



2.29 Numerical Fluid Mechanics Fall 2011 – Lecture 12

REVIEW Lecture 11:

- **End of (Linear) Algebraic Systems**
 - Gradient Methods
 - Krylov Subspace Methods
 - Preconditioning of $\mathbf{Ax}=\mathbf{b}$
- **FINITE DIFFERENCES**
 - Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations
 - Parabolic PDEs
 - Elliptic PDEs
 - Hyperbolic PDEs



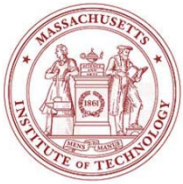
FINITE DIFFERENCES - Outline

- Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations
 - Parabolic PDEs, Elliptic PDEs and Hyperbolic PDEs
- Error Types and Discretization Properties
 - Consistency, Truncation error, Error equation, Stability, Convergence
- Finite Differences based on Taylor Series Expansions
 - Higher Order Accuracy Differences, with Example
 - Taylor Tables or Method of Undetermined Coefficients
- Polynomial approximations
 - Newton's formulas
 - Lagrange polynomial and un-equally spaced differences
 - Hermite Polynomials and Compact/Pade's Difference schemes
 - Equally spaced differences
 - Richardson extrapolation (or uniformly reduced spacing)
 - Iterative improvements using Romberg's algorithm



References and Reading Assignments

- Part 8 (PT 8.1-2), Chapter 23 on “Numerical Differentiation” and Chapter 18 on “Interpolation” of “Chapra and Canale, Numerical Methods for Engineers, 2010/2006.”
- Chapter 3 on “Finite Difference Methods” of “J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002”
- Chapter 3 on “Finite Difference Approximations” of “H. Lomax, T. H. Pulliam, D.W. Zingg, *Fundamentals of Computational Fluid Dynamics (Scientific Computation)*. Springer, 2003”



Classification of Partial Differential Equations

(2D case, 2nd order)

Quasi-linear PDE for $\phi(x, y)$

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F(x, y, \phi, \phi_x, \phi_y)$$

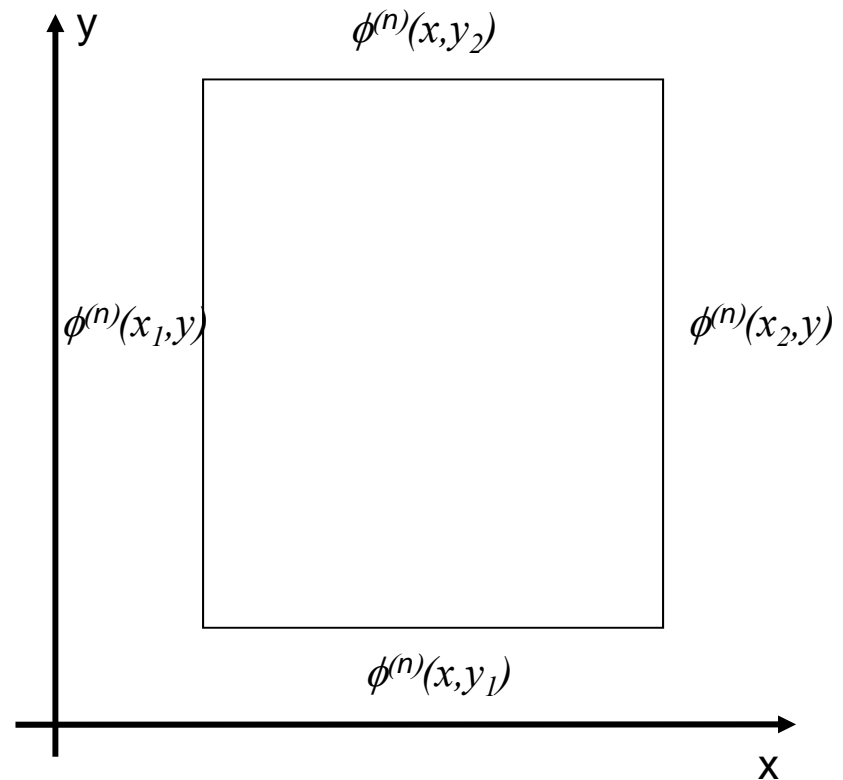
A, B and C Constants

$$B^2 - 4AC > 0 \quad \text{Hyperbolic}$$

$$B^2 - 4AC = 0 \quad \text{Parabolic}$$

$$B^2 - 4AC < 0 \quad \text{Elliptic}$$

(Only valid for two independent variables: x, y)



- In general: A, B and C are function of: $x, y, \phi, \phi_x, \phi_y$
- Equations may change of type from point to point if A, B and C vary with x, y, \dots etc
- Navier-Stokes, incomp., const. viscosity:
$$\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$



Partial Differential Equations

ELLIPTIC: $B^2 - 4AC < 0$

Quasi-linear PDE for $\phi(x, y)$

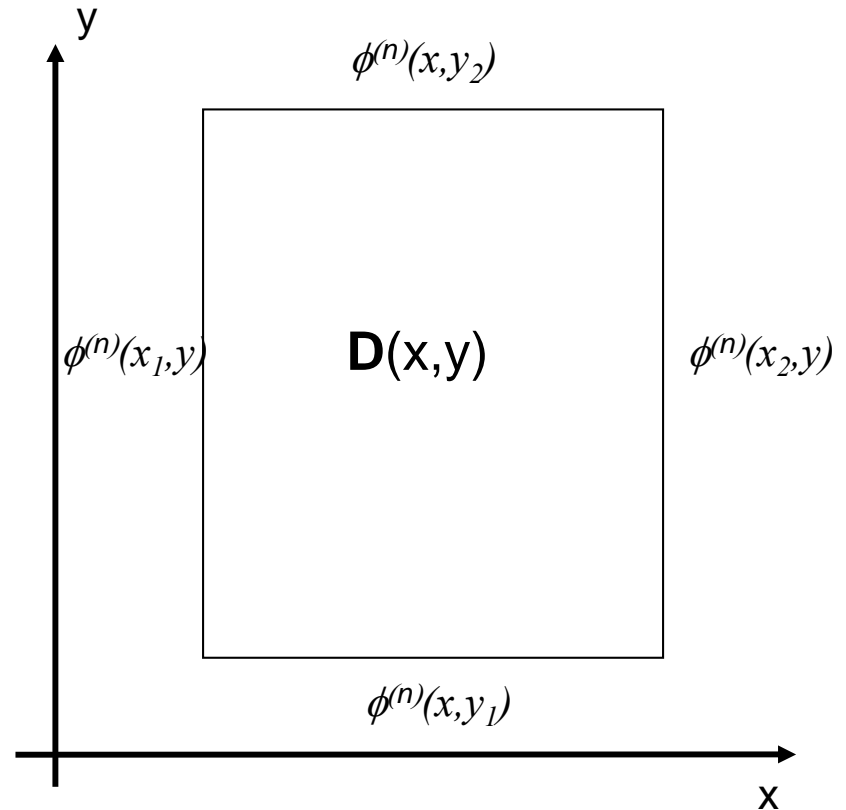
$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F(x, y, \phi, \phi_x, \phi_y)$$

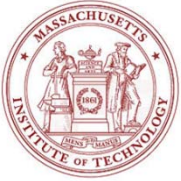
A, B and C Constants

$$B^2 - 4AC > 0 \quad \text{Hyperbolic}$$

$$B^2 - 4AC = 0 \quad \text{Parabolic}$$

$$B^2 - 4AC < 0 \quad \text{Elliptic}$$





Partial Differential Equations

Elliptic PDE

Laplace Operator

$$\nabla^2 \equiv u_{xx} + u_{yy}$$

Examples:

$$\nabla^2 u = 0$$

Laplace Equation – Potential Flow

$$\nabla^2 u = g(x, y)$$

Poisson Equation

- Potential Flow with sources
- Heat flow in plate

$$\nabla^2 u + f(x, y)u = 0$$

Helmholtz equation – Vibration of plates

$$\mathbf{U} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u}$$

Convection-Diffusion

- Smooth solutions (“diffusion effect”)
- Very often, steady state problems
- Domain of dependence of u is the full domain $\mathbf{D}(x,y) \Rightarrow$ “global” solutions
- Finite differ./volumes/elements, boundary integral methods (Panel methods)



Partial Differential Equations

Elliptic PDEs

$$0 \leq x \leq a, \quad 0 \leq y \leq b;$$

Equidistant Sampling

$$h = a/(n - 1)$$

$$h = b/(m - 1)$$

Discretization

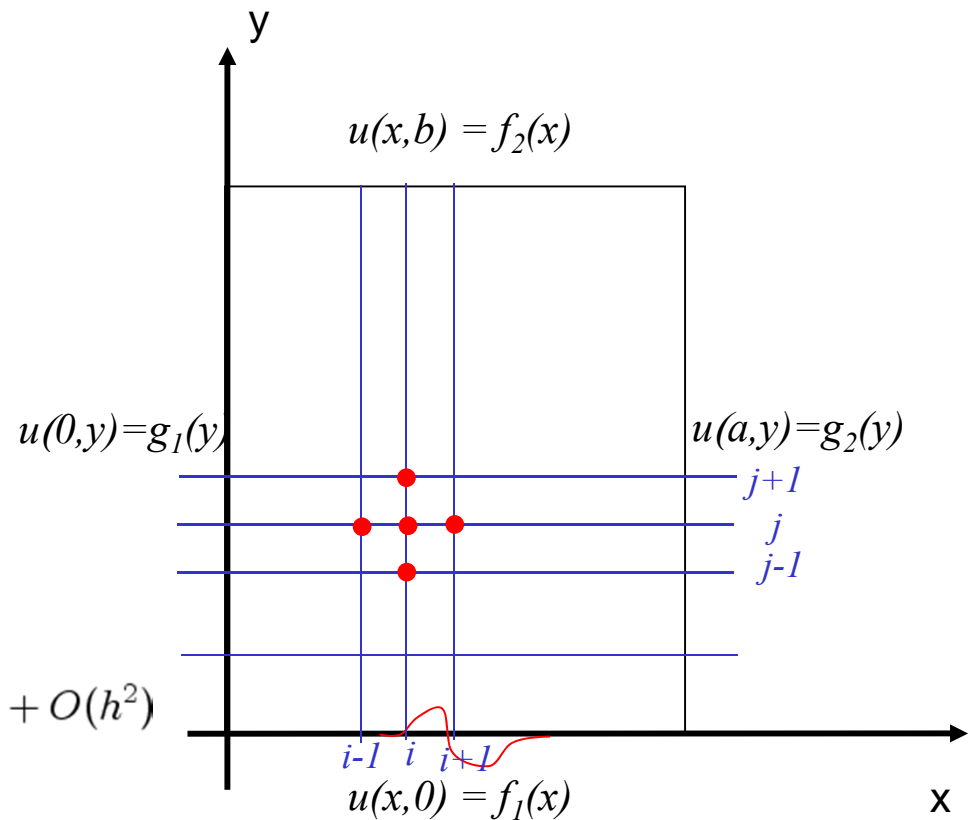
$$x_i = (i - 1)h, \quad i = 1, \dots, n$$

$$y_j = (j - 1)h, \quad j = 1, \dots, m$$

Finite Differences

$$u_{xx}(x, t) = \frac{u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j)}{h^2} + O(h^2)$$

$$u_{yy}(x, t) = \frac{u(x_i, y_{j-1}) - 2u(x_i, y_j) + u(x_i, y_{j+1}))}{h^2} + O(h^2)$$





Partial Differential Equations

Elliptic PDE

Discretized Laplace Equation

$$\nabla^2 u = \frac{u(x_{i-1}, y_j) + u(x_i, y_{j-1}) - 4u(x_i, y_j) + u(x_{i+1}, y_j) + u(x_i, y_{j+1}))}{h^2} = 0$$

$$u_{i,j} = u(x_i, y_j)$$

Finite Difference Scheme

$$u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = 0$$

Boundary Conditions

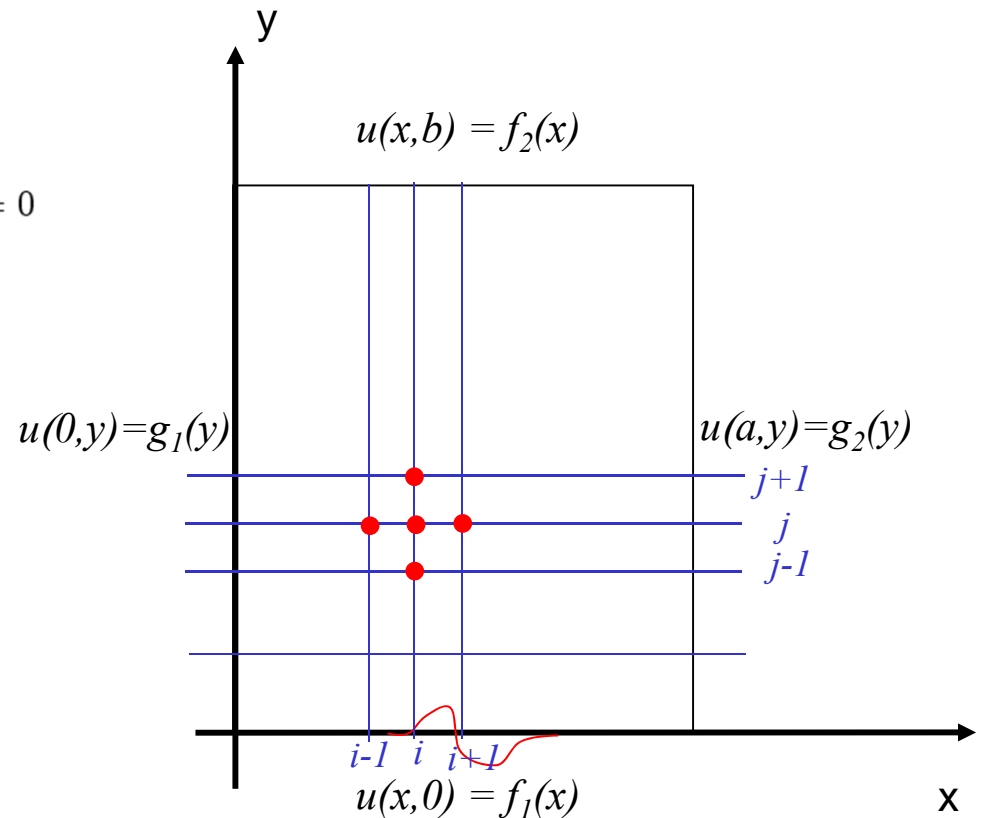
$$u(x_1, y_j) = u_{1,j}, \quad 2 \leq j \leq m-1$$

$$u(x_n, y_j) = u_{n,j}, \quad 2 \leq j \leq m-1$$

$$u(x_i, y_1) = u_{i,1}, \quad 2 \leq i \leq n-1$$

$$u(x_i, y_n) = u_{i,n}, \quad 2 \leq i \leq n-1$$

Global Solution Required





Elliptic PDE: Poisson Equation

$$\nabla^2 u = g(x, y)$$

$$g_{i,j} = g(x_i, y_j)$$

SOR Iterative Scheme, with Jacobi

$$\begin{aligned} u_{i,j}^{k+1} &= u_{i,j}^k + \omega r_{i,j}^k \\ &= u_{i,j}^k + \omega \frac{u_{n+1,j}^k + u_{n-1,j}^k + u_{n,j+1}^k + u_{n,j-1}^k - 4u_{n,j}^k - h^2 g_{i,j}}{4} \\ &= (1 - \omega)u_{i,j}^k + \omega \frac{u_{n+1,j}^k + u_{n-1,j}^k + u_{n,j+1}^k + u_{n,j-1}^k - h^2 g_{i,j}}{4} \end{aligned}$$



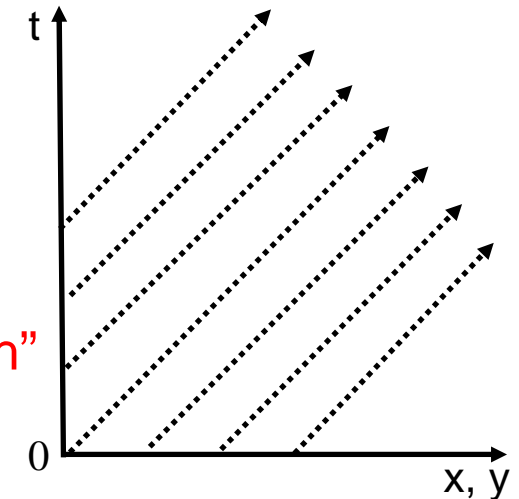
Partial Differential Equations

Hyperbolic PDE: $B^2 - 4AC > 0$

Examples:

- (1) $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$ ← Wave equation, 2nd order
- (2) $\frac{\partial u}{\partial t} \pm c \frac{\partial u}{\partial x} = 0$ ← Sommerfeld Wave/radiation equation, 1st order
- (3) $\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{u} = \mathbf{g}$ ← Unsteady (linearized) inviscid convection (Wave equation first order)
- (4) $(\mathbf{U} \cdot \nabla) \mathbf{u} = \mathbf{g}$ ← Steady (linearized) inviscid convection

- Allows non-smooth solutions
- Information travels along characteristics, e.g.:
 - For (3) above: $\frac{d \mathbf{x}_c}{dt} = \mathbf{U}(\mathbf{x}_c(t))$
 - For (4), along streamlines: $\frac{d \mathbf{x}_c}{ds} = \mathbf{U}$
- Domain of dependence of $\mathbf{u}(\mathbf{x}, T) =$ “characteristic path”
 - e.g., for (3), it is: $\mathbf{x}_c(t)$ for $0 < t < T$
- Finite Differences, Finite Volumes and Finite Elements





Partial Differential Equations

Hyperbolic PDE

Waves on a String

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \quad 0 < x < L, \quad 0 < t < \infty$$

Initial Conditions

$$u(x,0) = f(x), \quad 0 \leq x \leq L$$

$$u_t(x,0) = g(x), \quad 0 < x < L$$

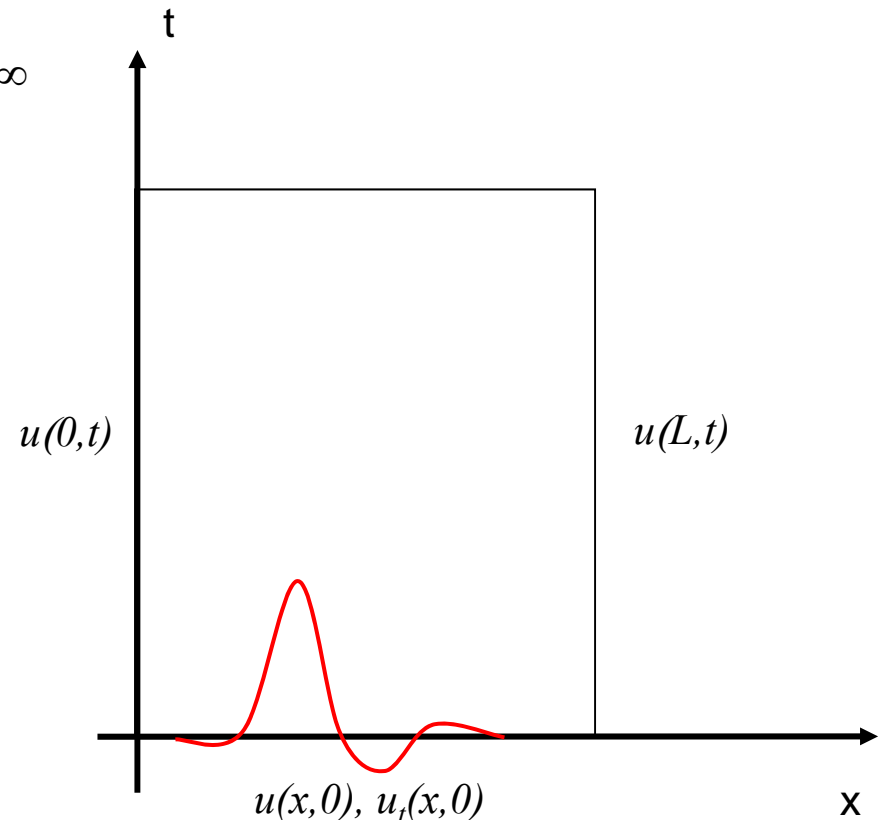
Boundary Conditions

$$u(0,t) = 0, \quad 0 < t < \infty$$

$$u(L,t) = 0, \quad 0 < t < \infty$$

Wave Solutions

$$u = \begin{cases} F(x - ct) & \text{Forward propagating wave} \\ G(x + ct) & \text{Backward propagating wave} \end{cases}$$



Typically Initial Value Problems in Time, Boundary Value Problems in Space
Time-Marching Solutions: Explicit Schemes Generally Stable



Partial Differential Equations

Hyperbolic PDE

Wave Equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \quad 0 < x < L, \quad 0 < t < \infty$$

Discretization:

$$h = L/n$$

$$k = T/m$$

$$x_i = (i-1)h, \quad i = 2, \dots, n-1$$

$$t_j = (j-1)k, \quad j = 1, \dots, m$$

Finite Difference Representations

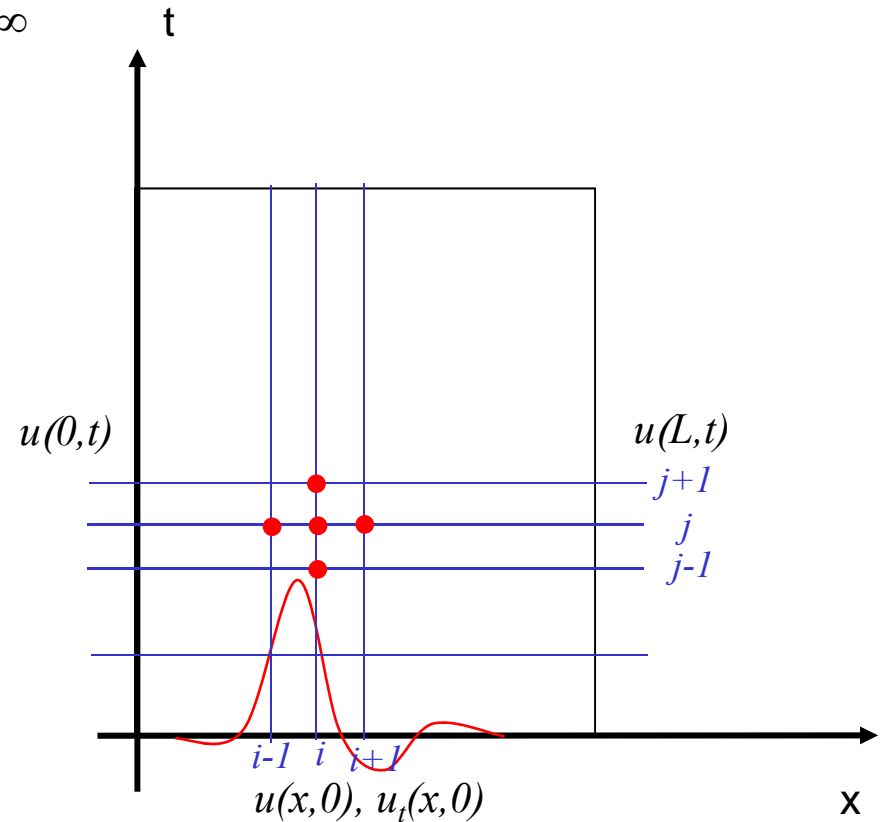
$$u_{tt}(x,t) = \frac{u(x_i, t_{j-1}) - 2u(x_i, t_j) + u(x_i, t_{j+1}))}{k^2} + O(k^2)$$

$$u_{xx}(x,t) = \frac{u(x_{i-1}, t_j) - 2u(x_i, t_j) + u(x_{i+1}, t_j))}{h^2} + O(h^2)$$

$$u_{i,j} = u(x_i, t_j)$$

Finite Difference Representations

$$\frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{k^2} = c^2 \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2}$$





Partial Differential Equations

Hyperbolic PDE

Introduce Dimensionless Wave Speed $C = \frac{ck}{h}$

Explicit Finite Difference Scheme

$$u_{i,j-1} - 2u_{i,j} + u_{i,j+1} = C^2(u_{i-1,j} - 2u_{i,j} + u_{i+1,j})$$

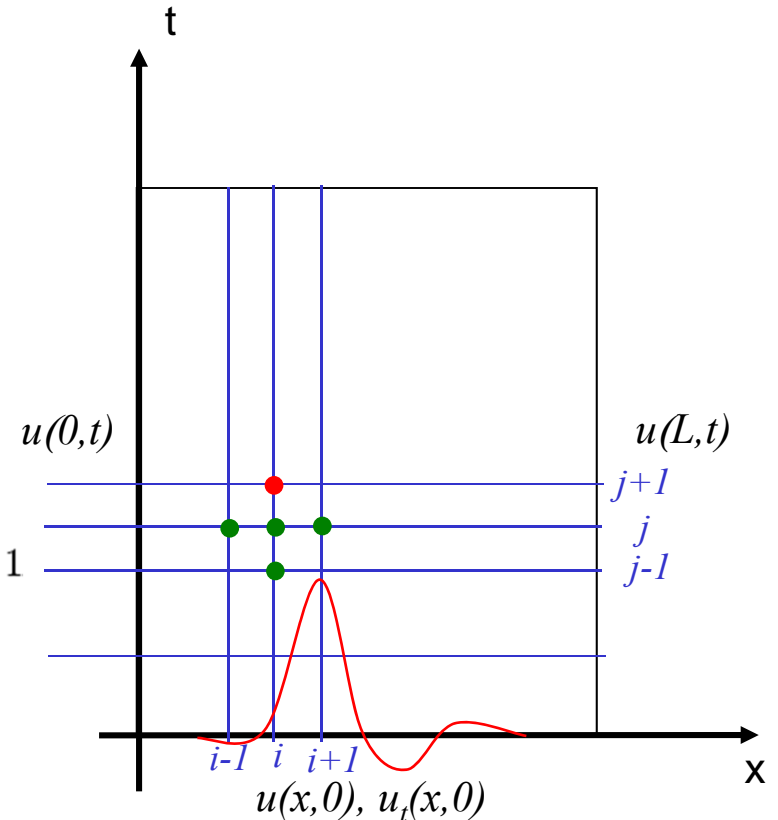
$$u_{i,j+1} = (2 - 2C^2)u_{i,j} + C^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1} \quad i = 2, \dots, n-1$$

Stability Requirement: $C = \frac{ck}{h} < 1$

$$C = \frac{c \Delta t}{\Delta x} < 1 \quad \text{Courant-Friedrichs-Lewy condition (CFL condition)}$$

Physical wave speed must be smaller than the largest numerical wave speed, or,
Time-step must be less than the time for the wave to travel to adjacent grid points:

$$c < \frac{\Delta x}{\Delta t} \quad \text{or} \quad \Delta t < \frac{\Delta x}{c}$$





Error Types and Discretization Properties: Consistency

Consider the differential equation (L symbolic operator)

$$L(\phi) = 0$$

and its discretization for any given difference scheme

$$L_{\Delta x}(\hat{\phi}) = 0$$

❖ **Consistency** (Property of the discretization)

- The discretization of a PDE should asymptote to the PDE itself as the mesh-size/time-step goes to zero, i.e

for all smooth functions ϕ :
$$\left| L(\phi) - L_{\Delta x}(\hat{\phi}) \right| \rightarrow 0 \quad \text{when } \Delta x \rightarrow 0$$

(the truncation error vanishes as mesh-size/time-step goes to zero)



Error Types and Discretization Properties: Truncation error and Error equation

❖ Truncation error

$$\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\phi)$$

Remember:

ϕ does not satisfy the FD eqn.

- Since $L(\phi) = 0$, the truncation error is the result of inserting the exact solution in the difference scheme
- If the FD scheme is consistent: $\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\phi) \rightarrow O(\Delta x^p)$ for $\Delta x \rightarrow 0$
- $p (> 0)$ is the order of accuracy for the FD scheme $\hat{L}_{\Delta x}$
- Order p indicates how fast the error is reduced when the grid is refined

❖ Error evolution equation

- From $\hat{L}_{\Delta x}(\hat{\phi}) = 0$ and $\phi = \hat{\phi} + \varepsilon$ where ε is the discretization error, for linear problems, we have:

$$\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\hat{\phi} + \varepsilon) = -\hat{L}_{\Delta x}(\varepsilon)$$

$$\Rightarrow \hat{L}_{\Delta x}(\varepsilon) = -\tau_{\Delta x}$$
- The truncation error acts as a source for the discretization error, which is convected and diffused by the operator $\hat{L}_{\Delta x}$



Error Types and Discretization Properties: Stability

❖ Stability

- A numerical solution scheme is said to be stable if it does not amplify errors that appear in the course of the numerical solution process
- For linear(-ized) problems, since $\hat{L}_{\Delta x}(\varepsilon) = -\tau_{\Delta x}$, stability implies:

$$\left\| \hat{L}_{\Delta x}^{-1} \right\| < \text{Const.} \quad \text{with the Const. not a function of } \Delta x$$

- If inverse was not bounded, discretization errors ε would increase with iterations
- In practice, infinite norm $\left\| \hat{L}_{\Delta x}^{-1} \right\|_{\infty} < \text{Const.}$ is often used.
- However, difficult to assess stability in real cases due to boundary conditions and non-linearities
 - It is common to investigate stability for linear problems, with constant coefficients and without boundary conditions
 - A widely used approach: von Neumann's method (see lectures 13-14)



Error Types and Discretization Properties: Convergence

❖ Convergence

– A numerical scheme is said to be convergent if the solution of the discretized equations tend to the exact solution of the (P)DE as the grid-spacing and time-step go to zero

– Error equation for linear(-ized) systems: $\varepsilon = -\hat{L}_{\Delta x}^{-1}(\tau_{\Delta x})$

– Error bounds for linear systems:

$$\|\varepsilon\| = \|\hat{L}_{\Delta x}^{-1}(\tau_{\Delta x})\| \leq \|\hat{L}_{\Delta x}^{-1}\| \|\tau_{\Delta x}\|$$

For a consistent scheme: $\|\tau_{\Delta x}\| \rightarrow O(\Delta x^p)$ for $\Delta x \rightarrow 0$

$$\text{Hence } \|\varepsilon\| \leq \|\hat{L}_{\Delta x}^{-1}\| \|\tau_{\Delta x}\| \leq \alpha O(\Delta x^p)$$

Convergence \Leftarrow Stability + Consistency (for linear systems)

= Lax Equivalence Theorem (for linear systems)

– For nonlinear equations, numerical experiments are often used

- e.g., iterate or approximate true solution with computation on successively finer grids, and compute resulting discretization errors and order of convergence



Finite Differences - Basics

- Finite Difference Approximation idea directly borrowed from the definition of a derivative.

$$\phi'(x_i) = \lim_{\Delta x \rightarrow 0} \frac{\phi(x_{i+1}) - \phi(x_i)}{\Delta x}$$

- Geometrical Interpretation

- Quality of approximation improves as stencil points get closer to x_i
- Central difference would be exact if ϕ was a second order polynomial and points were equally spaced

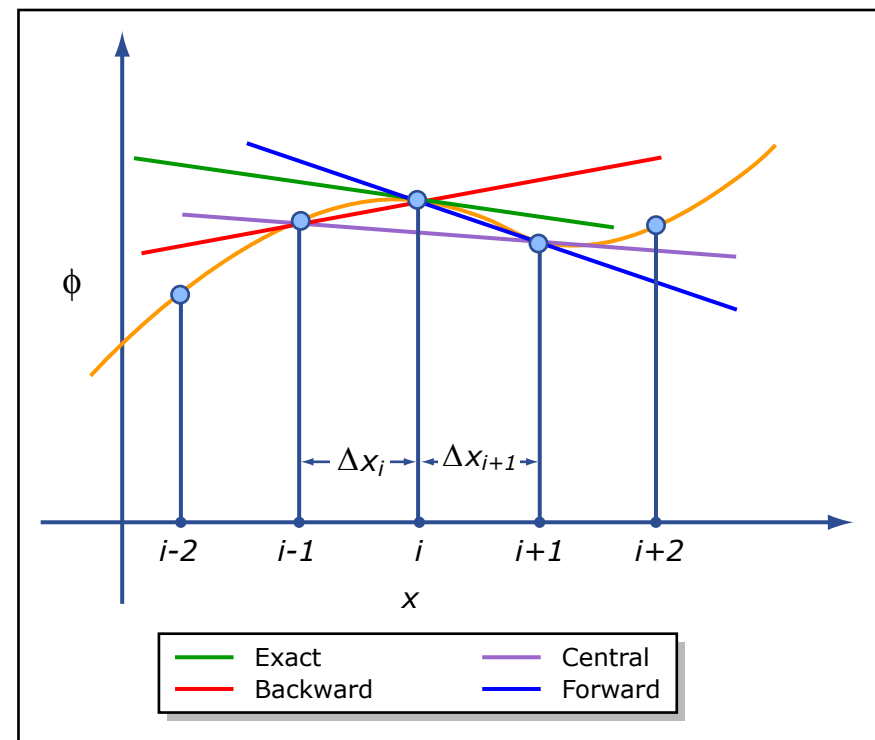


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FINITE DIFFERENCES: Taylor Series, Higher Order Accuracy

How to obtain differentiation formulas of arbitrary high accuracy?

1) First approach: Use Taylor series, introducing higher-order terms

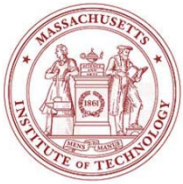
$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + \dots + \frac{\Delta x^n}{n!} f^n(x_i) + R_n$$

$$R_n = \frac{\Delta x^{n+1}}{n+1!} f^{(n+1)}(\xi)$$

- For example, how can we derive the forward finite-difference estimate of the first derivative at x_i with second order accuracy?

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + O(\Delta x^3) \left. \vphantom{f(x_{i+1})} \right\} \longrightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{\Delta x}{2!} \underline{f''(x_i)} + O(\Delta x^2)$$

- If we retain the second-derivative, and estimate it with first-order accuracy, the order of accuracy for the estimate of $f'(x_i)$ will be $p=2$



FINITE DIFFERENCES: Taylor Series, Higher Order Accuracy Cont'd

- Using $f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + \dots + \frac{\Delta x^n}{n!} f^n(x_i) + R_n$

$$R_n = \frac{\Delta x^{n+1}}{n+1!} f^{(n+1)}(\xi)$$

- Estimate the second-derivative with forward finite-differences at first-order accuracy:

$$\left. \begin{aligned} f(x_{i+1}) &= f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + O(\Delta x^3) \\ f(x_{i+2}) &= f(x_i) + 2\Delta x f'(x_i) + \frac{4\Delta x^2}{2!} f''(x_i) + O(\Delta x^3) \end{aligned} \right\} \begin{array}{l} * (-2) \\ * (1) \end{array} \Rightarrow f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{\Delta x^2} + O(\Delta x)$$

$$\rightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{\Delta x}{2!} f''(x_i) + O(\Delta x^2)$$

$$\Rightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{\Delta x}{2!} \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{\Delta x^2} + O(\Delta x^2) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2\Delta x} + O(\Delta x^2)$$



Forward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

Figure 23.1
Chapra and
Canale

Forward Differences

First Derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$$

Error

$O(h)$

$O(h^2)$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$$

$O(h)$

$O(h^2)$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$$

$O(h)$

$O(h^2)$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$$

$$f^{(4)}(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$$

$O(h)$

$O(h^2)$



Backward Differences

FIGURE 23.2

Backward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$$

Second Derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2}))}{h^2}$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3}))}{h^2}$$

Third Derivative

$$f'''(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3}))}{h^3}$$

$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4}))}{2h^3}$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4}))}{h^4}$$

$$f^{(4)}(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5}))}{h^4}$$

Error

$\mathcal{O}(h)$

$\mathcal{O}(h^2)$

$\mathcal{O}(h)$

$\mathcal{O}(h^2)$

$\mathcal{O}(h)$

$\mathcal{O}(h^2)$

$\mathcal{O}(h)$

$\mathcal{O}(h^2)$



FIGURE 23.3

Centered finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

Centered Differences

	<u>Error</u>
<u>First Derivative</u>	
$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h}$	$O(h^2)$
$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2}))}{12h}$	$O(h^4)$
<u>Second Derivative</u>	
$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{h^2}$	$O(h^2)$
$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2}))}{12h^2}$	$O(h^4)$
<u>Third Derivative</u>	
$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2}))}{2h^3}$	$O(h^2)$
$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3}))}{8h^3}$	$O(h^4)$
<u>Fourth Derivative</u>	
$f^{(4)}(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2}))}{h^4}$	$O(h^2)$
$f^{(4)}(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3}))}{6h^4}$	$O(h^4)$



FINITE DIFFERENCES

Taylor Series, Higher Order Accuracy: EXAMPLE

Problem: Estimate 1st derivative of $f = -0.1*x^4 - 0.15*x^3 - 0.5*x^2 - 0.25*x + 1.2$ at $x=0.5$, with a step size of 0.25 and using successively higher order schemes. How does the solution improve?

```
L11_FD.m
%Define the function
f=@(x) -0.1*x^4 - 0.15*x^3-0.5*x^2-0.25*x +1.2;
%Define Step size
h=0.25;
%Set point at which to evaluate the derivative
x = 0.5;
%% Using forward difference
%First order:
df=(f(x+h)-f(x)) / h;
fprintf('\n\n First order Forward difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
%Second order:
df=(-f(x+2*h)+4*f(x+h)-3*f(x)) / (2*h);
fprintf('Second order Forward difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
%% Backwards difference
%First order:
df=(-f(x-h)+f(x)) / (h);
fprintf('First order Backwards difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
%Second order:
df=(f(x-2*h)-4*f(x-h)+3*f(x)) / (2*h);
fprintf('Second order Backwards difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
```

```
%% Central difference
%Second order:
df=(f(x+h)-f(x-h)) / (2*h);
fprintf('Second order Central difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
%Fourth order:
df=(-f(x+2*h)+8*f(x+h)-8*f(x-h)+f(x-2*h)) /
(12*h);
fprintf('Fourth order Central difference: %g, with
error:%g%% \n',df,abs(100*(df+0.9125)/0.9125))
```

Output

```
First order Forward difference: -1.15469, with error:26.5411%
Second order Forward difference: -0.859375, with error:5.82192%
First order Backwards difference: -0.714063, with error:21.7466%
Second order Backwards difference: -0.878125, with error:3.76712%
Second order Central difference: -0.934375, with error:2.39726%
Fourth order Central difference: -0.9125, with error:2.43337e-014%
Why is the 4th order "exact"?
```




FINITE DIFFERENCES: Taylor Series, Higher Order Accuracy Summary

- Approach:
 - Incorporate more higher-order terms of the Taylor series expansion than strictly needed and express them as finite differences themselves
 - e.g. for finite difference of m^{th} derivative at order of accuracy p , express the $m+1^{\text{th}}$, $m+2^{\text{th}}$, $m+p-1^{\text{th}}$ derivatives at an order of accuracy $p-1, \dots, 2, 1$.
 - General approximation:
$$\left(\frac{\partial^m u}{\partial x^m} \right)_j - \sum_{i=-r}^s a_i u_{j+i} = \tau_{\Delta x}$$
 - Can be used for forward, backward, skewed or central differences
 - Can be computer automated
 - Independent of coordinate system and extends to multi-dimensional finite differences (each coordinate is usually treated separately)
- Remember: order p of approximation indicates how fast the error is reduced when the grid is refined (not the magnitude of the error)



FINITE DIFFERENCES: Interpolation Formulas for Higher Order Accuracy

2nd approach: Generalize Taylor series using interpolation formulas

- Fit the unknown function solution of the (P)DE to an interpolation curve and differentiate the resulting curve. For example:

- Fit a parabola to data at points x_{i-1}, x_i, x_{i+1} ($\Delta x_i = x_i - x_{i-1}$), then differentiate to obtain:

$$f'(x_i) = \frac{f(x_{i+1})(\Delta x_i)^2 - f(x_{i-1})(\Delta x_{i+1})^2 + f(x_i)[(\Delta x_{i+1})^2 - (\Delta x_i)^2]}{\Delta x_{i+1} \Delta x_i (\Delta x_i + \Delta x_{i+1})}$$

- This is a 2nd order approximation
- For uniform spacing, reduces to centered difference seen before
- In general, approximation of first derivative has truncation error of the order of the polynomial
- All types of polynomials or numerical differentiation methods can be used to derive such interpolations formulas
 - Polynomial fitting, Method of undetermined coefficients, Newton's interpolating polynomials, Lagrangian and Hermite Polynomials, etc

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