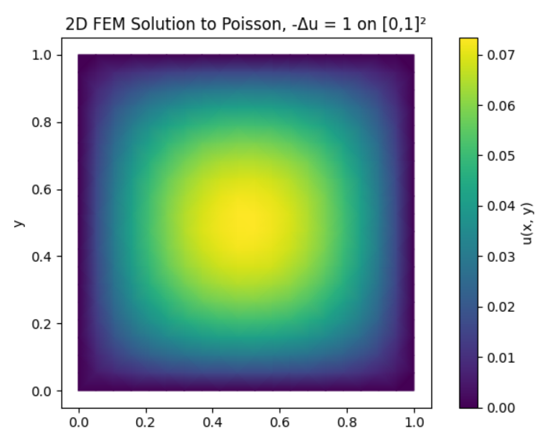




2.2. **FEM.** In a simple demonstration of FEM, we modeled the 1D Poisson equation with $f(x) = 1$ with Dirichlet boundary conditions using FEM, employing 20 equally spaced nodes, which approximate $u(x)$ piecewise using simple basis functions. The resulting solution had the characteristic inverted parabolic shape, matching the expected analytical solution.

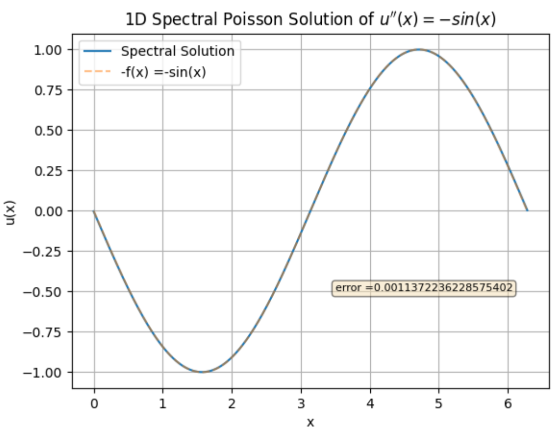
For the 2D Poisson equation with the same $f(x)$, we note that the Dirichlet boundary conditions fixed the edges of the graph at 0 and had a 2D raised paraboloid shape in the center, much like its 1D counterpart's visualization.

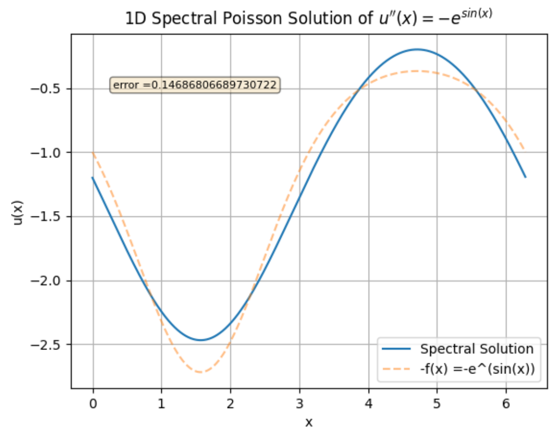




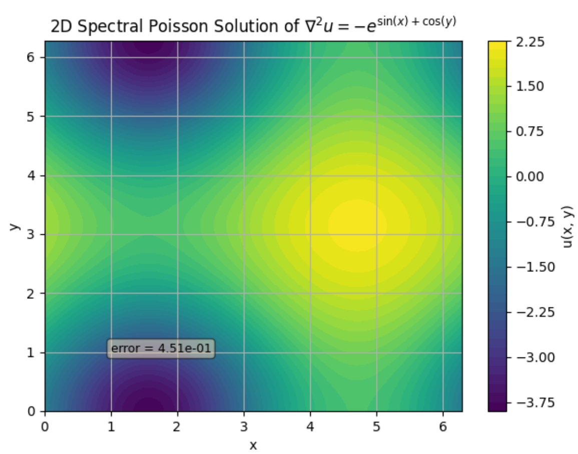
2.3. **Fourier Spectral Methods.** To first demonstrate the high accuracy of this method with periodic, smooth PDEs, we began by applying 1D spectral methods to the function $f(x) = \sin(x)$, which yielded accurate results with a relatively low error of approximately 0.01 when using $N = 1000$ points. Increasing N further reduced the error, showcasing the method's strength in handling smooth periodic functions.

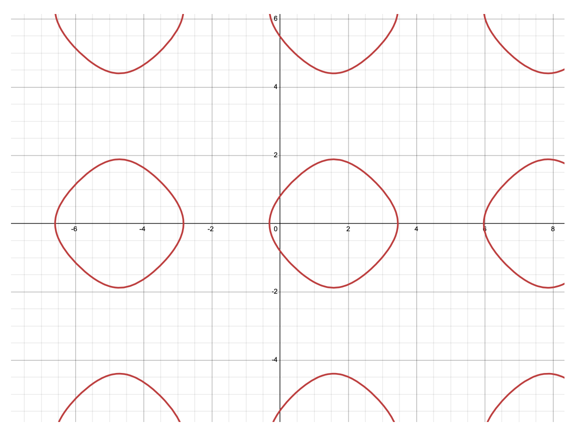
However, performance decreased when we tested the more complex function $f(x) = e^{\sin(x)}$, a deliberately non-sinusoidal function. In this case, the error plateaued at around 0.15 even with larger values of N, indicating limited improvement with resolution and suggesting that spectral methods are more sensitive to the analytic properties of our target function.





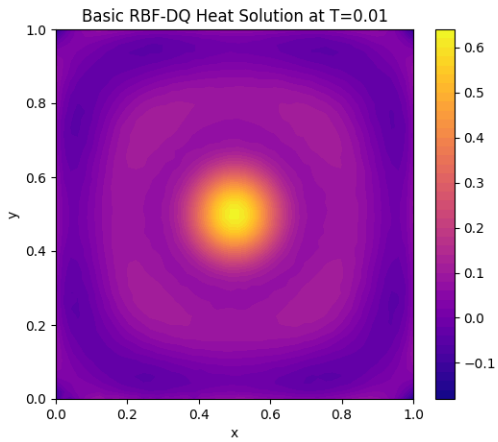
Extending the approach to two dimensions, we applied 2D spectral methods to $f(x, y) = e^{\sin(x)+\cos(y)}$. With $N = 1000$, the method produced a qualitatively correct shape but a relatively high error of 0.45, reflecting the increased computational complexity and challenges of spectral methods in higher dimensions. However, the smooth 2D surface of the solution aligns well with the behavior of the function, graphed on a 2D plane, showing the efforts behind the spectral method in 2D.

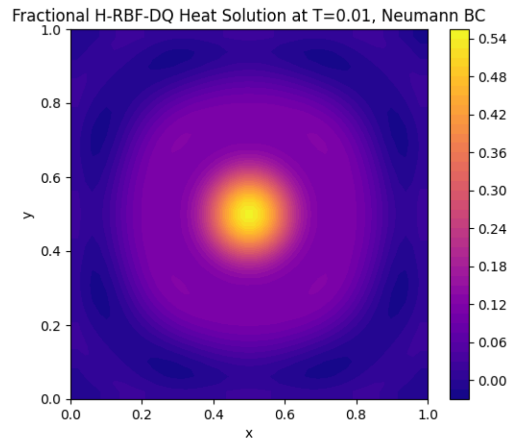




2.4. **H-RBF-DQ.** To focus on the H-RBF-DQ method for the variable-order time fractional advection-diffusion equation on complex geometries with Neumann boundary conditions, we simulated the diffusion of the the heat equation (a diffusion equation) over time with Gaussian RBF as our base, using L1 weights from the differential quadrature to incorporate the time-fractional derivatives. First, we start with a basic RBF-DQ method, without set boundary conditions. Note the rings around the solution fluctuating in magnitude instead of a steady outwards fade.

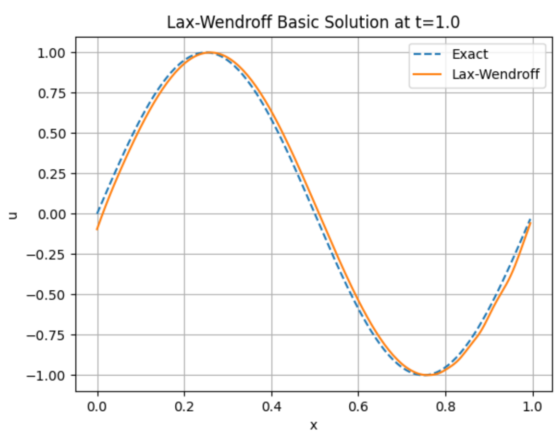
Next, we utilize Hermite interpolation with RBF-DQ as well as setting Neumann boundary conditions to visualize a more accurate solution to the problem. Both graphs use differential quadratures to create weight coefficient matrices from the derivatives, with diffusion starting at the center and later time steps visually matching expected theoretical behavior. While the two visualizations for the heat equation solution look very similar with small differences, there are expected greater differences for other time fractional equations like Caputo derivative, for example. [Jia23]

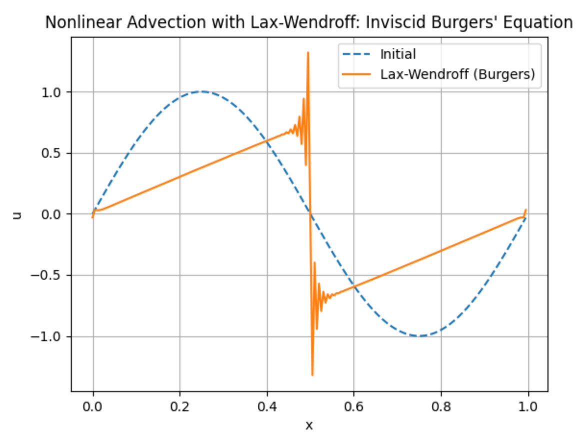




2.5. **Lax-Wendroff.** Finally, we apply the Lax-Wendroff scheme to advection equations. We start with the linear advection equation $u_t + au_x = 0$. It successfully captured the propagation of the initial sine wave $\sin(2\pi x)$ using only 200 points for $t = 0.1$. As the given PDE was a smooth function, it gives the accuracy expected from the basic Lax-Wendroff scheme.

For the nonlinear Inviscid Burgers equation $u_t + \left(\frac{u^2}{2}\right)_x = 0$ that assumes zero viscosity, this PDE posed more difficulties, and the numerical results deviated significantly from the expected solution, as shown in the below visualization. This equation is made to work with advection-diffusion equations, so when the scheme's linear approximation was combined to this non-linear case, shocks were created. Any change of sign or slope creates oscillations, partially due to using Taylor Series (which over-corrects in both directions). This highlights the challenges of applying the Lax-Wendroff scheme to nonlinear problems.





3. Final Thoughts

This study demonstrates the diverse capabilities and limitations of various numerical methods for solving partial differential equations. For our explored basic methods, spectral methods achieved the highest degrees of accuracy (regarding error from expected solutions) for smooth, periodic problems, especially in one dimension, but quickly encountered difficulties with non-analytic functions and higher-dimensional domains. Finite difference methods proved to be an accessible and reliable option for simulating both wave propagation and diffusion, despite minor limitations in smoothness and resolution. Finite element methods excelled in approximating solutions for elliptic problems, particularly within irregular or bounded domains, producing smooth and consistent results. The advanced methods introduced in this project offered a deeper look into mesh-free and hyperbolic PDE solutions. The Hermite RBF-DQ method provided high-order accuracy and adaptability to irregular domains, though it required careful implementation of boundary conditions, as well as having the longest run-times out of all methods. The classical Lax-Wendroff scheme performed well for linear advection but fell short when applied to nonlinear dynamics, where numerical artifacts became significant. These observations are in line with general findings of these methods' trade-offs found in our research, proved with explicit PDE examples in our repository code.

Ultimately, the effectiveness of any numerical method depends on the properties of the PDE being solved, including smoothness, domain complexity, and boundary conditions. There is no universally optimal method, and informed choices must be made based on problem-specific criteria. Future directions may include the exploration of hybrid methods that combine the strengths of individual techniques or the use of adaptive meshing to dynamically refine solutions, achievable through our repository's solid structure. Our project reinforces the importance of a solid conceptual and computational understanding of numerical methods for advancing applied mathematics and computational science.

References

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