Ordinary Differential Equations

Lecture Notes

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1 Lecture 7: Numerical Methods for Differential Equations

1.0.1 Introduction to Numerical Methods

The vast majority of differential equations encountered in scientific and engineering applications cannot be solved analytically. Even when analytical solutions exist, they may be too complex for practical use or may not provide insight into system behavior. Numerical methods bridge this gap by providing approximate solutions with controlled accuracy, enabling the study of complex systems that would otherwise remain intractable.

Numerical methods for differential equations have evolved dramatically since the pioneering work of Euler in the 18th century. Modern algorithms incorporate sophisticated error control, adaptive step sizing, and specialized techniques for different classes of problems. The development of high-performance computing has further expanded the scope of problems that can be addressed numerically, from weather prediction and climate modeling to molecular dynamics and financial risk analysis.

The fundamental challenge in numerical integration is balancing accuracy, stability, and computational efficiency. Different methods excel in different regimes: explicit methods are simple and efficient for non-stiff problems, while implicit methods are essential for stiff systems. Adaptive methods automatically adjust step sizes to maintain accuracy while minimizing computational cost.

Understanding the theoretical foundations of numerical methods is crucial for their effective application. Concepts such as consistency, stability, and convergence provide the mathematical framework for analyzing method performance and selecting appropriate algorithms for specific problems.

1.0.2 Fundamental Concepts

Before examining specific algorithms, we establish the basic framework for numerical integration of initial value problems. Consider the general first-order system:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}) \tag{1}$$

$$\mathbf{y}(t_0) = \mathbf{y}_0 \tag{2}$$

where $\mathbf{y} \in \mathbb{R}^n$ is the state vector and $\mathbf{f} : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is the vector field. Higher-order equations can always be converted to this first-order form through the introduction of auxiliary variables.

Numerical methods approximate the solution at discrete time points $t_n = t_0 + nh$ where h is the step size. The approximate solution at t_n is denoted $\mathbf{y}_n \approx \mathbf{y}(t_n)$. The goal is to construct a sequence $\{\mathbf{y}_n\}$ that converges to the true solution as $h \to 0$.

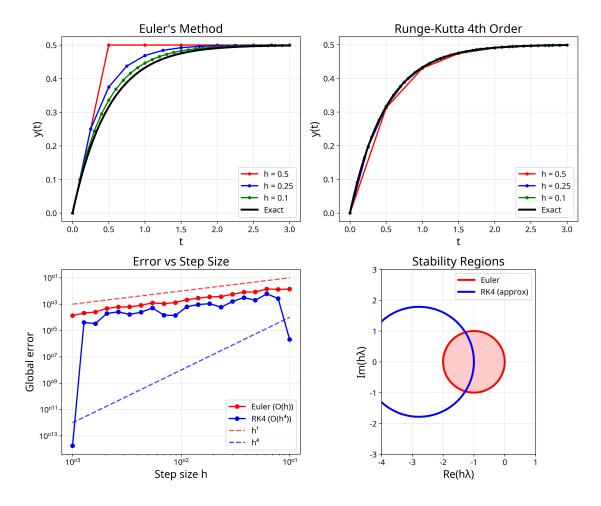


Figure 1: Numerical method comparison: Euler vs RK4 accuracy for different step sizes, global error analysis showing theoretical convergence rates, and stability region analysis for different integration schemes.

Local Truncation Error: The error introduced in a single step, assuming all previous values are exact. For a method with local truncation error $O(h^{p+1})$, we say the method has order p.

Global Error: The accumulated error after many steps, typically $O(h^p)$ for a method of order p.

Stability: The property that small perturbations in the initial data or intermediate calculations do not grow unboundedly. Stability is essential for reliable long-term integration.

1.0.3 Single-Step Methods

Single-step methods compute \mathbf{y}_{n+1} using only information from the current point $(\mathbf{t}_n, \mathbf{y}_n)$. These methods are self-starting and have simple error analysis, making them the foundation for more advanced techniques.

1.0.4 Euler's Method and Its Variants

Euler's method is the simplest numerical integration scheme, based on the first-order Taylor expansion:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n) \tag{3}$$

Geometrically, this follows the tangent line at (t_n, \mathbf{y}_n) for a distance h. The method has order 1, meaning the global error is O(h).

Backward Euler Method: The implicit variant uses the derivative at the new point:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) \tag{4}$$

This requires solving a nonlinear system at each step but provides superior stability properties, especially for stiff problems.

Improved Euler Method (Heun's Method): This predictor-corrector scheme achieves second-order accuracy:

$$\mathbf{y}_{n+1}^{(0)} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n) \quad \text{(predictor)}$$
 (5)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2} [\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}^{(0)})] \quad \text{(corrector)}$$

The predictor step estimates the solution at t_{n+1} , while the corrector uses this estimate to compute a more accurate derivative average.

1.0.5 Runge-Kutta Methods

Runge-Kutta methods achieve higher-order accuracy by evaluating the derivative at multiple points within each step. The general s-stage explicit Runge-Kutta method has the form:

$$\mathbf{k}_{i} = \mathbf{f} \left(t_{n} + c_{i}h, \mathbf{y}_{n} + h \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_{j} \right), \quad i = 1, 2, \dots, s$$
 (7)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i \tag{8}$$

The coefficients a_{ij} , b_i , and c_i are chosen to maximize the order of accuracy. These coefficients are typically presented in a Butcher tableau:

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} \tag{9}$$

Classical Fourth-Order Runge-Kutta (RK4): The most widely used Runge-Kutta method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n) \tag{10}$$

$$\mathbf{k}_2 = \mathbf{f}(t_n + h/2, \mathbf{y}_n + h\mathbf{k}_1/2) \tag{11}$$

$$\mathbf{k}_3 = \mathbf{f}(t_n + h/2, \mathbf{y}_n + h\mathbf{k}_2/2) \tag{12}$$

$$\mathbf{k}_4 = \mathbf{f}(t_n + h, \mathbf{y}_n + h\mathbf{k}_3) \tag{13}$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$
(14)

RK4 achieves fourth-order accuracy with four function evaluations per step, providing an excellent balance of accuracy and computational cost for many problems.

Example. Consider the Duffing oscillator:

$$\frac{dx}{dt} = y \tag{15}$$

$$\frac{dy}{dt} = -x - x^3 - 0.1y + 0.3\cos(t) \tag{16}$$

Converting to vector form: $\mathbf{y} = (x, y)^T$ and

$$\mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} y \\ -x - x^3 - 0.1y + 0.3\cos(t) \end{pmatrix}$$
 (17)

The RK4 method provides accurate integration of this chaotic system, capturing the complex dynamics that would be missed by lower-order methods or large step sizes.

1.0.6 Embedded Runge-Kutta Methods

Embedded methods compute two approximations of different orders using the same function evaluations, enabling automatic error estimation and step size control. The Runge-Kutta-Fehlberg method (RKF45) embeds a fourth-order and fifth-order method:

The error estimate is:

$$\mathbf{e}_{n+1} = \mathbf{y}_{n+1}^{(5)} - \mathbf{y}_{n+1}^{(4)} = h \sum_{i=1}^{s} (b_i^{(5)} - b_i^{(4)}) \mathbf{k}_i$$
(18)

This error estimate guides adaptive step size selection without additional function evaluations.

1.0.7 Multi-Step Methods

Multi-step methods use information from several previous points to achieve higher accuracy or better stability properties. These methods can be more efficient than single-step methods for smooth problems but require special starting procedures.

1.0.8 Adams Methods

Adams methods are based on polynomial interpolation of the derivative. The Adams-Bashforth methods are explicit:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{j=0}^{k-1} \beta_j \mathbf{f}_{n-j}$$

$$\tag{19}$$

where $\mathbf{f}_{n-j} = \mathbf{f}(t_{n-j}, \mathbf{y}_{n-j})$ and the coefficients β_j are determined by the interpolation conditions. The Adams-Moulton methods are implicit:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{j=-1}^{k-1} \beta_j^* \mathbf{f}_{n+1-j}$$
 (20)

Predictor-Corrector Schemes: Combining Adams-Bashforth (predictor) and Adams-Moulton (corrector) methods provides the efficiency of explicit methods with the stability of implicit methods:

$$\mathbf{y}_{n+1}^{(0)} = \mathbf{y}_n + h \sum_{j=0}^{k-1} \beta_j \mathbf{f}_{n-j} \quad \text{(predict)}$$
(21)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \left[\beta_{-1}^* \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}^{(0)}) + \sum_{j=0}^{k-1} \beta_j^* \mathbf{f}_{n-j} \right]$$
 (correct) (22)

1.0.9 Backward Differentiation Formulas (BDF)

BDF methods are particularly effective for stiff problems. They approximate the derivative using backward differences:

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+1-j} = h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1})$$
(23)

The coefficients α_j are chosen so that the method has maximum order for the given number of steps. BDF methods up to order 6 are stable, making them suitable for stiff problems where stability is more important than high-order accuracy.

1.0.10 Stiff Differential Equations

Stiff equations are characterized by the presence of multiple time scales, with some components evolving much faster than others. These problems pose significant challenges for explicit methods, which require impractically small step sizes to maintain stability.

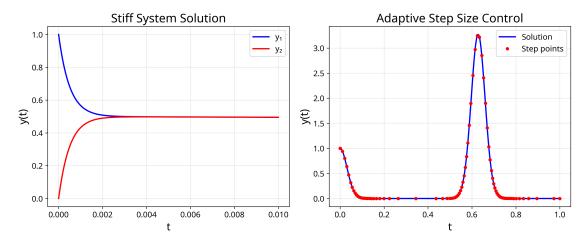


Figure 2: Advanced numerical techniques: (left) stiff system solution showing multiple time scales, (right) adaptive step size control demonstrating automatic error management.

1.0.11 Characterization of Stiffness

A system is stiff if the eigenvalues of the Jacobian matrix $\frac{\partial \mathbf{f}}{\partial \mathbf{y}}$ have widely separated magnitudes. The stiffness ratio is defined as:

$$S = \frac{\max_{i} |\operatorname{Re}(\lambda_{i})|}{\min_{i} |\operatorname{Re}(\lambda_{i})|}$$
(24)

where λ_i are the eigenvalues. Large stiffness ratios $(S \gg 1)$ indicate stiff problems.

Physical Origins of Stiffness: Stiffness commonly arises in: - Chemical kinetics with fast and slow reactions - Electrical circuits with different RC time constants - Structural dynamics with high-frequency vibrations - Fluid dynamics with boundary layers - Control systems with fast actuator dynamics

Example. The Van der Pol equation with large μ :

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + x = 0 {25}$$

For $\mu \gg 1$, the system exhibits relaxation oscillations with fast transitions and slow evolution phases. Explicit methods require step sizes $h \sim 1/\mu$ for stability, making integration extremely expensive.

Converting to first-order form and analyzing the Jacobian reveals eigenvalues of order μ , confirming the stiff nature of the problem.

1.0.12 Implicit Methods for Stiff Problems

Implicit methods are essential for stiff problems because their stability regions include large portions of the left half-plane. The backward Euler method, despite its low order, is often preferred for highly stiff problems due to its excellent stability properties.

A-Stability: A method is A-stable if its stability region includes the entire left half-plane $\{\lambda : \text{Re}(\lambda) < 0\}$. This ensures stability for any step size when applied to the test equation $y' = \lambda y$ with $\text{Re}(\lambda) < 0$.

L-Stability: A stronger condition requiring that the amplification factor approaches zero as $|\lambda h| \to \infty$. L-stable methods effectively damp high-frequency components.

Solving Nonlinear Systems: Implicit methods require solving nonlinear systems at each step. Newton's method is typically used:

$$\mathbf{G}(\mathbf{y}_{n+1}) = \mathbf{y}_{n+1} - \mathbf{y}_n - h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) = \mathbf{0}$$
(26)

The Newton iteration is:

$$\mathbf{y}_{n+1}^{(k+1)} = \mathbf{y}_{n+1}^{(k)} - \left[\mathbf{I} - h\frac{\partial \mathbf{f}}{\partial \mathbf{v}}\right]^{-1} \mathbf{G}(\mathbf{y}_{n+1}^{(k)})$$
(27)

1.0.13 Adaptive Step Size Control

Adaptive methods automatically adjust the step size to maintain a specified accuracy while minimizing computational cost. This is essential for problems with varying solution smoothness or when high accuracy is required over long integration intervals.

1.0.14 Error Estimation and Control

Most adaptive methods use embedded formulas to estimate the local truncation error. Given error tolerance tol, the step size is adjusted according to:

$$h_{\text{new}} = h_{\text{old}} \left(\frac{\text{tol}}{|\mathbf{e}|}\right)^{1/(p+1)} \cdot \text{safety factor}$$
 (28)

where p is the order of the lower-order method and the safety factor (typically 0.8-0.9) provides a margin for error.

Error Norms: For vector problems, appropriate error norms must be chosen. Common choices include: - Maximum norm: $|\mathbf{e}|_{\infty} = \max_i |e_i|$ - Weighted RMS norm: $|\mathbf{e}|_{\text{RMS}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (e_i/w_i)^2}$ where weights w_i account for the different scales of solution components.

1.0.15 Step Size Selection Strategies

Effective step size control requires balancing several competing objectives:

Accuracy Control: Maintain local error below specified tolerance Efficiency: Use the largest possible step size consistent with accuracy requirements Stability: Avoid step sizes that lead to numerical instability Smoothness: Prevent excessive step size variations that can degrade accuracy

Advanced controllers use PI (proportional-integral) or PID (proportional-integral-derivative) control theory to achieve smooth, efficient step size adaptation.

1.0.16 Geometric Integration

Traditional numerical methods focus on achieving high-order accuracy but may not preserve important geometric properties of the continuous system. Geometric integrators are designed to preserve specific structural properties such as energy, momentum, or symplectic structure.

1.0.17 Symplectic Integration

Hamiltonian systems have a special geometric structure that should be preserved during numerical integration. Symplectic integrators maintain the symplectic structure, ensuring long-term stability and energy conservation properties.

For separable Hamiltonian systems H(p,q) = T(p) + V(q), the Störmer-Verlet method is a simple symplectic integrator:

$$p_{n+1/2} = p_n - \frac{h}{2}V'(q_n) \tag{29}$$

$$q_{n+1} = q_n + hT'(p_{n+1/2}) (30)$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2}V'(q_{n+1})$$
(31)

This method exactly preserves the symplectic structure and exhibits excellent long-term energy behavior.

1.0.18 Energy-Preserving Methods

For conservative systems, preserving energy exactly can be more important than achieving highorder accuracy. Energy-preserving methods are designed to satisfy discrete energy conservation laws.

The discrete gradient method for systems $\frac{d\mathbf{y}}{dt} = \nabla H(\mathbf{y})$ uses:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\bar{\nabla}H(\mathbf{y}_n, \mathbf{y}_{n+1}) \tag{32}$$

where ∇H is a discrete gradient satisfying:

$$(\mathbf{y}_{n+1} - \mathbf{y}_n) \cdot \bar{\nabla} H(\mathbf{y}_n, \mathbf{y}_{n+1}) = H(\mathbf{y}_{n+1}) - H(\mathbf{y}_n)$$
(33)

This ensures exact energy conservation: $H(\mathbf{y}_{n+1}) = H(\mathbf{y}_n)$.

1.0.19 Boundary Value Problems

Many applications require solving boundary value problems (BVPs) where conditions are specified at multiple points. Unlike initial value problems, BVPs generally require global methods that satisfy all boundary conditions simultaneously.

1.0.20 Shooting Methods

Shooting methods convert BVPs to sequences of initial value problems. For the two-point BVP:

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad t \in [a, b] \tag{34}$$

$$\mathbf{g}(\mathbf{y}(a), \mathbf{y}(b)) = \mathbf{0} \tag{35}$$

The shooting method guesses initial conditions $\mathbf{y}(a) = \mathbf{s}$ and integrates to t = b. The parameter \mathbf{s} is adjusted using Newton's method to satisfy the boundary conditions.

Multiple Shooting: For better numerical stability, the interval can be divided into subintervals with continuity conditions enforced at the interfaces. This reduces sensitivity to initial condition errors and improves convergence for difficult problems.

1.0.21 Finite Difference Methods

Finite difference methods discretize the differential equation directly on a grid. For the BVP y'' = f(t, y, y') with $y(a) = \alpha$, $y(b) = \beta$, the second derivative is approximated by:

$$y''(t_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \tag{36}$$

This leads to a system of nonlinear algebraic equations that can be solved using Newton's method or other root-finding techniques.

1.0.22 Partial Differential Equations: Method of Lines

Many PDEs can be solved by discretizing in space to obtain a system of ODEs, which is then integrated using standard ODE methods. This approach, called the method of lines, leverages the sophisticated ODE solvers developed for temporal integration.

1.0.23 Spatial Discretization

Consider the heat equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{37}$$

Discretizing in space using finite differences:

$$\frac{du_i}{dt} = \alpha \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$
 (38)

This produces a system of ODEs that can be integrated using any suitable method. The choice of spatial discretization (finite differences, finite elements, spectral methods) depends on the problem geometry and accuracy requirements.

1.0.24 Stability Considerations

The method of lines can produce stiff ODE systems, especially for parabolic PDEs with fine spatial grids. The stiffness arises from the high-frequency spatial modes, which have large eigenvalues proportional to $1/(\Delta x)^2$.

Implicit time integration is often necessary for stability, leading to the need to solve large linear systems at each time step. Efficient linear algebra techniques and preconditioning become crucial for computational performance.

1.0.25 Software and Implementation

Modern scientific computing relies heavily on robust, efficient ODE solver libraries. Understanding the capabilities and limitations of these tools is essential for effective problem solving.

1.0.26 Popular ODE Solver Libraries

MATLAB: The ode45, ode15s, and related functions provide high-quality adaptive Runge-Kutta and BDF methods with automatic stiffness detection and method switching.

Python: The scipy.integrate module includes solve_ivp with multiple method options, event detection, and dense output capabilities.

Fortran/C: Libraries like ODEPACK, SUNDIALS, and CVODE provide highly optimized implementations for production computing environments.

Julia: The Differential Equations. jl ecosystem offers a unified interface to numerous solvers with excellent performance and extensive method selection.

1.0.27 Method Selection Guidelines

Choosing appropriate methods requires understanding problem characteristics:

Non-stiff problems: Explicit Runge-Kutta methods (RK45, Dormand-Prince) provide excellent accuracy and efficiency.

Stiff problems: BDF methods or implicit Runge-Kutta methods are essential for stability.

Conservative systems: Symplectic or energy-preserving methods maintain physical properties over long integrations.

Oscillatory problems: Specialized methods that account for the oscillatory nature can be more efficient than general-purpose solvers.

Computational Note: The file lecture?.py provides comprehensive implementations of the numerical methods discussed in this lecture. The code includes basic methods (Euler, RK4), adaptive algorithms (RKF45), stiff solvers (backward Euler with Newton iteration), and geometric integrators (Störmer-Verlet). Error analysis, stability region plotting, and performance comparisons demonstrate the practical aspects of method selection and implementation.

1.0.28 Error Analysis and Convergence Theory

Understanding the theoretical foundations of numerical methods is crucial for reliable implementation and effective problem solving. Convergence theory provides the mathematical framework for analyzing method performance and predicting behavior as step sizes decrease.

1.0.29 Consistency, Stability, and Convergence

The fundamental theorem of numerical analysis for ODEs establishes the relationship between these three concepts:

Consistency: A method is consistent if the local truncation error approaches zero as the step size decreases. Formally, the method $\mathbf{y}_{n+1} = \mathbf{y}_n + h\Phi(t_n, \mathbf{y}_n, h)$ is consistent if:

$$\lim_{h \to 0} \frac{1}{h} [\mathbf{y}(t_n + h) - \mathbf{y}(t_n) - h\Phi(t_n, \mathbf{y}(t_n), h)] = \mathbf{0}$$
(39)

Stability: A method is stable if small perturbations in the initial data or intermediate calculations do not grow unboundedly. For linear problems, this can be analyzed using the amplification factor.

Convergence: A method converges if the global error approaches zero as the step size decreases: $\lim_{h\to 0} \max_n |\mathbf{y}_n - \mathbf{y}(t_n)| = 0.$

Theorem 1.1. For a consistent numerical method applied to a well-posed linear initial value problem, stability is necessary and sufficient for convergence.

This theorem provides the theoretical foundation for numerical method analysis and guides the development of new algorithms.

1.0.30 Order of Accuracy and Error Bounds

The order of accuracy determines how rapidly the error decreases as the step size is reduced. For a method of order p, the global error satisfies:

$$|\mathbf{y}_n - \mathbf{y}(t_n)| \le Ch^p \tag{40}$$

for some constant C independent of h (but depending on the problem and integration interval). Higher-order methods provide better accuracy for smooth problems but may not be advantageous for problems with limited smoothness or when high precision is not required.

1.0.31 Advanced Topics and Current Research

The field of numerical methods for differential equations continues to evolve, driven by new applications and computational architectures. Several areas represent active research frontiers with significant practical impact.

1.0.32 Exponential Integrators

For problems with linear stiff components, exponential integrators can provide excellent efficiency by treating the linear part exactly. These methods have the form:

$$\mathbf{y}_{n+1} = e^{h\mathbf{A}}\mathbf{y}_n + h\varphi_1(h\mathbf{A})\mathbf{N}(\mathbf{y}_n)$$
(41)

where **A** is the linear part and **N** represents nonlinear terms. The function $\varphi_1(z) = (e^z - 1)/z$ and its generalizations can be computed efficiently using Krylov subspace methods.

1.0.33 Structure-Preserving Methods

Beyond symplectic integration, researchers have developed methods that preserve other important structures:

Lie Group Methods: For problems evolving on manifolds, methods that respect the geometric structure can provide superior long-term behavior.

Discrete Variational Methods: Based on discrete versions of variational principles, these methods automatically preserve conservation laws and symplectic structure.

Energy-Momentum Methods: For mechanical systems, methods that preserve both energy and momentum provide excellent long-term stability.

1.0.34 Parallel and High-Performance Computing

Modern computational demands require methods that can exploit parallel architectures:

Parallel-in-Time Methods: Techniques like parareal and PFASST enable temporal parallelization by solving multiple time intervals simultaneously.

GPU Acceleration: Explicit methods with high arithmetic intensity can achieve significant speedups on graphics processing units.

Adaptive Mesh Refinement: For PDE applications, dynamic grid adaptation can focus computational effort where needed most.

This lecture has provided a comprehensive overview of numerical methods for differential equations, covering both fundamental algorithms and advanced techniques. The key insights include:

Method Selection: The choice of numerical method depends critically on problem characteristics such as stiffness, required accuracy, conservation properties, and computational constraints. No single method is optimal for all problems.

Adaptive Control: Modern solvers automatically adjust step sizes and even switch methods to maintain accuracy while minimizing computational cost. Understanding these adaptive mechanisms is crucial for effective use of numerical software.

Stability and Accuracy: The interplay between stability and accuracy determines method performance. Stiff problems require implicit methods despite their higher computational cost per step.

Geometric Structure: For problems with special structure (Hamiltonian, conservative, etc.), specialized methods that preserve these properties often provide superior long-term behavior compared to general-purpose methods.

Implementation Considerations: Practical implementation involves many details beyond the basic algorithm: error control, linear algebra, event detection, and output management all affect overall performance and reliability.

The numerical solution of differential equations remains an active area of research, with new methods and applications continually emerging. The principles and techniques covered in this lecture provide the foundation for understanding both current methods and future developments in this essential area of scientific computing.

The next lecture will explore applications of these numerical methods to real-world problems in science and engineering, demonstrating how the theoretical concepts translate to practical problem solving.