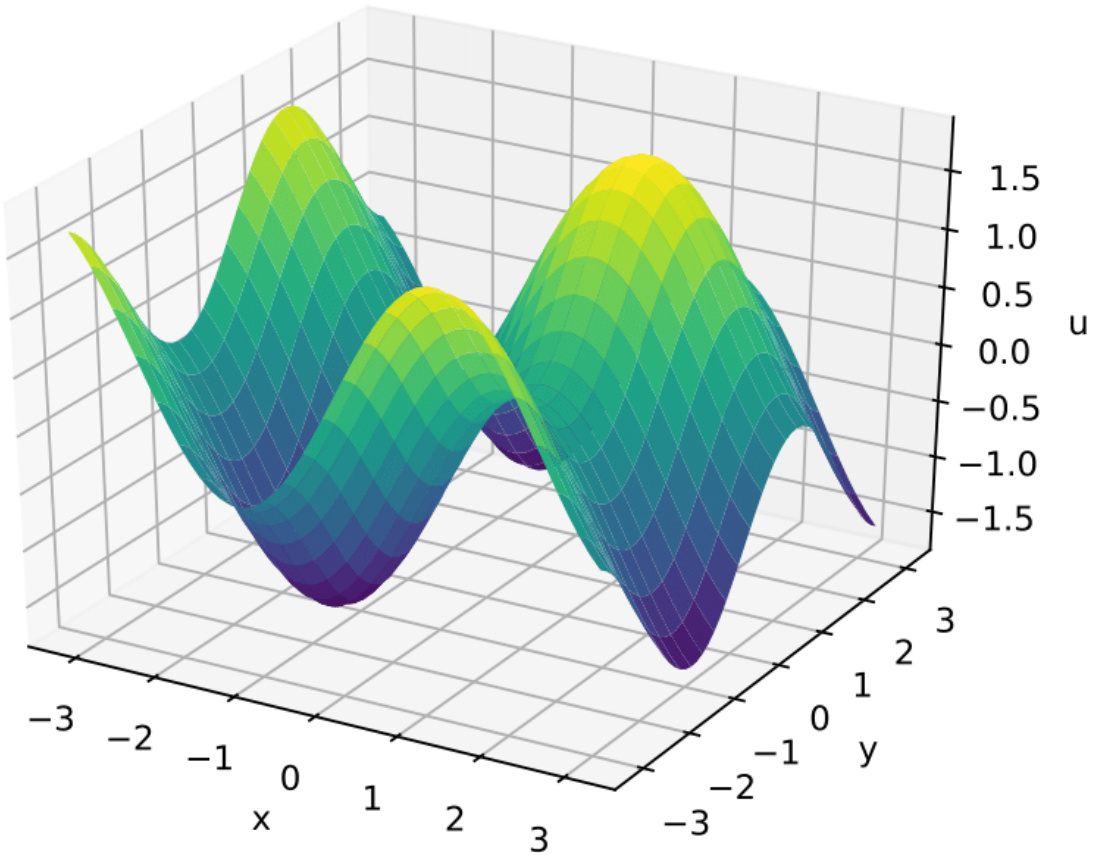
# Spectral Methods for Partial Differential Equations

CMOR 523 Numerical Methods for Partial Differential Equations

Uzochi Gideon
ug6@rice.edu

Kiara Richardson
kar15@rice.edu

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# 1 Introduction

## 1.1 What is 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, also known as trial functions. These basis functions are carefully chosen to possess desirable mathematical properties, such as orthogonality, smoothness, and global support, making them well-suited for accurately approximating the behavior of the solution across the entire domain of interest.

Unlike finite difference or finite element methods, which typically use local approximations over small regions of the domain, the spectral method considers the entire domain as a unified entity. In practice, finite-element methods are particularly well suited to problems in complex geometries, whereas spectral methods can provide superior accuracy, at the expense of domain flexibility [1]. This method is particularly great for problems characterized by smooth solutions and regular domains. However, spectral methods may exhibit limitations in terms of domain flexibility, as they are generally less adaptable to irregular geometries.

In the realm of numerical techniques for solving differential equations, spectral methods are categorized within the weighted residual methods (WRMs) framework. WRMs, a cornerstone in various numerical methodologies like finite element, spectral, finite volume, and boundary element methods, encapsulate a distinct set of approximation [1]. These methods aim to minimize residuals or errors in a defined manner, giving rise to specific approaches such as Galerkin, Petrov-Galerkin, collocation, and tau formulations.

When understanding WRMs, we consider the general problem

$$\partial_t u(x,t) - \mathcal{L}u(x,t) = \mathcal{N}(u)(x,t), \quad t > 0, x \in \Omega, \tag{1}$$

where $\mathcal{L}$ is a leading spatial derivative operator, and $\mathcal{N}$ is a lower-order linear or nonlinear operator involving only spatial derivatives [1]. In this definition $\Omega$ denotes a bounded domain of $\mathbb{R}^d$, where $d = 1, 2, 3$. Equation 1 requires an initial condition along with appropriate boundary conditions for completeness.

We focus solely on spatial discretization using the WRM method, while assuming an appropriate time-stepping scheme for discretizing the time derivative. Commonly, semi-implicit or linearly implicit schemes are preferred, as they handle principal linear operators implicitly to mitigate stability issues, while treating nonlinear terms explicitly to avoid solving costly nonlinear equations at each time step [1].

If we let $\tau$ be the time step size, we can use a Crank-Nicolson leap-frog scheme for 1. This writes

$$\mathbf{L}u(x) := \alpha u(x) - \mathcal{L}u(x) = f(x), \quad x \in \Omega \tag{2}$$

where $u = \frac{u^{n+1}+u^{n-1}}{2}$, $\alpha = \tau^{-1}$, and $f = \alpha u^{n-1} + \mathcal{N}(u^n)$ from the abusively notated scheme [1].

The initial step in the WRM involves approximating the solution $u(x)$ of equation 1 by a finite sum

$$u(x) \approx u_N(x) = \sum_{k=0}^{N} a_k \phi_k(x) \tag{3}$$

where $\phi_k$ are the basis functions and $a_k$ are the to be determined expansion coefficients. Substituting

$u_N$ for $u$ in 1 leads to the residual equation

$$\mathbf{R}_N = \mathbf{L}u_N(x) - f(x) \neq 0, \quad x \in \Omega \tag{4}$$

The concept of the WRM is to drive the residual to zero by enforcing

$$\langle \mathbf{R}_N, \psi \rangle_{N,\omega} = \sum_{N}^{k=0} \mathbf{R}_N(x_k)\psi_j(x_k)\omega_k = 0, \quad 0 \leq j \leq N \tag{5}$$

where the $x_k$'s are a set of collocation points and the $\omega_k$'s are the numerical quadrature formula weights.

## 1.2 Definition of Terms

### 1.2.1 Basis Function

Spectral Methods rely on representing the solution to any problem as a linear combination of some basis function. These functions are very important when determining the accuracy and efficiency of the Spectral Method itself. There are many types of basis functions that the method employs when solving a problem and utilizing its boundary/initial conditions[1] .

**Fourier Basis Functions:** $\phi_k(x) = e^{ikx}$. Any repeating function, like Sine or Cosine, that have different frequencies $k$ fall under this category. This method, known as the Fourier Spectral Method, is suitable for problems with periodic boundary conditions.

**Chebyshev Basis Functions:** $\phi_k(x) = T_k(x)$. Chebyshev polynomials are orthogonal on the interval [1,1] and cluster near the boundaries. This method is suitable for solving problems with non-periodic domains with layered boundary or boundary singularities.

**Legendre Basis Functions:** $\phi_k(x) = L_k(x)$. Legendre polynomials are also orthogonal on the interval [-1,1] but have a uniform distribution of nodes. This method is suitable for solving problems with symmetric domains.

**Laguerre Basis Functions:** $\phi_k(x) = \mathcal{L}_k(x)$. Legendre polynomials are orthogonal on the interval $[0, \infty]$ with weight $e^{-x}$. This method is suitable for solving problems defined on unbounded domains or problems with exponential decay.

**Hermite Basis Functions:** $\phi_k(x) = H_k(x)$. Hermite polynomials are orthogonal on the entire real line with weight $e^{-x^2}$. This method is suitable for solving problems with Gaussian-like solutions, meaning the solution resembles a Gaussian distribution or normal distribution.

## 1.3 Physical Space

In the physical space, the spectral method is a great numerical approach for tackling diverse partial differential equations. Operating across the entire domain, it harnesses global approximations by using basis functions customized to the unique traits of each problem. In essence, within this space, functions and their derivatives are represented throughout the spatial domain via selected basis functions. This methodology ensures precision and efficiency.

## 1.4 Frequency Space

In the frequency space, the spectral method goes beyond the limitations of traditional numerical techniques by harnessing the power of Fourier analysis and other spectral transformations. Un-

[1]This paper will focus on the Fourier Spectral method, as the problem chosen has a periodic domain/conditions.

like finite difference or finite element methods, which operate primarily in the physical space, the spectral method exploits the frequency domain to decompose functions into a series of eigenfunctions. This transition enables a global approximation approach, where the solution is expressed as a weighted sum of basis functions, each representing a distinct frequency component we can denote $k$.

In this space lies the Fourier transform, a mathematical tool that decomposes a function into its constituent sinusoidal components. By representing functions in terms of Fourier modes or other spectral basis functions, the spectral method facilitates efficient computation of derivatives and integrals. This approach not only provides a natural framework for solving differential equations but also unlocks the ability to analyze the frequency content of the solution.

### 1.5 Time-Stepping Scheme

Time stepping schemes in the spectral method are used to numerically integrate time-dependent partial differential equations over discrete time intervals. Time stepping schemes are essential for advancing the solution from one time level to the next. Once the spatial domain is discretized and the initial condition is specified, the time stepping scheme is applied to advance the solution from the initial time $t_0$ to subsequent time levels $t_1, t_2, \cdots$. These schemes can be implicit, explicit, or even fractional-step. There exist many different types of time stepping schemes; for example Runge-Kutta, Leap-Frog, and Euler. Because this project explores the Euler method as its time stepping scheme, we will briefly cover it now.

The Euler method involves taking a single time step forward from the current state to the next state based on the derivative at the current time. Mathematically, for a differential equation $dy/dt = f(y,t)$, where $y$ is the solution and $f$ is the derivative function, the Euler method updates the solution as follows:

$$y_{n+1} = y_n + hf(y_n, t_n)$$

where $h$ is the time step size, $t_n$ is the current time, and $y_n$ is the current state of the solution.

### 1.6 Fourier Transforms

The Fourier Transform is a mathematical technique that converts a function of time $x(t)$ to a function in the frequency space. It is a generalization of the Fourier series from a finite domain to an infinite sized domain. Given any arbitrary function $f(x)$ that is periodic on some domain say $(-L, L)$, we can expand $f(x)$ as linear combination of sine and cosine, or equivalently, as a complex Fourier series

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

that is $2L$ periodic, where

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

are the Fourier coefficients. Define

$$\omega_k = \frac{k\pi}{L} = k\Delta\omega$$

as the frequencies of the sine and cosine,

$$\Delta\omega = \frac{\pi}{L}$$

So, the Fourier Transform extends to $L$, meaning it represents the function $u(x)$ as $L \to \infty$, which is the same as $\Delta\omega \to 0$.

$$u(x) = \lim_{\Delta\omega \to 0} \sum_{k=-\infty}^{\infty} \frac{\Delta\omega}{2\pi} \int_{-\frac{\pi}{\Delta\omega}}^{\frac{\pi}{\Delta\omega}} u(\eta) e^{-ik\Delta\omega\eta} d\eta e^{ik\Delta\omega x}$$

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

With the expression above, we obtain the Fourier transform of $f(x)$:

$$\hat{u}(x) = U(x) = \int_{-\infty}^{\infty} u(x) e^{-i\omega x} dx$$

which is a function of the frequency $\omega$ and the inverse Fourier transform :

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

This transformation enables us to work in any space we like. We can transform our problem to the frequency space using the Fourier transform. After solving the problem, we use inverse Fourier Transform to change back to the physical domain. We will see later that working in the frequency space is computationally less expensive than working in the physical space. The last two equations are known as the Fourier Transform Pair.

### 1.7 Discrete Fourier

Discrete Fourier Transform is the Fourier series on finite data. It represents the data as sum of sine and cosine components. Given any integer $N$, the set of discrete points on a domain that is $2\pi$ periodic is given by

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

with its corresponding function values:

$$\{u(x_j)\}_{j=0}^{N-1}$$

The Discrete Fourier Transform is :

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

and the Inverse Discrete Fourier Transform is :

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

This transformation leads to a large matrix multiplication which requires $O(N^2)$ operations. The Fast Fourier Transform (FFT) is a technique for calculating the discrete Fourier Transform which is computationally less expensive because it requires $O(N \log_2 N)$.

# 2 Implementation of the Spectral Method

## 2.1 Differentiation in Physical Space

Differentiation can be done either in the physical space or in the frequency space. The following differentiation is given by our textbook → Spectral Methods: Algorithms, Analysis and Applications [1].

Starting in the physical space, we use Fourier techniques to set

$$\mathcal{I}_N = \{u = \sum_{k=-N/2}^{N/2} \tilde{u}_k e^{ikx} : \tilde{u}_{-N/2} = \tilde{u}_{N/2}\} \tag{6}$$

and define the mapping $I_N : C[0, 2\pi] \to \mathcal{I}_N$ by

$$(I_N u)(x) = \sum_{k=-N/2}^{N/2} \tilde{u}_k e^{ikx}. \tag{7}$$

Here, $\tilde{u}_k$ is defined as

$$\tilde{u}_k = \frac{1}{Nc_k} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j}, \quad k = -N/2, \cdots, N/2. \tag{8}$$

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

$$(I_N u)(x_j) = u(x_j), \quad x_j = \frac{2\pi j}{N}, \quad 0 \le j \le N-1 \tag{9}$$

**Lemma 2.1** *Therefore, for any $u \in C(0, 2\pi)$,*

$$(I_N u)(x) = \sum_{j=0}^{N-1} u(x_j) h_j(x) \tag{10}$$

*where*

$$h_j(x) = \frac{1}{N} \sin[N\frac{x - x_j}{2}] \cot[\frac{x - x_j}{2}] \in \mathcal{I}_N \tag{11}$$

*satisfies*

$$h_j(x_k) = \delta_{jk}, \quad \forall j, k = 0, 1, \cdots, N-1. \tag{12}$$

The lemma is proven on page 28 of the Spectral Methods textbook [1]. By letting $x_j$ and $h_j$ be defined as above, we can set

$$u(x) = \sum_{j=0}^{N-1} u(x_j) h_j(x) \tag{13}$$

and take the m-th derivative to get

$$u^{(m)}(x) = \sum_{j=0}^{N-1} u(x_j) h_j^{(m)}(x). \tag{14}$$

The process of equations 13 and 14 can be expressed as a matrix-vector multiplication

$$\mathbf{u}^{(m)} = D^{(m)}\mathbf{u}, \quad m \geq 0$$

$$D^{(m)} = (d^(m)_{kj} := h_j^{(m)}(x_k))_{k,j=0,\cdots,N-1}$$

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

$$\mathbf{u}^{(m)} = (u^{(m)}(x_0), u^{(m)}(x_1), \cdots, u^{(m)}(N-1))^T.$$

This matrix differentiation procedure requires $O(N^2)$ operations. In the frequency space, this can be performed with $O(N \log_2 N)$ operations using the Fast Fourier Transform.

## 2.2 Differentiation in Frequency (Fourier) Space

Given any function $u(x)$ with a periodic domain, its finite Fourier series can be expressed as:

$$u(x) = \sum_{k=\frac{-N}{2}}^{\frac{N}{2}} \hat{u}_k e^{ikx}, \quad \hat{u}_{N/2} = \hat{u}_{-N/2}$$

The n-th derivative is computed as follows:

$$u^n(x_j) = \sum_{k=\frac{-N}{2}}^{\frac{N}{2}-1} (ik)^n * \hat{u}_k e^{ikx_j}$$

where $k$ is the wave number vector given by $k = (\frac{-N}{2}, ..., \frac{N}{2} - 1)$ and $i$ is the imaginary number $\sqrt{-1}$. So, when we move into the frequency space using FFT, we initiate the wave number vector and compute the multiplicative factor $(ik)^n$ and then use it to multiply the frequency vector $\hat{u} = (\hat{u}_1, ..., \hat{u}_N)$. The Fourier spectral method adopts this property in its implementation.

## 2.3 How Does the Fourier Spectral works

Given any PDEs with a periodic boundary condition and initial data, the Fourier Spectral method adopts the following steps:

1. Discretize the spatial domain and evaluate the initial condition at the discrete points.
2. Use FFT to transform the initial condition into the frequency space.
3. In the frequency space, compute the multiplicative factors of the derivatives using the wave number vector $i * k$.
4. Unlike in the method of differentiation in the frequency space where the multiplicative factor is being multiplied to $\hat{u}(k, t)$, the Fourier Spectral method reverses the process by dividing with this factor, where the component with 0 value remains unchanged. This reverses the process of differentiation.
5. Next, use a time-stepping scheme to obtain the solution at the next time level.
6. Use IFFT to move out of the Frequency space. The solution at this point becomes the initial condition and this process is repeated until the final time is reached.

## 2.4 Solving the 1D Heat Equation using Fourier Spectral Method

Here, we consider the 1D Heat Equation:

$$u_t = \alpha^2 u_{xx}, \quad \alpha = 1$$

$$u(x,0) = \sin(x), \quad 0 \leq x \leq 2\pi, \quad t > 0$$

The plots below show the exact solution with the numerical solutions obtained using both the Fourier Spectral method and the Finite Difference approach, providing a comprehensive comparison. Upon visual inspection, discerning variations between the two numerical methods and the exact solution proves challenging. Therefore, section 3 of this paper dives into a thorough error analysis and comparison of these numerical solutions, shedding light on their respective accuracy's and performance characteristics.

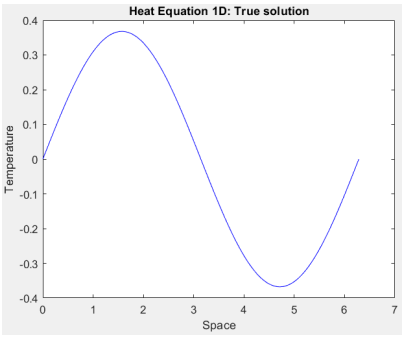


Figure 1: Finite Difference

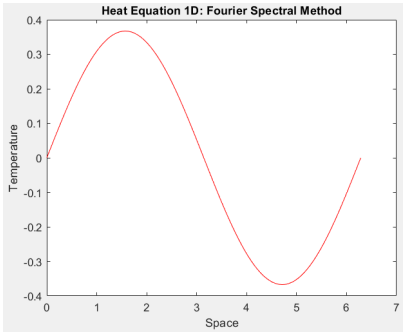


Figure 2: Fourier Spectral

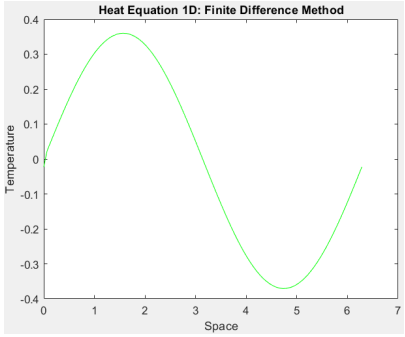


Figure 3: Exact Solution

## 2.5 Solving the 2D Heat Equation using Fourier Spectral Method

Next, we also consider the 2D Heat Equation:

$$u_t = \alpha^2(u_{xx} + u_{yy}), \quad \alpha = 1$$

$$u(x,y,0) = \sin(x)\sin(y), \quad 0 \leq x \leq 2\pi, \quad 0 \leq y \leq 2\pi, \quad t > 0$$

which results in the following 3D plots. Again, they are hard to discern between so we turn to the next section to discuss errors.

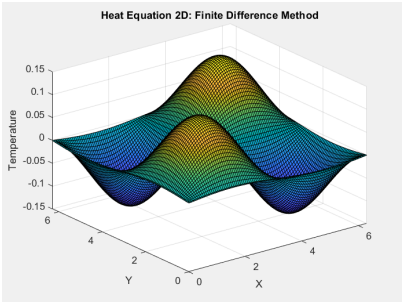


Figure 4: Finite Difference

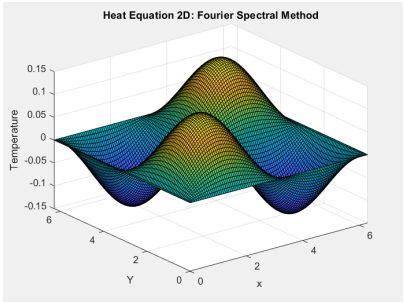


Figure 5: Fourier Spectral

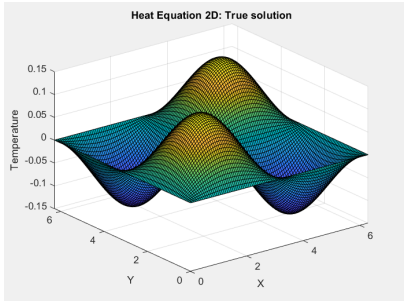


Figure 6: Exact Solution

## 3 Error Analysis and Comparison

For the 1D heat equation: Table 1 below shows the L2 error in Fourier spectral method and the finite difference method. The former gives a better approximation to our solution than the later. In this table, we plot the L2 error against N. It is clear from Figure 7 that the Fourier Spectral method indicates a minimal error than the finite difference method.

To get a more accurate result, we decreased the time step, for the finite difference method, this time step is $\Delta t \approx 0.5\Delta x^2$. Keeping N constant and decreasing the time step gave a more accurate result in the Fourier spectral method with less effect on the finite difference. To get a better result using the finite difference, we increased N while maintaining $\Delta t \approx 0.5\Delta x^2$, and we obtain the CPU time taken for both methods to reach the same accuracy. We discovered as shown in Table 1, that the Fourier Spectral is still a better choice than the Finite difference.

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 |

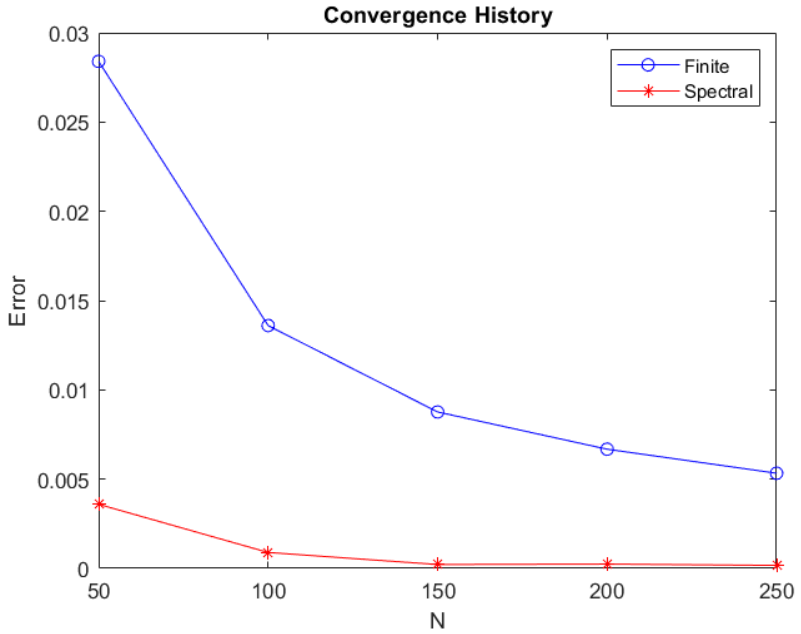


Figure 7: 1D: Fourier Spectral Method vs. Finite Difference Method

Table 2: CPU Time for Accuracy of $10^{-5}$

| Method | Error | CPU Time |
|---|---|---|
| Fourier Spectral | 8.09474e-05 | 0.0222 |
| Finite Difference | 6.02044e-05 | 19.478 |

For the 2D case: Table 3 shows the L2 error in our numerical solution to the 2D heat equation. As expected the Fourier Spectral method gave a better approximation to our solution than the finite difference method. This is also obvious from Figure 8 where we plotted the L2 error against N. A more accurate result can also be obtained by decreasing the time step. For the Finite difference, we ensure that $\Delta t \approx 0.25\Delta x^2$ in order to maintain stability.

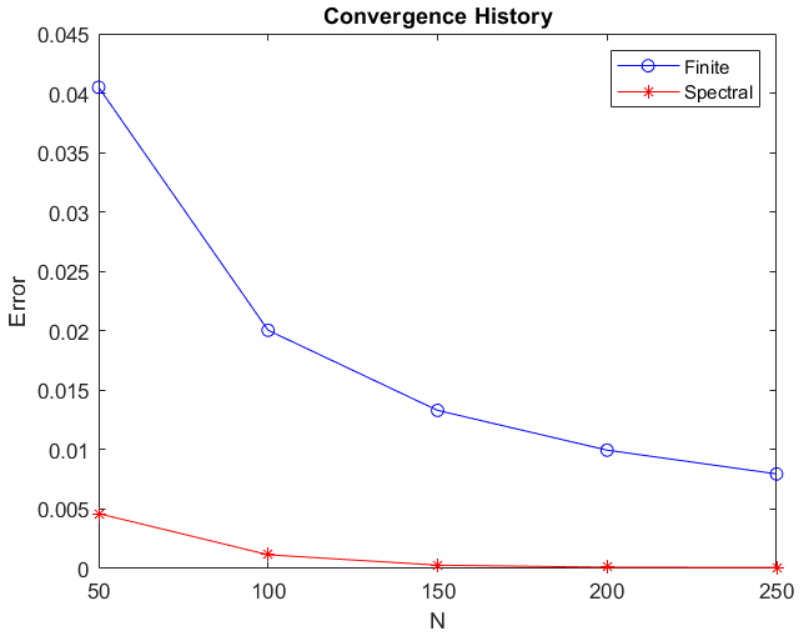


Figure 8: 2D Error: Fourier Spectral Method vs. Finite Difference Method

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 |

# 4 Conclusion

Given a problem with a periodic boundary condition and a smooth solution, the Fourier Spectral Method achieves a high accuracy and with good convergence rate. Whenever accuracy and convergence rates are a matter of concern when solving a problem with the above properties, the Fourier Spectral is a choice method to adopt.

The ability to represent functions in the frequency domain enables the efficient computation of multiplicative factors [2] [3] which facilitates superior convergence and allows for the analysis of solutions with unprecedented precision. This is shown through our comparison with the Finite Difference method. This high accuracy comes from the use of globally smooth basis functions.

## References


[1] Jie Shen, Tao Tang, Li-Lian Wang (2011) *Spectral Methods: Algorithms, Analysis and Applications*, Springer Publishing Company, 1st ed.

[2] Lloyd Trefethen (2000) *Spectral Methods in Matlab*, Society for Industrial and Applied Mathematics, 1st ed.

[3] 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