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Spectral Methods for PDEs

Rice University ✦ CMOR 523 ✦ Spring 2024

Overview

The Spectral Method

Fourier Transforms

Implementation

Comparison

Error Analysis

Conclusion

The Spectral Method

The spectral method is a numerical technique used for solving differential equations. It accomplishes this task by representing the solution to the differential equation as a weighted combination of basis functions. Unlike the finite difference method, which uses local approximation in a finite domain, the spectral method uses global approximations and achieves superior accuracy. The chosen basis function depends on the PDE being solved.

The Spectral Method

The Spectral Method approximates the solution of our PDE as a linear combination of this sum:

$$u(x) \approx u_N(x) = \sum_{k=0}^{N} a_k \phi_k(x)$$

where $\phi_k(x)$ are the basis functions that are most commonly chosen to be orthogonal. The choice of the basis function depends on the PDE being solved. A basis function can be any of the following:

$$\begin{aligned}
&\phi_k(x) = e^{ikx} \text{ (Fourier spectral method)} \\
&\phi_k(x) = T_k(x) \text{ (Chebyshev spectral method)} \\
&\phi_k(x) = L_k(x) \text{ (Legendre spectral method)} \\
&\phi_k(x) = \mathscr{L}_k(x) \text{ (Laguerre spectral method)} \\
&\phi_k(x) = H_k(x) \text{ (Hermite spectral method)}
\end{aligned}$$

The domain of the chosen PDE for this project is periodic, therefore we will be using the Fourier Spectral Method.

Fourier Transforms

Given any arbitrary function f(x) that is periodic on some domain (-L, L) we can expand f(x) as linear combination of sine and cosine, or equivalently as a complex Fourier series:

$$f(x) = \sum_{k=-\infty}^{\infty} C_k e^{\frac{ik\pi x}{L}}$$

that is 2L periodic where

$$C_k = \frac{1}{2\pi} \int_{-L}^{L} f(x) e^{\frac{-ik\pi x}{L}} dx$$

We can transform our PDE to the frequency space using the Fourier transform:

$$\hat{f}(x) = F(x) = \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx$$ where $$\omega_k = \frac{k\pi}{L}$$

After solving the problem in the frequency space, we use the inverse Fourier Transform to return to the physical domain:

$$f(x) = F^{-1}(\hat{f}(\omega)) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{i\omega x} d\omega$$

Discrete Fourier Transforms

The Discrete Fourier Transform is the Fourier Transform on a set of data. Given a positive integer N, let

$$x_j = jh = j\frac{2\pi}{N}, \quad 0 \le j \le N-1$$

with its corresponding function values $\{f(x_j)\}_{j=0}^{N-1}$, the Discrete Fourier Transform is:

$$\hat{f}_k = \sum_{j=0}^{N-1} f(x_j) e^{-ikx_j}, \quad k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1$$

and the Inverse Discrete Fourier Transform is given by:

$$f(x_j) = \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{-ikx_j}, \quad j = 0, \ldots, N-1$$

The Discrete Fourier Transform leads to a matrix multiplication requiring $O(N^2)$ operations. The Fast Fourier Transform (FFT) is a technique for calculating the Discrete Fourier Transform which is less computationally expensive, requiring $O(N \log_2 N)$ operations in the frequency space.

Differentiation in Physical Space

Define the interpolation operator $I_N : C[0,2\pi] \to \mathcal{I}_N$ as

$$(I_N f)(x) = \sum_{k=-N/2}^{N/2} \tilde{f}_k e^{ikx}$$

where

$$\mathcal{I}_N = \{f = \sum_{k=-N/2}^{N/2} \tilde{f}_k e^{ikx} : \tilde{f}_{-N/2} = \tilde{f}_{N/2}\}$$

I_N is the interpolation operator from $C[0,2\pi)$ to $\mathcal{I}_N$ such that

$$(I_N f)(x_j) = f(x_j), \quad x_j = \frac{2\pi j}{N}, \quad 0 \le j \le N-1$$

The following proof is shown extensively in the research paper: for any f in $C[0,2\pi)$

$$(I_N f)(x) = \sum_{j=0}^{N-1} f(x_j) h_j(x)$$

where

$$h_j(x) = \frac{1}{N} \sin\left[N\frac{x-x_j}{2}\right] \cot\left[\frac{x-x_j}{2}\right] \in \mathcal{I}_N$$

which satisfies $h_j(x_k) = \delta_{jk}, \quad \forall j,k = 0,1,\ldots,N-1$

Differentiation in Physical Space

Let $\{x_j\}$ and $\{h_j\}$ be defined as in the last slide. By setting

$$f(x) = \sum_{j=0}^{N-1} f(x_j) h_j(x)$$

and taking the m-th derivative, we get

$$f^{(m)}(x) = \sum_{j=0}^{N-1} f(x_j) h_j^{(m)}(x)$$

This process can be formulated as a matrix-vector multiplication $\mathbf{f}^{(m)} = D^{(m)} \mathbf{f}, \quad m \geq 0$ where

$$D^{(m)} = \left(d_{kj}^{(m)} := h_j^{(m)}(x_k)\right)_{k,j=0,\dots,N-1}$$

$$\mathbf{f} = (f(x_0), f(x_1), \dots, f(N-1))^T$$

$$\mathbf{f}^{(m)} = (f^{(m)}(x_0), f^{(m)}(x_1), \dots, f^{(m)}(N-1))^T$$

This matrix differentiation procedure requires $O(N^2)$ operations. We shall demonstrate in the next slide how to perform the differentiation in the frequency space with $O(N \log_2 N)$ operations.

Differentiation in Frequency Space

Given a function with a periodic domain, its finite Fourier series can be expressed as:

$$u(x) = \sum_{k=-N/2}^{N/2} \tilde{u}_k e^{ikx}, \qquad \text{where} \qquad \tilde{u}_{N/2} = \tilde{u}_{-N/2}$$

Thus, the derivative is:

$$u'(x_j) = \sum_{k=-N/2}^{N/2} ik\tilde{u}_k e^{ikx_j},$$

With the known physical values, the approximation of the derivative values follows:

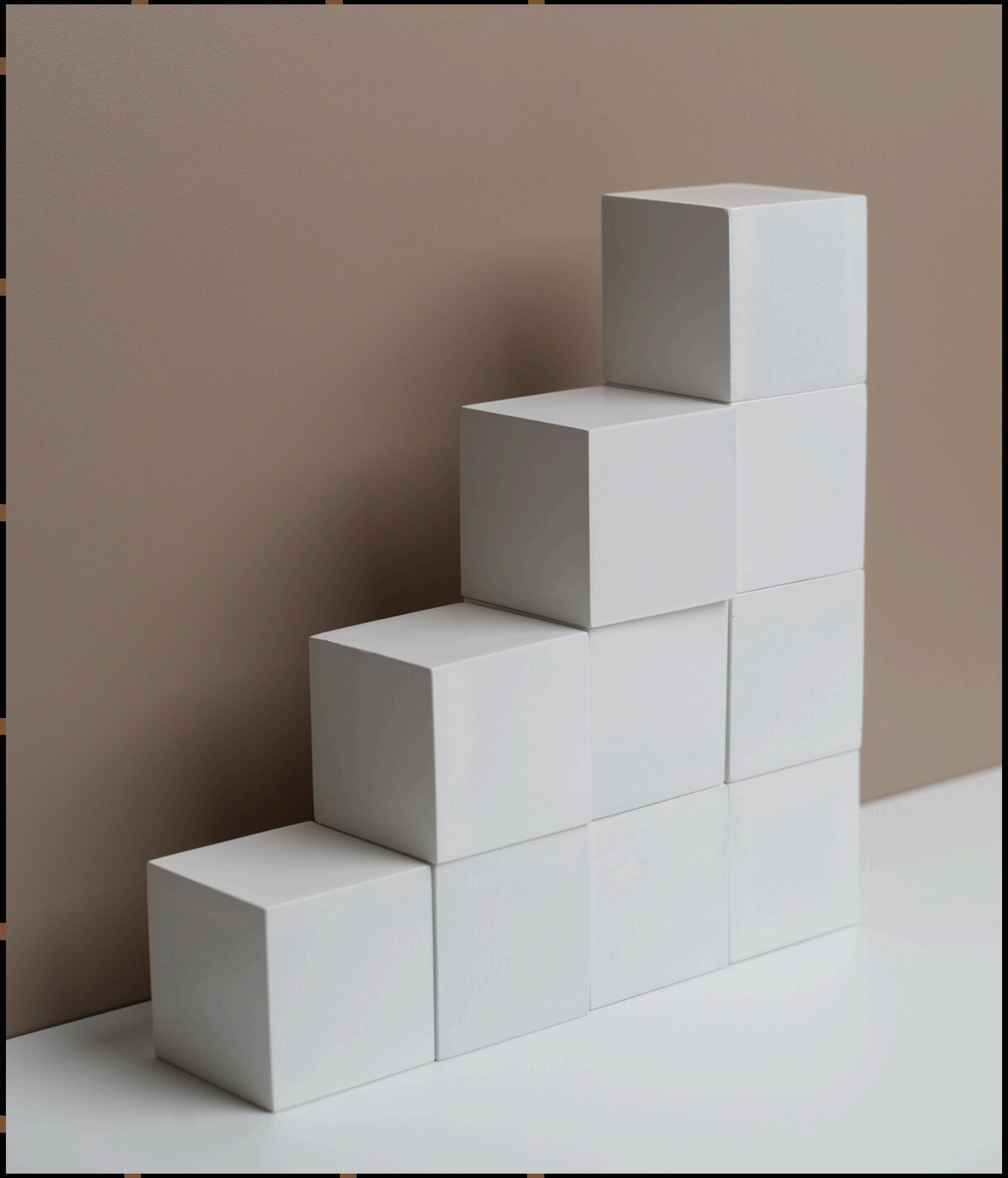
1. Call $\tilde{u} = \mathrm{fft}(u)$ which will return the frequency vector

$$\tilde{u} = (\tilde{u}_1, \tilde{u}_1, \ldots, \tilde{u}_N)$$

2. Compute the coefficients of the expansion of the derivative

$$\tilde{u}^{(1)} = ik * \tilde{u}$$ where the multiplicative vector k is $$\mathbf{k} = (0, 1, \ldots, N/2-1, 0, -N/2+1, \ldots, -1)$$

How the Fourier Spectral Method Works



01 We start with an initial condition, which represents the solution at time t = 0.

02 Discretization the spatial domain and evaluate the initial condition at those points.

03 Apply FFT to the initial condition, meaning our problem is transformed to the frequency space. While in this space, we compute the multiplication factor for the derivative from the wave number vector k and use it to divide .

04 Use a time-stepping scheme to solve for the Fourier coefficients at the next time level while still in the frequency space.

05 Use the Inverse Fast Fourier Transform to come back to the physical space at that next time level.

06 Use the solution obtained at the next time level as the new initial condition for the next time step. Repeat this until the final time is reached.

Implementation in 1D

Given the 1D Heat Equation problem:

$$u_t = \alpha^2 u_{xx}, \quad \alpha = 1$$
$$u(x,0) = \sin(x), \quad 0 \le x \le 2\pi, \quad t > 0$$

We use FFT to transform into the frequency space and compute the multiplicative factor for the derivatives as:

$$\hat{u}(k,t) = FFTu(x,0)$$
$$u_x = ik\hat{u}(k,t)$$
$$u_{xx} = -k^2\hat{u}(k,t)$$

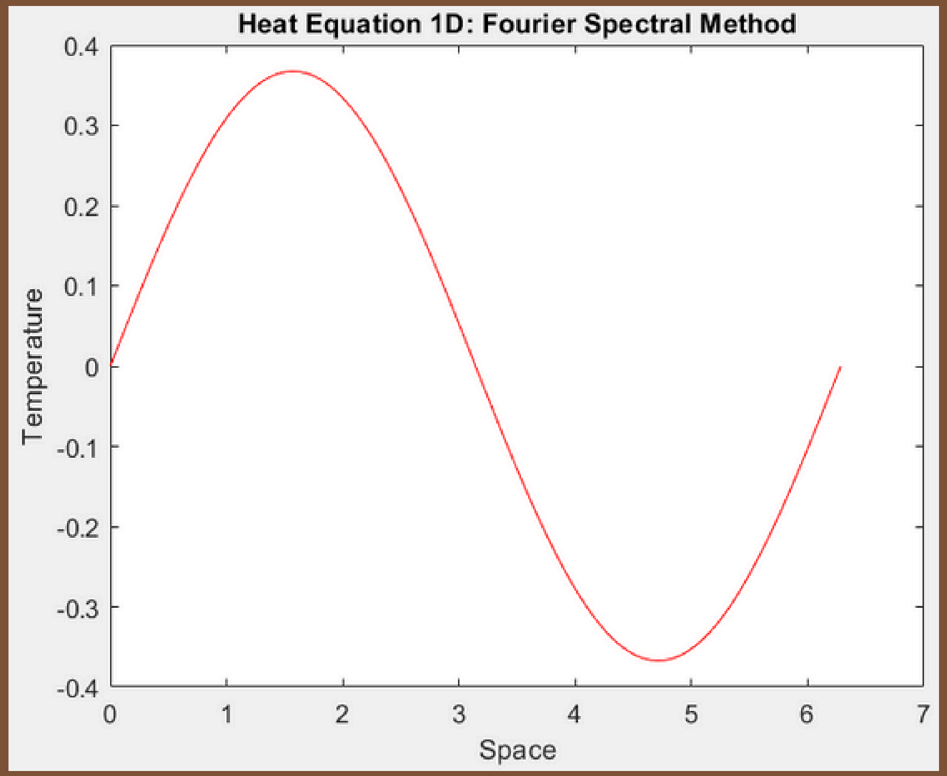
Using an explicit time-stepping scheme, we solve the problem and obtain the solution at the next time level:

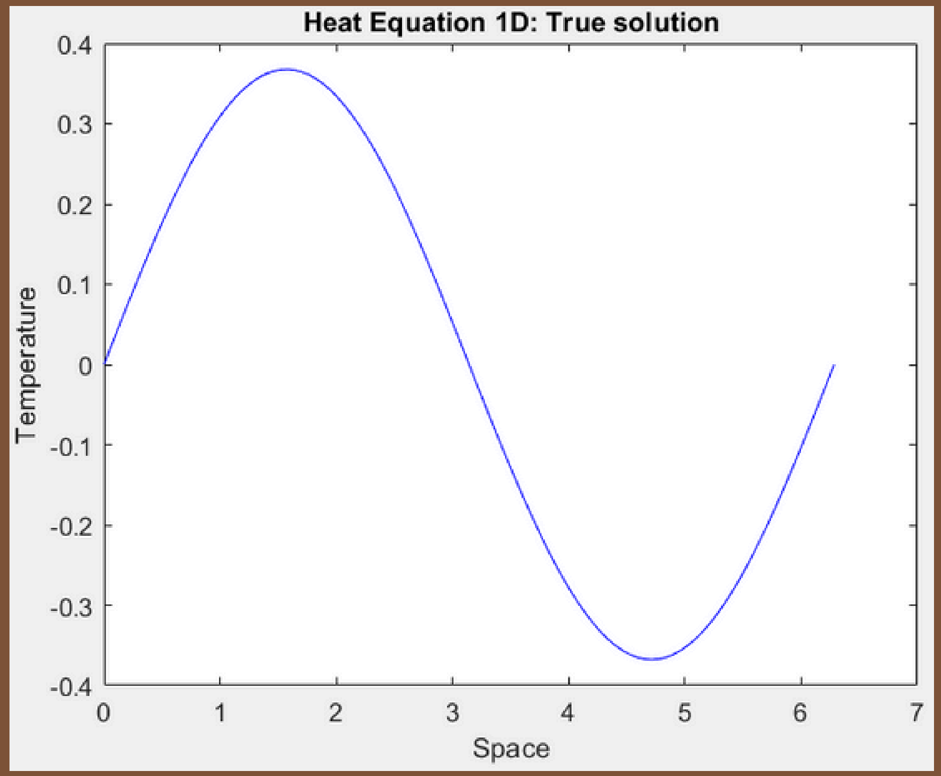
$$\hat{u}_t = -\alpha^2 k^2 \hat{u}(k,t)$$
$$U^{n+1} = U^n + dt(-\alpha^2 k^2 \hat{u}(k,t))$$

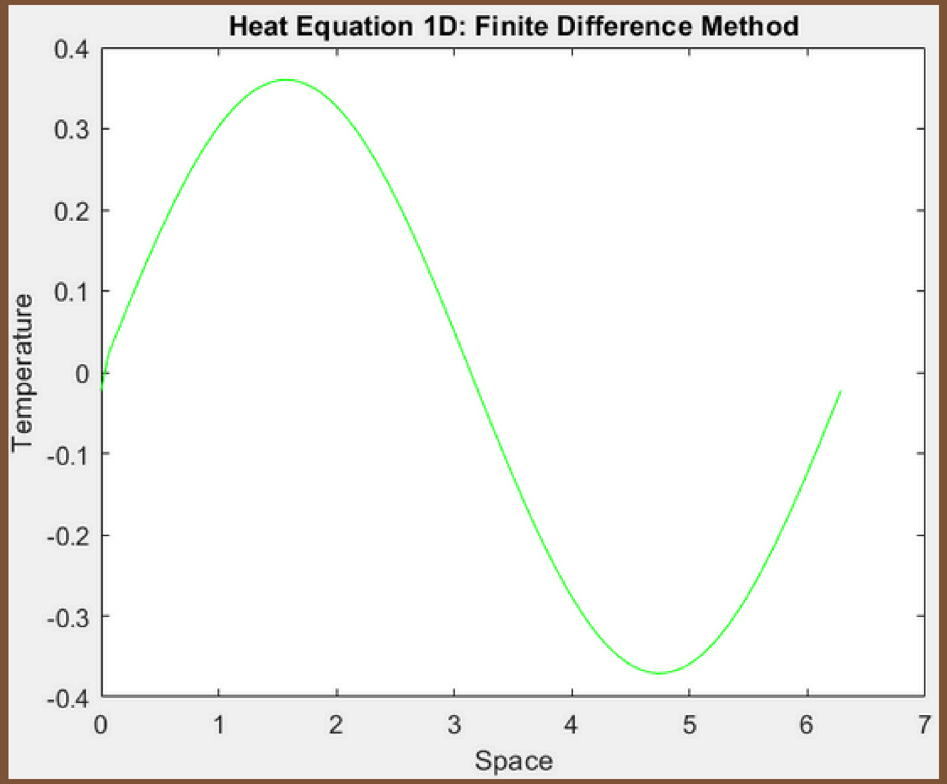
Repeat this process until the final time is reached.

Comparison: 1D

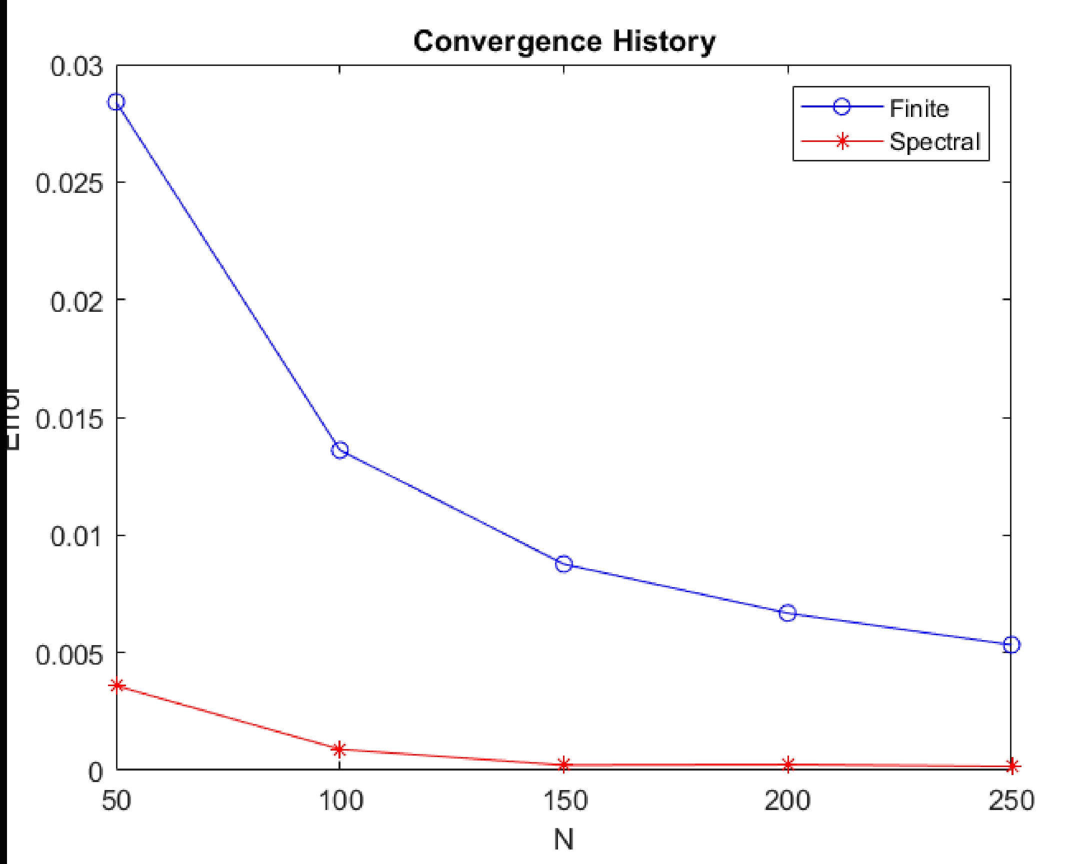
1D Heat Equation solution implemented with Fourier Spectral Method and the Finite Difference Method

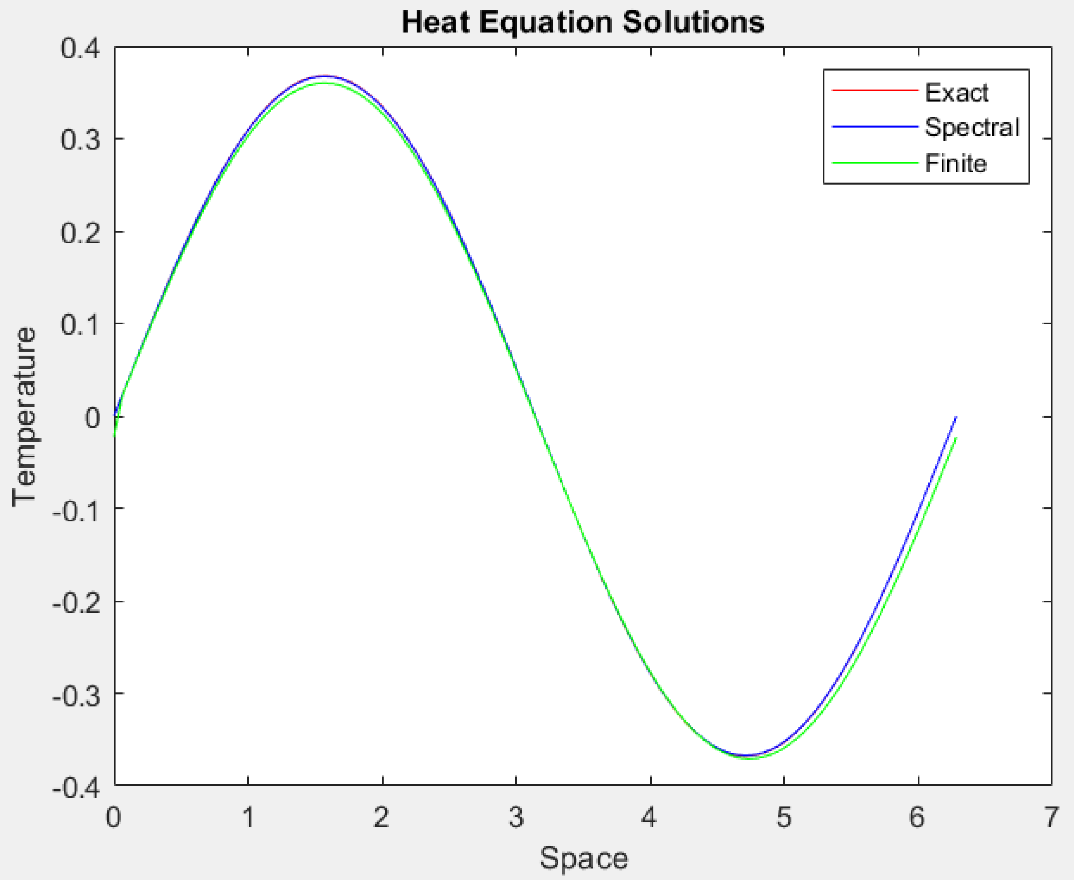






Error Analysis: 1D





From the plots, we can observe that the Spectral Method achieves a lower error and better accuracy.

Table 1: 1D Error

N	Finite Difference Error	Fourier Spectral Error
50	0.0284	0.0035924
100	0.013603	0.00089347
150	0.0087631	0.00021831
200	0.006678	0.000242
250	0.0053318	0.00016966

Similarly, this can also be seen on the convergence table below.

Implementation in 2D

Given the 2D Heat Equation problem:

$$u_{xy} = \alpha^2(u_{xx} + u_{yy}), \quad \alpha = 1$$
$$u(x,y,0) = \sin(x)\sin(y), \quad 0 \leq x \leq 2\pi, \quad 0 \leq y \leq 2\pi, \quad t > 0$$

We use FFT2 to transform into the frequency space and compute the derivatives as:

$$\hat{u}(k,t) = FFT2u(x,y,0)$$
$$u_{xx} + u_{yy} = -(kx^2 + ky^2)\hat{u}(k,t)$$

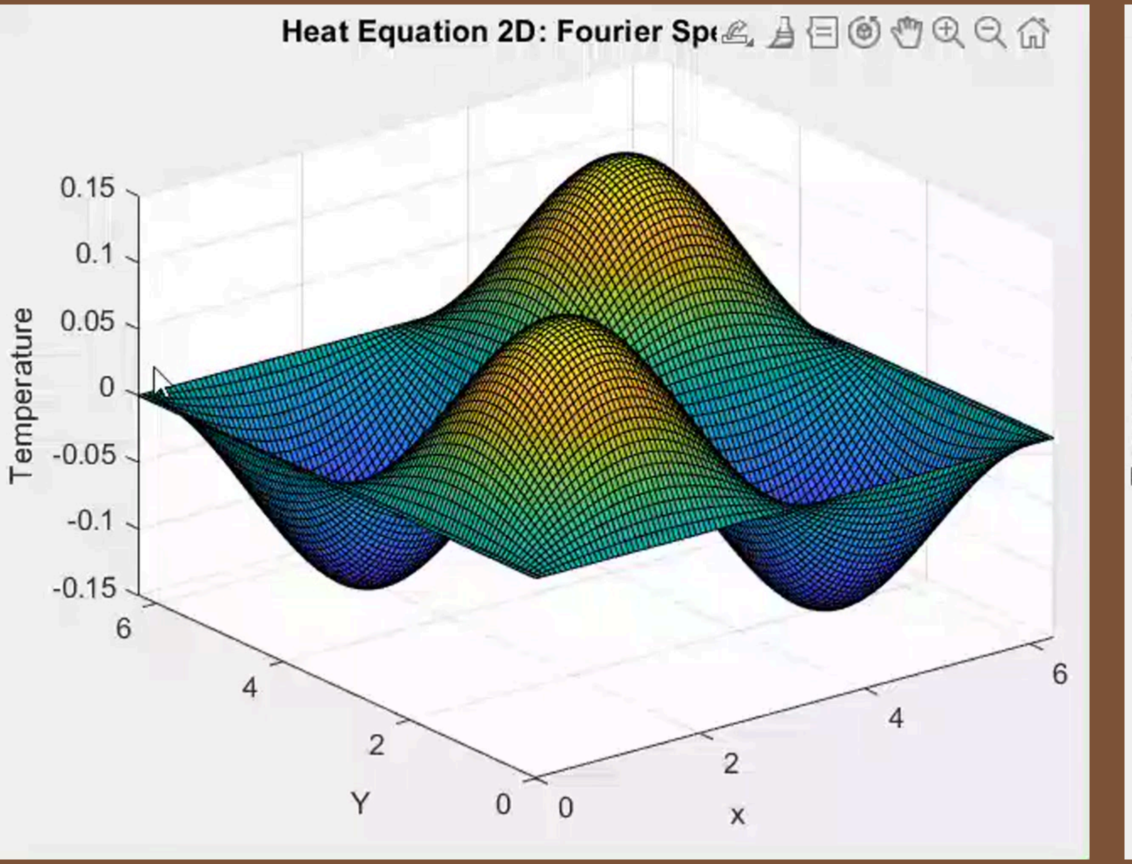
Using an explicit time-stepping scheme, we solve the problem and obtain the solution at the next time level:

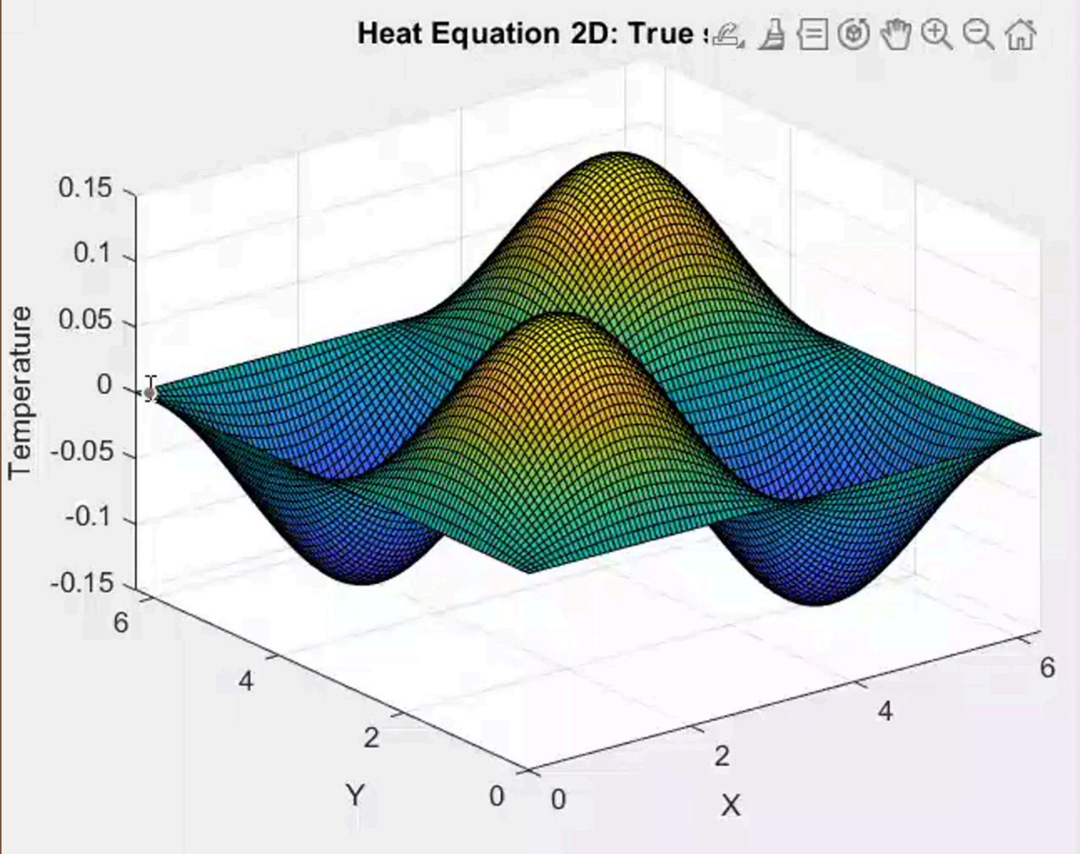
$$\hat{u}_t = -\alpha^2(kx^2 + ky^2)\hat{u}(k,t)$$
$$U^{n+1} = U^n + dt(-\alpha^2(kx^2 + ky^2)\hat{u}(k,t))$$

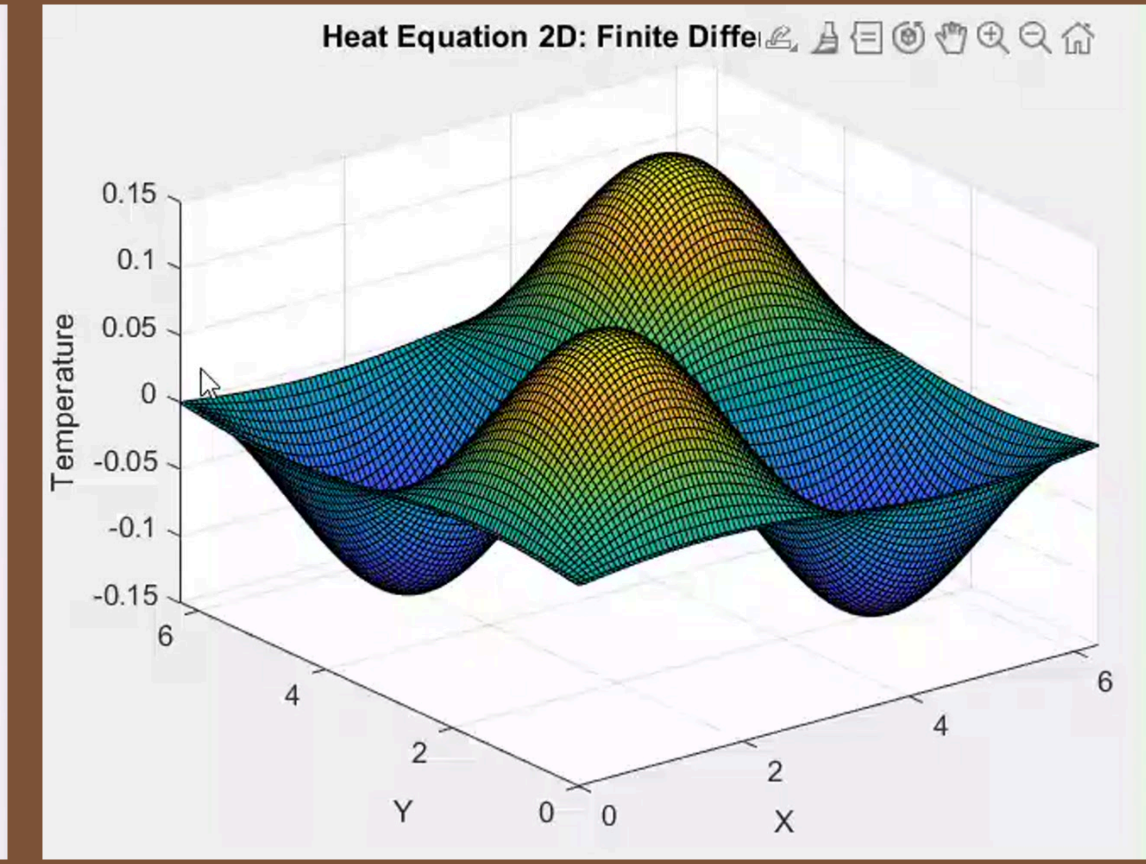
Repeat this process until the final time is reached.

Comparison: 2D

2D Heat Equation solution implemented with Fourier Spectral Method and the Finite Difference Method







Error Analysis: 2D

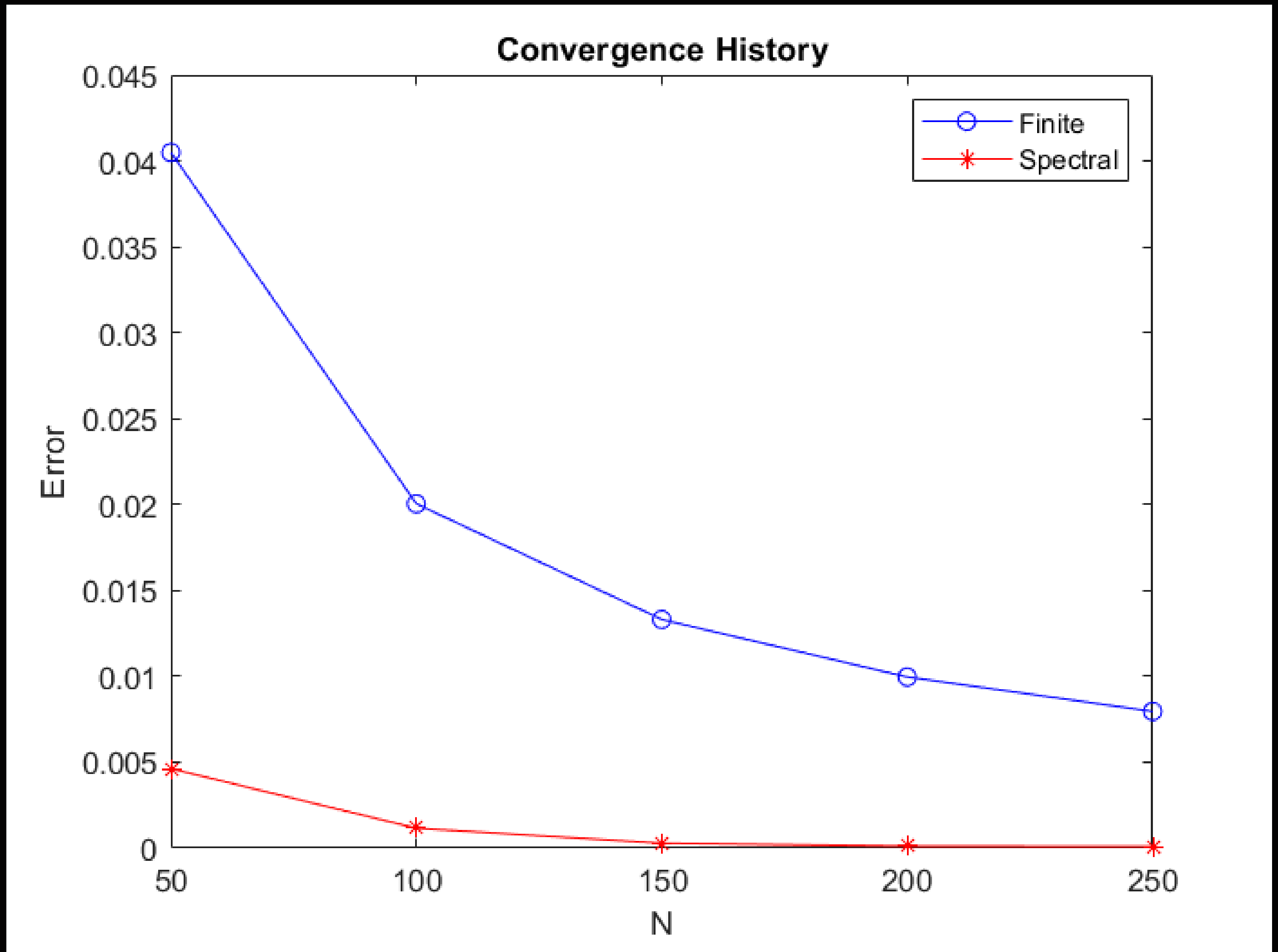


Table 3: 2D Error

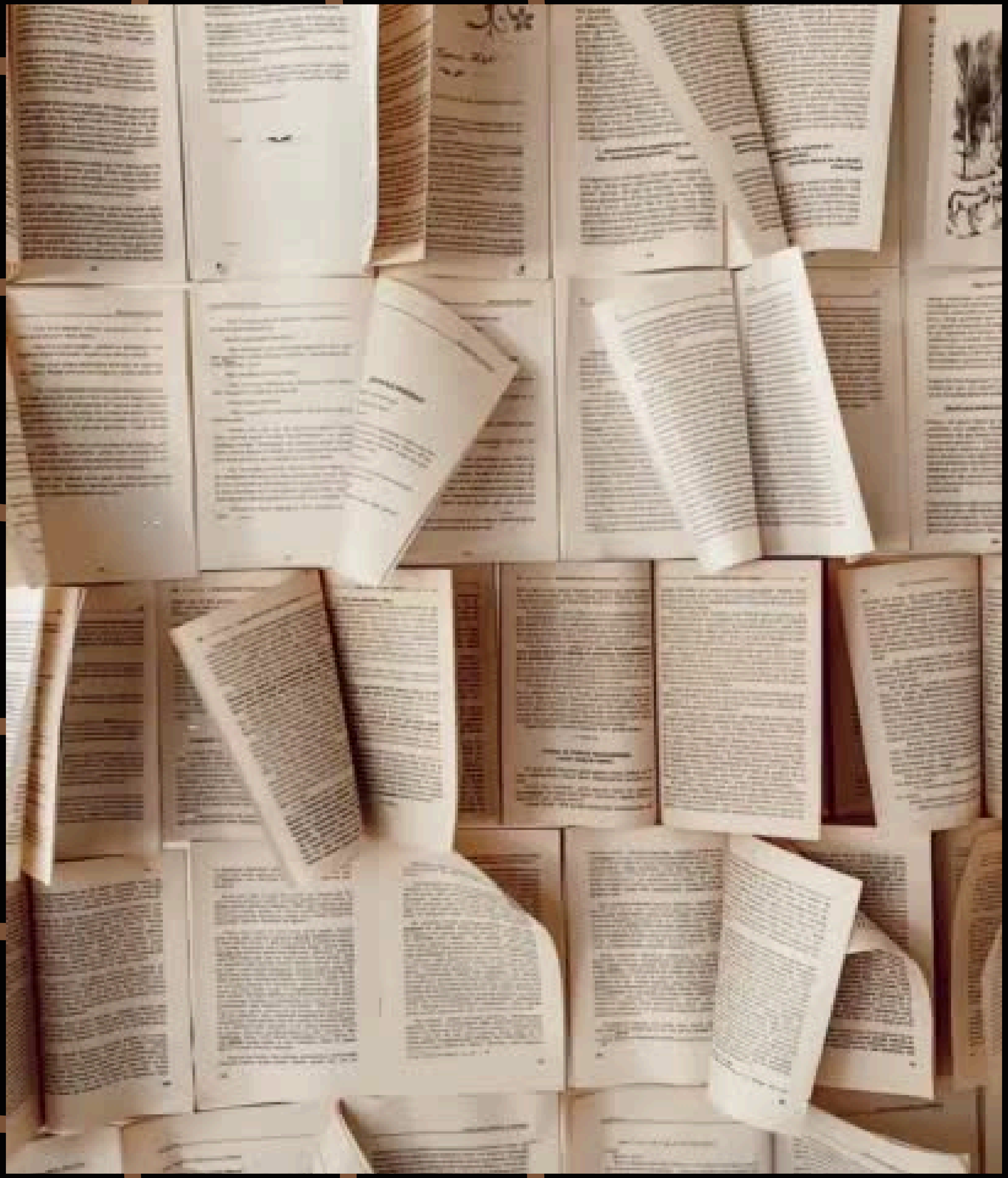
N	Finite Difference Error	Fourier Spectral Error
50	0.040494	0.0046257
100	0.020046	0.0011586
150	0.013307	0.0002837
200	0.0099612	0.0001081
250	0.0079595	8.8126e-05

From the error plot, we can observe that the Spectral Method achieves a lower error and converges to 0 quickly.

Similarly, this can also be seen on the convergence table below.

Conclusion

Given a problem with a periodic domain and smooth solution, the Spectral Method achieves a higher accuracy and convergence rate. This higher accuracy comes from the use of globally smooth basis functions and the spectral convergence properties of Fourier series.



Sources

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03 Fourier Spectral Methods in MATLAB and Python. Fourier spectral methods in Matlab and Python. (2013, November 6). http://faculty.washington.edu/rjl/classes/am590a2013/ static/Fourier-Spectral.pdf

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thank you!

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