2.29 Numerical Fluid Mechanics
Spring 2015 – **Lecture 10**

REVIEW Lecture 9:

- End of (Linear) Algebraic Systems
  - Gradient Methods
  - Krylov Subspace Methods
  - Preconditioning of $\mathbf{Ax=b}$
- 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 Roomberg's algorithm

References and Reading Assignments

- Chapter 23 on “Numerical Differentiation” and Chapter 18 on “Interpolation” of “Chapra and Canale, Numerical Methods for Engineers, 2006/2010/2014.”
- 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”

Partial Differential Equations

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

Examples:

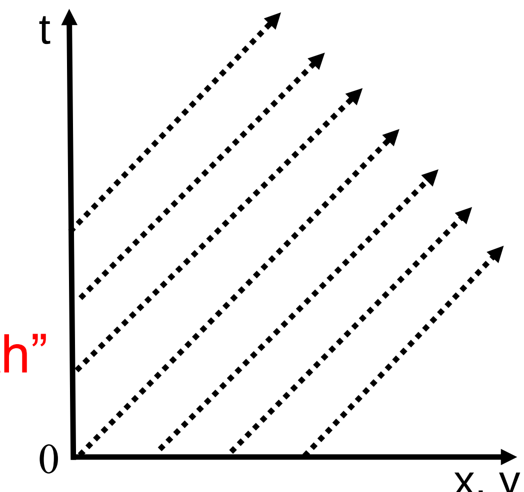
(1) $$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$ ← Wave equation, 2nd order

(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
  - Upwind schemes



Partial Differential Equations
Hyperbolic PDE - Example

Waves on a String

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

Initial Conditions

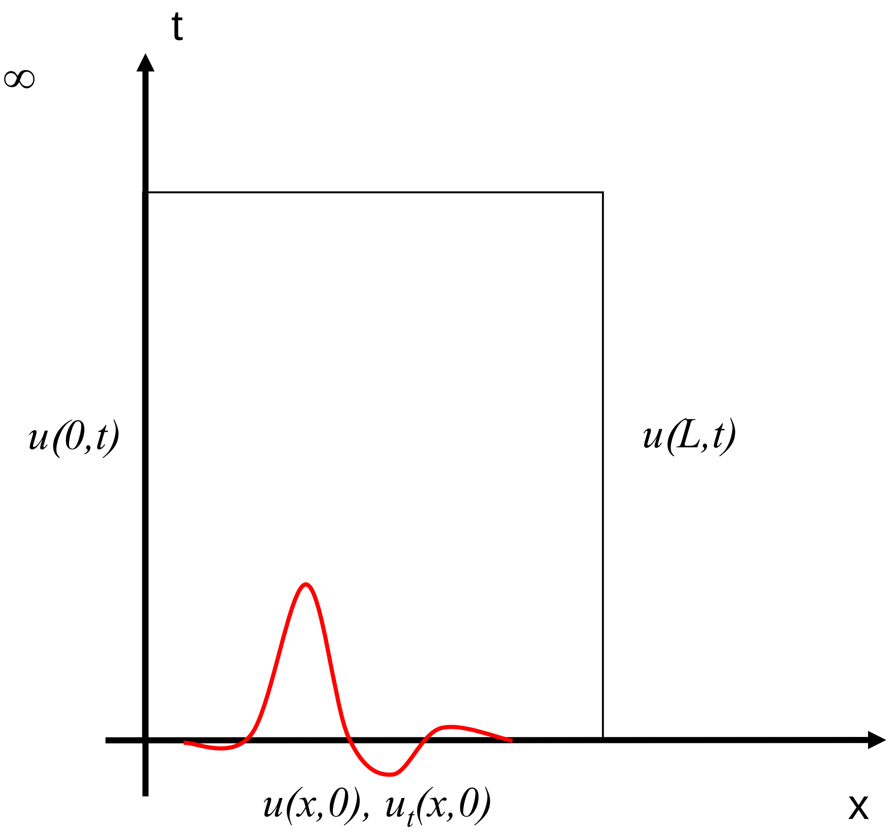
$$\begin{aligned} u(x,0) &= f(x), \;\; 0 \le x \le L \\ u_t(x,0) &= g(x), \;\; 0 < x < L \end{aligned}$$

Boundary Conditions

$$\begin{aligned} u(0,t) &= 0, \;, \; 0 < t < \infty \\ u(L,t) &= 0, \;, \; 0 < t < \infty \end{aligned}$$

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:

- Implicit schemes generally stable
- Explicit sometimes stable under certain conditions

Partial Differential Equations
Hyperbolic PDE - Example

Wave Equation

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

Discretization:

$$\begin{aligned} h &= L/n \\ k &= T/m \\ x_i &= (i-1)h, \; i = 2, \ldots, n-1 \\ t_j &= (j-1)k, \; j = 1, \ldots, m \end{aligned}$$

Finite Difference Representations (centered)

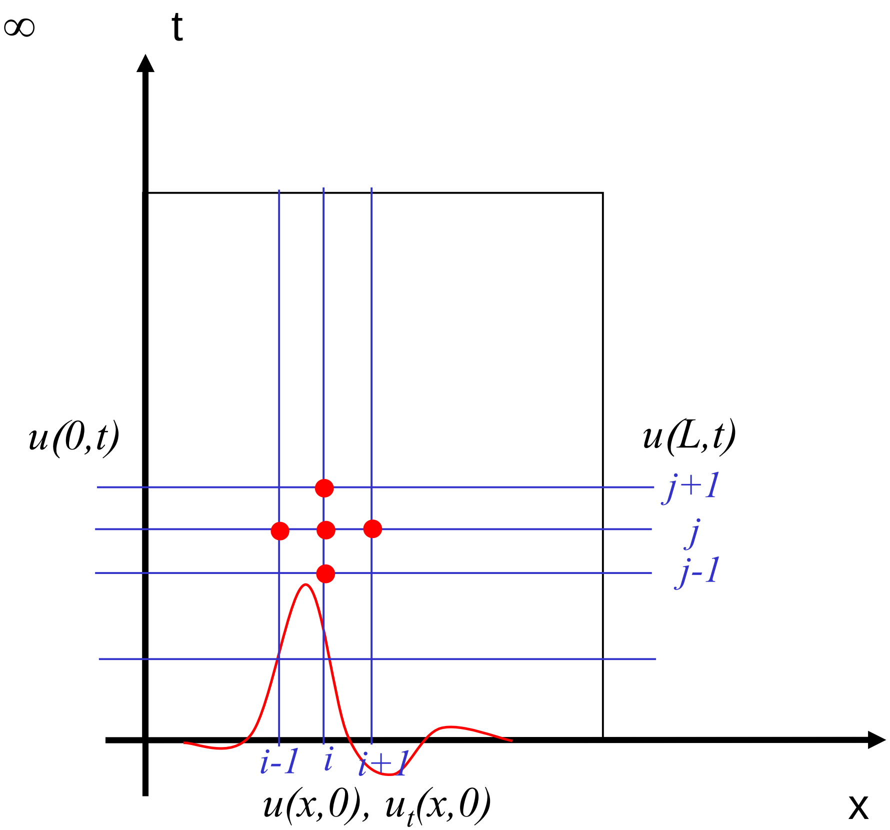
$$u_{tt}(x,t) = \frac{u(x_i,t_{j-1}) - 2u(x_i,t_j) + u(x_i,t_{j+1})}{k^2} + O(k^2)$$

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

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

Finite Difference Representations

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



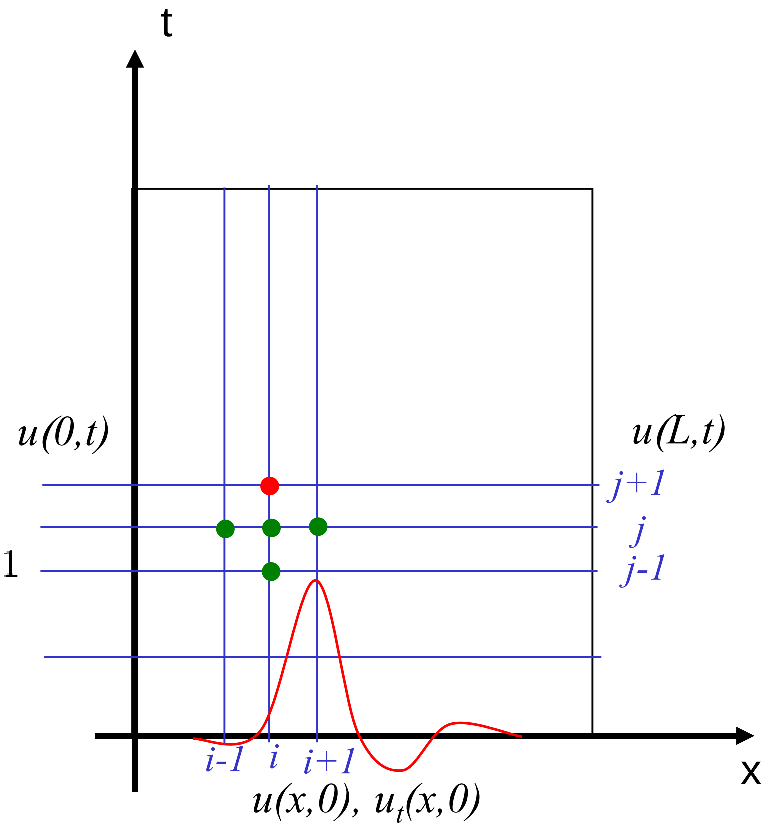
Partial Differential Equations
Hyperbolic PDE - Example

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

Explicit Finite Difference Scheme

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

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



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

$C = \frac{c\,\Delta t}{\Delta x} < 1$ 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 ($\mathcal{L}$ symbolic operator)

$$\mathcal{L}(\phi) = 0$$

and its discretization for any given difference scheme

$$\hat{\mathcal{L}}_{\Delta x}(\hat{\phi}) = 0$$

❖ **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: $\left| \mathcal{L}(\phi) - \hat{\mathcal{L}}_{\Delta x}(\phi) \right| \to 0 \quad \text{when } \Delta x \to 0$

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

Error Types and Discretization Properties: Truncation error and Error equation

❖ Truncation error

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

Remember:
ϕ does not satisfy the FD eqn.

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

❖ Error evolution equation

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

$$\Rightarrow \hat{\mathcal{L}}_{\Delta x}(\varepsilon) = -\tau_{\Delta x}$$

- The truncation error acts as a source for the discretization error, which is convected, diffused, evolved, etc., by the operator $\hat{\mathcal{L}}_{\Delta x}$

Error Types and Discretization Properties: Stability

❖ Stability

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

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

  - If inverse was not bounded, discretization errors ε would increase with iterations
- In practice, infinite norm $\left\| \hat{\mathcal{L}}_{\Delta x}^{-1} \right\|_{\infty} < \text{Const.}$ 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 12-13)

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

– Error bounds for linear systems:

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

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

Hence $\|\varepsilon\| \leq \left\|\hat{\mathcal{L}}_{\Delta x}^{-1}\right\| \; \|\tau_{\Delta x}\| \leq \alpha \, O(\Delta x^p)$

Convergence <= Stability + Consistency (for linear systems)

= Lax Equivalence Theorem (for linear systems)

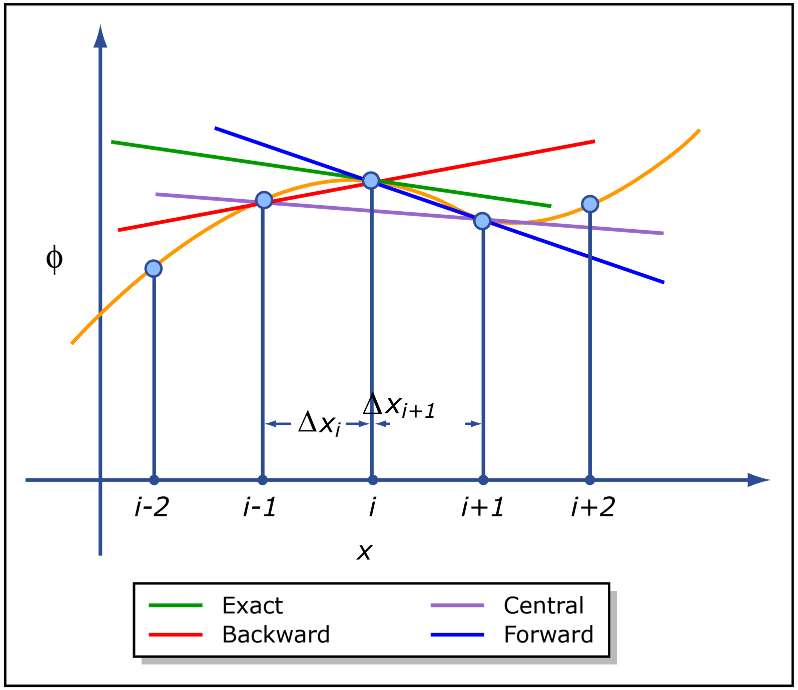
– For nonlinear equations, numerical experiments are often used
  - e.g., iterate or approximate true solution with computation on successively finer grids, and compute resulting discretization errors and order of convergence

Finite Differences - Basics

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

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

- 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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On the definition of a derivative and its approximations

FINITE DIFFERENCES: Taylor Series, Higher Order Accuracy

How to obtain differentiation formulas of arbitrary high accuracy?

1) First approach: Use Taylor series, keep more higher-order terms than strictly needed and express these higher-order terms as finite-differences themselves

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

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

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

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

- 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

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

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

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

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

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

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

Figure 23.1 Chapra and Canale

Forward Differences

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.

First Derivative	**Error**
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Backward Differences

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

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.

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

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

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 grid cell size of $h=0.25$ 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-14%

Why is the 4th order "exact"?

FINITE DIFFERENCES: Taylor Series, Higher Order Accuracy Summary

- 1st 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 $p-1, .., 2, 1$.
  - 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 often treated separately)
- Remember: order p of approximation indicates how fast the error is **reduced** when the grid is **refined (**not necessarily 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 "f data" at points x_{i-1}, x_i, x_{i+1} $\quad (\Delta x_i = x_i - x_{i-1})$, then differentiate to obtain:

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

  - This is a 2nd order approximation (parabola approx. is of order 3)
  - For uniform spacing, reduces to centered difference seen before
  - In general, approximation of first derivative has a truncation error of the order of the polynomial (here 2)
- 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

FINITE DIFFERENCES Higher Order Accuracy: Taylor Tables or Method of Undetermined Coefficients

Taylor Tables: Convenient way of forming linear combinations of Taylor Series on a term-by-term basis

Table 3.1. Taylor table for centered 3-point Lagrangian approximation to a second derivative

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j - \frac{1}{\Delta x^2}(a\,u_{j-1} + b\,u_j + c\,u_{j+1}) = ?$$

What we are looking for, in 1st column:

Taylor series at:

		u_j	$\Delta x \left(\frac{\partial u}{\partial x}\right)_j$	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_j$	$\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_j$	$\Delta x^4 \left(\frac{\partial^4 u}{\partial x^4}\right)_j$
	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_j$			1		
j-1	$-a \cdot u_{j-1}$	$-a$	$-a \cdot (\text{-}1) \cdot \frac{1}{1}$	$-a \cdot (\text{-}1)^2 \cdot \frac{1}{2}$	$-a \cdot (\text{-}1)^3 \cdot \frac{1}{6}$	$-a \cdot (\text{-}1)^4 \cdot \frac{1}{24}$
j	$-b \cdot u_j$	$-b$				
j+1	$-c \cdot u_{j+1}$	$-c$	$-c \cdot (1) \cdot \frac{1}{1}$	$-c \cdot (1)^2 \cdot \frac{1}{2}$	$-c \cdot (1)^3 \cdot \frac{1}{6}$	$-c \cdot (1)^4 \cdot \frac{1}{24}$

Sum each column starting from left, force the sums to zero and so choose a, b, c, etc

FINITE DIFFERENCES
Higher Order Accuracy: Taylor Tables Cont'd

Table 3.1. Taylor table for centered 3-point Lagrangian approximation to a second derivative

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j - \frac{1}{\Delta x^2}(a\,u_{j-1} + b\,u_j + c\,u_{j+1}) = ?$$

Sum each column starting from left and force the sums to be zero by proper choice of a, b, c, etc:

$$\begin{bmatrix} -1 & -1 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -2 \end{bmatrix} \Rightarrow \begin{bmatrix} a & b & c \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 \end{bmatrix}$$

= Familiar 3-point central difference

Truncation error is first column in the table that does not vanish, here fifth column of table:

$$\tau_{\Delta x} = \frac{1}{\Delta x^2}\left[\frac{-a}{24} + \frac{-c}{24}\right]\Delta x^4 \left(\frac{\partial^4 u}{\partial x^4}\right)_j = -\frac{\Delta x^2}{12}\left(\frac{\partial^4 u}{\partial x^4}\right)_j$$

Higher Order Accuracy: Taylor Tables Cont'd

Table 3.2. Taylor table for backward 3-point Lagrangian approximation to a first derivative

$$\left(\frac{\partial u}{\partial x}\right)_j - \frac{1}{\Delta x}(a_2 u_{j-2} + a_1 u_{j-1} + b\, u_j) = ?$$

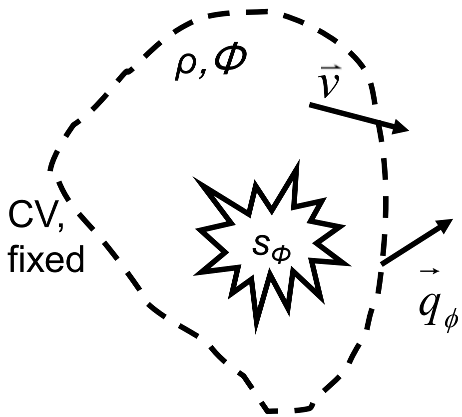
	u_j	$\Delta x \left(\frac{\partial u}{\partial x}\right)_j$	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_j$	$\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_j$	$\Delta x^4 \left(\frac{\partial^4 u}{\partial x^4}\right)_j$
$\Delta x \left(\frac{\partial u}{\partial x}\right)_j$		1			
$-a_2 \cdot u_{j-2}$	$-a_2$	$-a_2 \cdot (\text{-}2) \cdot \frac{1}{1}$	$-a_2 \cdot (\text{-}2)^2 \cdot \frac{1}{2}$	$-a_2 \cdot (\text{-}2)^3 \cdot \frac{1}{6}$	$-a_2 \cdot (\text{-}2)^4 \cdot \frac{1}{24}$
$-a_1 \cdot u_{j-1}$	$-a_1$	$-a_1 \cdot (\text{-}1) \cdot \frac{1}{1}$	$-a_1 \cdot (\text{-}1)^2 \cdot \frac{1}{2}$	$-a_1 \cdot (\text{-}1)^3 \cdot \frac{1}{6}$	$-a_1 \cdot (\text{-}1)^4 \cdot \frac{1}{24}$
$-b \cdot u_j$	$-b$				

$\Rightarrow \begin{bmatrix} a_2 & a_1 & b \end{bmatrix} = \begin{bmatrix} 1 & -4 & 3 \end{bmatrix}/2$ and $\tau_{\Delta x} = \frac{1}{\Delta x}\left[\frac{8a_2}{6} + \frac{a_1}{6}\right]\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_j = \frac{\Delta x^2}{3}\left(\frac{\partial^3 u}{\partial x^3}\right)_j$

(as before)

Integral Conservation Law for a scalar ϕ

$$\left\{\frac{d}{dt}\int_{CM}\rho\phi dV=\right\} \quad \frac{d}{dt}\int_{CV_{\text{fixed}}}\rho\phi dV+\underbrace{\int_{CS}\rho\phi\,(\vec{v}.\vec{n})dA}_{\substack{\text{Advective fluxes}\\ \text{(Adv.\& diff. fluxes }\Rightarrow\text{ convection)}}}=\underbrace{-\int_{CS}\vec{q}_{\phi}.\vec{n}\,dA}_{\text{Other transports (diffusion, etc)}}+\underbrace{\sum\int_{CV_{\text{fixed}}}s_{\phi}\,dV}_{\substack{\text{Sum of sources and}\\ \text{sinks terms (reactions, etc)}}}$$



Applying the Gauss Theorem, for any arbitrary CV gives:

$$\frac{\partial\rho\phi}{\partial t}+\nabla.(\rho\phi\vec{v})=-\nabla.\,\vec{q}_{\phi}+s_{\phi}$$

For a common diffusive flux model (Fick's law, Fourier's law):

$$\vec{q}_{\phi}=-k\nabla\phi$$

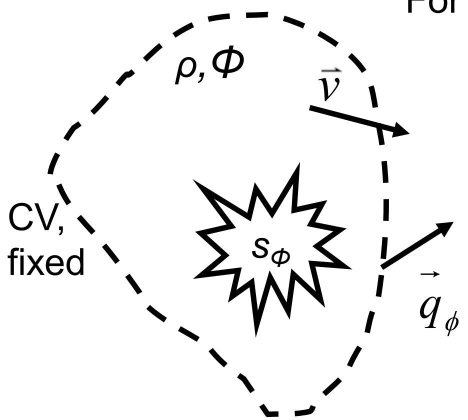
Conservative form of the PDE →

$$\frac{\partial\rho\phi}{\partial t}+\nabla.\,(\rho\phi\vec{v})=\nabla.\,(k\nabla\phi)+s_{\phi}$$

Strong-Conservative form of the Navier-Stokes Equations ($\phi \Rightarrow \boldsymbol{v}$)

Cons. of Momentum: $$\frac{d}{dt}\int_{CV} \rho\vec{v}dV + \int_{CS} \rho\vec{v}(\vec{v}.\vec{n})dA = \underbrace{\int_{CS} -p\,\vec{n}dA + \int_{CS} \vec{\vec{\tau}}.\vec{n}dA + \int_{CV} \rho\vec{g}dV}_{=\sum\vec{F}}$$

Applying the Gauss Theorem gives: $$= \int_{CV}\left(-\nabla p + \nabla.\vec{\vec{\tau}} + \rho\vec{g}\right)dV$$



For any arbitrary CV gives: $$\frac{\partial\rho\vec{v}}{\partial t} + \nabla.(\rho\vec{v}\ \vec{v}) = -\nabla p + \nabla.\vec{\vec{\tau}} + \rho\vec{g}$$ Cauchy Mom. Eqn.

With Newtonian fluid + incompressible + constant μ:

Momentum: $$\frac{\partial\rho\vec{v}}{\partial t} + \nabla.(\rho\vec{v}\ \vec{v}) = -\nabla p + \mu\nabla^2\vec{v} + \rho\vec{g}$$

Mass: $$\nabla.\vec{v} = 0$$

Equations are said to be in "strong conservative form" if all terms have the form of the divergence of a vector or a tensor. For the i^{th} Cartesian component, in the general Newtonian fluid case:

With Newtonian fluid only: $$\frac{\partial\rho v_i}{\partial t} + \nabla.(\rho v_i\ \vec{v}) = \nabla.\left(-p\ \vec{e}_i + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\vec{e}_j - \frac{2}{3}\mu\frac{\partial u_j}{\partial x_j}\vec{e}_i + \rho g_i x_i \vec{e}_i\right)$$