

Week #12: Partial Differential Equations

Numerical Methods: Mathematical Foundations

June 22, 2025

Overview

Partial differential equations (PDEs) model phenomena involving multiple independent variables, from heat conduction and wave propagation to fluid dynamics and quantum mechanics. This week we develop the mathematical foundations for numerical PDE methods, exploring finite difference, finite element, and spectral approaches while analyzing their stability, accuracy, and computational properties.

The numerical solution of PDEs presents unique challenges compared to ODEs, including the curse of dimensionality, the need for appropriate boundary condition treatment, and the delicate balance between accuracy and computational efficiency. We examine how different discretization strategies address these challenges and investigate the mathematical principles that guide method selection.

Our analysis emphasizes the mathematical theory underlying PDE discretizations, the crucial role of stability analysis in multidimensional problems, and the convergence theory that ensures reliable numerical solutions.

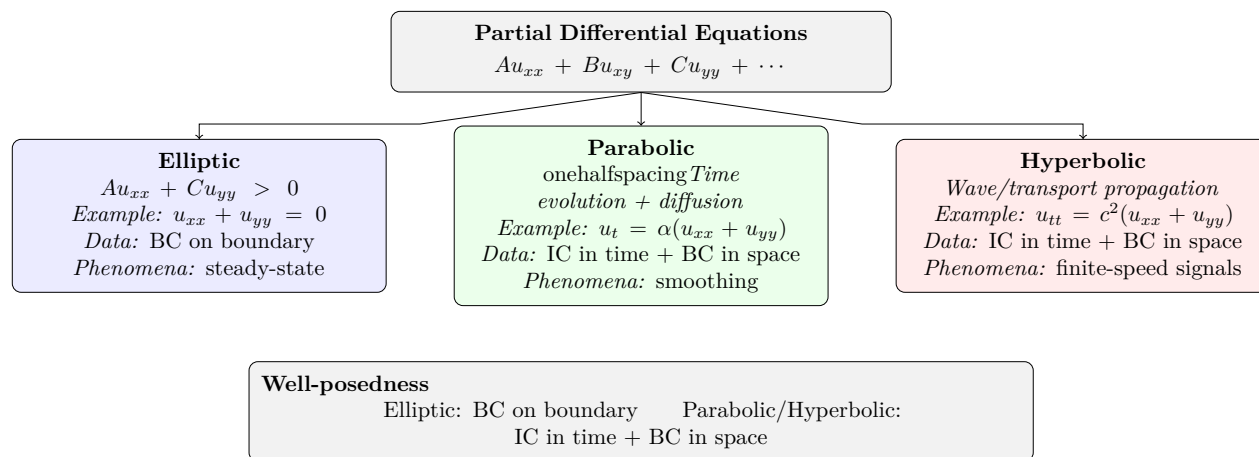


Figure 1: Compact classification: elliptic (steady-state), parabolic (diffusion), hyperbolic (waves), with canonical examples and data requirements.

1 Classification of PDEs

1.1 Mathematical Classification

Definition. Second-Order Linear PDE

A general second-order linear PDE in two variables has the form:

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G$$

where A, B, C, D, E, F, G may depend on x and y .

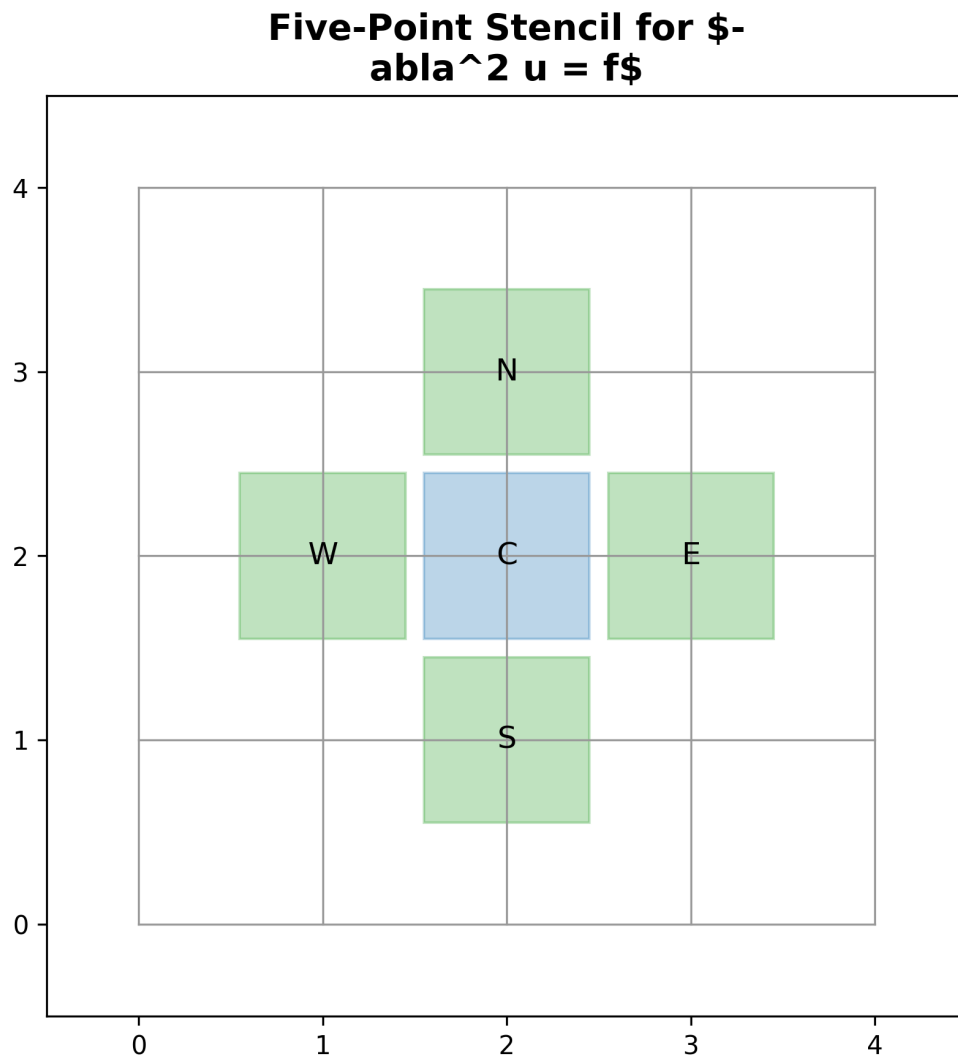


Figure 2: Five-point stencil layout on a uniform grid for the Poisson equation.

Definition. PDE Classification

The PDE is classified by the discriminant $\Delta = B^2 - 4AC$:

- **Elliptic:** $\Delta < 0$ (e.g., Laplace equation)
- **Parabolic:** $\Delta = 0$ (e.g., heat equation)
- **Hyperbolic:** $\Delta > 0$ (e.g., wave equation)

1.2 Model Problems

Definition. Heat Equation (Parabolic)

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

Models diffusion processes with initial condition $u(x, 0) = f(x)$ and boundary conditions.

Definition. Wave Equation (Hyperbolic)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Models wave propagation with initial conditions $u(x, 0) = f(x)$ and $u_t(x, 0) = g(x)$.

Definition. Laplace Equation (Elliptic)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Models steady-state phenomena with boundary conditions on the domain boundary.

2 Finite Difference Methods

2.1 Basic Finite Difference Approximations

Definition. Finite Difference Operators

For uniform grid spacing h :

$$\delta_+ u_i = u_{i+1} - u_i \quad (\text{forward difference}) \quad (1)$$

$$\delta_- u_i = u_i - u_{i-1} \quad (\text{backward difference}) \quad (2)$$

$$\delta_0 u_i = \frac{u_{i+1} - u_{i-1}}{2} \quad (\text{central difference}) \quad (3)$$

Theorem 2.1 (Finite Difference Accuracy). *The truncation errors are:*

$$u'(x_i) - \frac{\delta_+ u_i}{h} = -\frac{h}{2} u''(x_i) + O(h^2) \quad (4)$$

$$u'(x_i) - \frac{\delta_0 u_i}{h} = -\frac{h^2}{6} u'''(x_i) + O(h^4) \quad (5)$$

$$u''(x_i) - \frac{\delta_+ \delta_- u_i}{h^2} = -\frac{h^2}{12} u^{(4)}(x_i) + O(h^4) \quad (6)$$

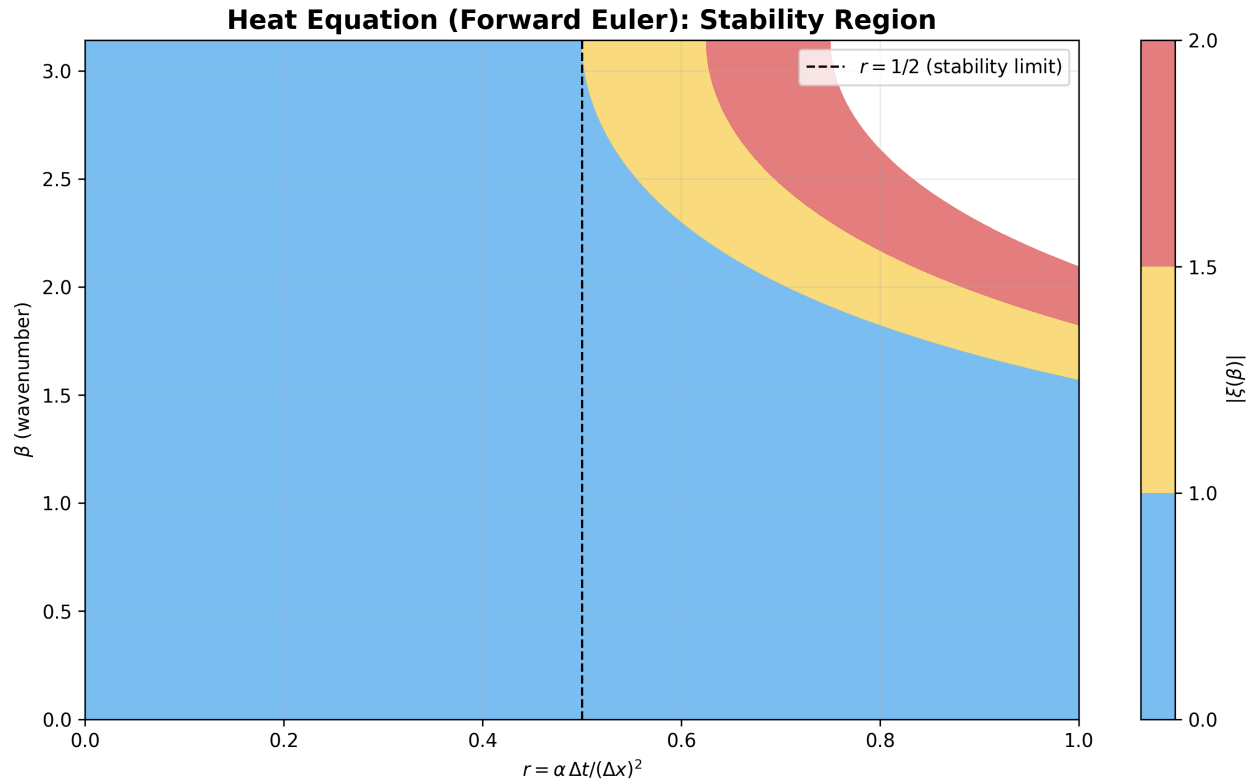


Figure 3: Von Neumann amplification factor $|\xi(\beta)|$ for the forward Euler heat scheme as a function of $r = \alpha\Delta t/(\Delta x)^2$ and wavenumber. Stable for $r \leq 1/2$.

2.2 Heat Equation Discretization

Definition. Forward Euler for Heat Equation

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \alpha \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2}$$

where $U_i^n \approx u(x_i, t_n)$.

Theorem 2.2 (Stability of Forward Euler for Heat Equation). *The forward Euler scheme is stable if and only if:*

$$r = \frac{\alpha\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$$

Definition. Backward Euler for Heat Equation

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \alpha \frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{(\Delta x)^2}$$

This implicit scheme is unconditionally stable.

2.3 Wave Equation Discretization

Definition. Leapfrog Scheme for Wave Equation

$$\frac{U_i^{n+1} - 2U_i^n + U_i^{n-1}}{(\Delta t)^2} = c^2 \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2}$$

Theorem 2.3 (CFL Condition for Wave Equation). *The leapfrog scheme is stable if and only if:*

$$c \frac{\Delta t}{\Delta x} \leq 1$$

This is the Courant-Friedrichs-Lewy (CFL) condition.

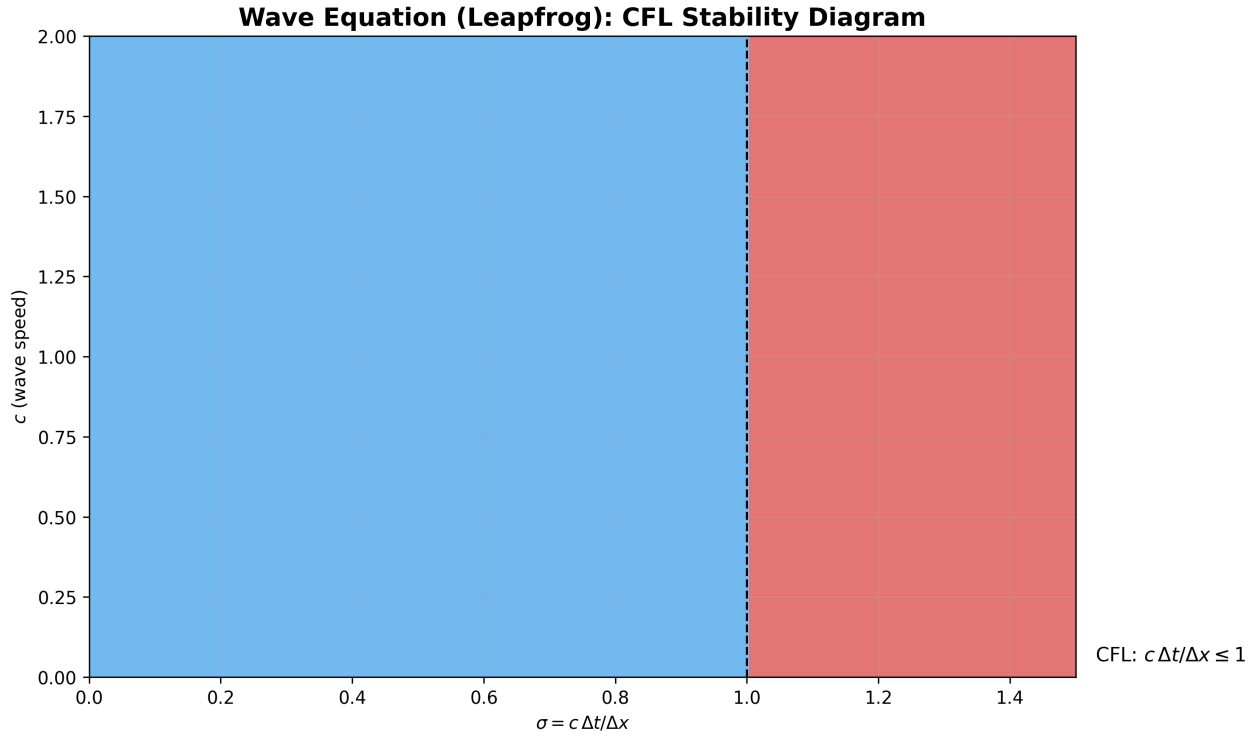


Figure 4: CFL diagram for the leapfrog scheme showing the stable region $c \Delta t / \Delta x \leq 1$.

3 Stability Analysis

3.1 Von Neumann Stability Analysis

Definition. Fourier Mode Analysis

Assume solutions of the form $U_j^n = \xi^n e^{i\beta j \Delta x}$ where ξ is the amplification factor and β is the wave number.

Theorem 3.1 (Von Neumann Stability Condition). *A finite difference scheme is stable if $|\xi(\beta)| \leq 1$ for all wave numbers β .*

Example 3.1 (Forward Euler Stability Analysis). *For the forward Euler heat equation scheme:*

$$\xi = 1 - 4r \sin^2 \left(\frac{\beta \Delta x}{2} \right)$$

Stability requires $|\xi| \leq 1$, giving $r \leq 1/2$.

3.2 Matrix Stability Analysis

Definition. Method of Lines

Semi-discretize in space to obtain a system of ODEs:

$$\frac{d\mathbf{U}}{dt} = A\mathbf{U} + \mathbf{b}$$

where A is the spatial discretization matrix.

Theorem 3.2 (Stability via Eigenvalue Analysis). *For the forward Euler time discretization, stability requires $1 + \Delta t \lambda_i \geq -1$ for all eigenvalues λ_i of A .*

4 Elliptic Problems

4.1 Poisson Equation

Definition. Five-Point Stencil for Poisson Equation

For $-\nabla^2 u = f$ on a rectangular grid:

$$-\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} - \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} = f_{i,j}$$

This leads to a large sparse linear system $AU = b$.

4.2 Iterative Methods for Elliptic Problems

Definition. Gauss-Seidel for Poisson Equation

$$U_{i,j}^{(k+1)} = \frac{1}{4} \left[U_{i+1,j}^{(k)} + U_{i-1,j}^{(k+1)} + U_{i,j+1}^{(k)} + U_{i,j-1}^{(k+1)} + h^2 f_{i,j} \right]$$

Definition. Successive Over-Relaxation (SOR)

$$U_{i,j}^{(k+1)} = (1 - \omega)U_{i,j}^{(k)} + \frac{\omega}{4} \left[U_{i+1,j}^{(k)} + U_{i-1,j}^{(k+1)} + U_{i,j+1}^{(k)} + U_{i,j-1}^{(k+1)} + h^2 f_{i,j} \right]$$

Theorem 4.1 (Optimal SOR Parameter). *For the Poisson equation on a rectangle with Dirichlet boundary conditions, the optimal relaxation parameter is:*

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho^2}}$$

where ρ is the spectral radius of the Jacobi iteration matrix.

5 Finite Element Methods

5.1 Weak Formulation

Definition. Weak Form of Poisson Equation

Find $u \in H_0^1(\Omega)$ such that:

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx$$

for all $v \in H_0^1(\Omega)$.

5.2 Galerkin Approximation

Definition. Finite Element Approximation

Seek $u_h \in V_h \subset H_0^1(\Omega)$ such that:

$$\int_{\Omega} \nabla u_h \cdot \nabla v_h \, dx = \int_{\Omega} f v_h \, dx$$

for all $v_h \in V_h$, where V_h is a finite-dimensional subspace.

5.3 Linear Elements

Definition. Piecewise Linear Elements

On a triangulation $\mathcal{T}_h$ of Ω :

$$V_h = \{v \in C(\bar{\Omega}) : v|_T \text{ is linear for each } T \in \mathcal{T}_h, v = 0 \text{ on } \partial\Omega\}$$

Theorem 5.1 (Finite Element Error Estimate). *If $u \in H^2(\Omega)$ and u_h is the finite element approximation using linear elements:*

$$\|u - u_h\|_{H^1(\Omega)} \leq Ch \|u\|_{H^2(\Omega)}$$

where h is the maximum element diameter.

6 Spectral Methods

6.1 Fourier Spectral Methods

Definition. Fourier Series Approximation

For periodic problems, approximate:

$$u(x, t) \approx \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx}$$

Theorem 6.1 (Spectral Accuracy). *For smooth periodic functions, Fourier spectral methods achieve exponential convergence: the error decreases faster than any polynomial in $1/N$.*

6.2 Chebyshev Spectral Methods

Definition. Chebyshev Polynomial Approximation

For non-periodic problems on $[-1, 1]$:

$$u(x, t) \approx \sum_{k=0}^N a_k(t) T_k(x)$$

where $T_k(x)$ are Chebyshev polynomials.

Intuition: Why Spectral Methods Work

Spectral methods use global basis functions (trigonometric or polynomial) that can represent smooth functions very efficiently. They achieve high accuracy with relatively few degrees of freedom, but require smooth solutions to be effective.

7 Advanced Topics

7.1 Adaptive Mesh Refinement

Definition. h-Refinement

Reduce element size h in regions where the error is large, maintaining the same polynomial degree.

Definition. p-Refinement

Increase polynomial degree p while keeping the mesh fixed.

Definition. hp-Refinement

Optimally combine h and p refinement based on solution regularity.

7.2 Multigrid Methods

Definition. Geometric Multigrid

Use a hierarchy of grids to accelerate convergence:

1. Smooth on fine grid
2. Restrict residual to coarse grid
3. Solve coarse grid problem
4. Interpolate correction to fine grid

Theorem 7.1 (Multigrid Convergence). *Under appropriate smoothing and approximation properties, multigrid methods achieve convergence rates independent of grid size, leading to optimal $O(N)$ complexity.*

7.3 Discontinuous Galerkin Methods

Definition. Discontinuous Galerkin Formulation

Allow discontinuities across element boundaries and enforce continuity weakly through numerical fluxes.

DG methods combine advantages of finite elements (geometric flexibility) and finite differences (local conservation).

8 Nonlinear PDEs

8.1 Newton's Method for PDEs

Definition. Newton Iteration for Nonlinear PDEs

For $F(u) = 0$, iterate:

$$\begin{aligned} J(u^{(k)})\delta u^{(k)} &= -F(u^{(k)}) \\ u^{(k+1)} &= u^{(k)} + \delta u^{(k)} \end{aligned}$$

where J is the Jacobian matrix.

8.2 Time-Dependent Nonlinear Problems

Definition. Implicit-Explicit (IMEX) Methods

Treat stiff linear terms implicitly and nonlinear terms explicitly:

$$\frac{u^{n+1} - u^n}{\Delta t} = Lu^{n+1} + N(u^n)$$

where L is linear and N is nonlinear.

Practice Problems

1. Derive the stability condition for the forward Euler scheme applied to the heat equation using von Neumann analysis.
2. Prove that the backward Euler scheme for the heat equation is unconditionally stable.
3. Implement the five-point stencil for the Poisson equation and solve using SOR with optimal relaxation parameter.
4. Analyze the dispersion properties of finite difference schemes for the wave equation.
5. Compare the accuracy of finite difference and spectral methods for solving the heat equation with smooth initial data.