Review of Numerical Analysis

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Computational Fluid Dynamics

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Outline

- Review last week
- Numerical analysis basics
  - Derivative expressions
  - Round-off and truncation errors
  - Order of the error
  - Solutions of ordinary differential equation boundary value problems
  - Finite differences and finite elements
  - Accuracy of results

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Turbulence Models

- Cannot compute turbulence exactly except for simple flows
  - Need to use turbulence models
  - Based on combination of theory and empirical measurements
  - Many models available
    - No model correct for all flows
  - Basic approach is to model turbulent viscosity
    - Averages of turbulent fluctuation products are assumed to be proportional to mean gradients

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General Equation

- Reynolds (time) averaged Navier-Stokes

$$\frac{\partial\left(u_i\overline{\varphi}+\overline{u_i'\varphi'}\right)}{\partial x_i}=\frac{\partial}{\partial x_i}\gamma^{(\varphi)}\frac{\partial\overline{\varphi}}{\partial x_i} \quad\Rightarrow\quad \frac{\partial u_i\overline{\varphi}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\gamma^{(\varphi)}+\gamma_t^{(\varphi)}\right)\frac{\partial\overline{\varphi}}{\partial x_i}$$

$$\frac{\partial\overline{u_i}\,\overline{u_j}}{\partial x_i}=-\frac{1}{\rho}\frac{\partial\overline{p}}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\nu+\nu_t\right)\frac{\partial\overline{u_j}}{\partial x_i} \qquad \frac{\partial\overline{u_i}\,\overline{\varphi}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\gamma_{lam}^{(\varphi)}+\frac{\nu_t}{\sigma_t^{(\varphi)}}\right)\frac{\partial\overline{\varphi}}{\partial x_i}$$

- Turbulence models obtain values for ν_t
  - Dimensionally n_t = C l V, *e.g.*, $C_\mu(k^{3/2}/\varepsilon)k^{1/2}$
- Turbulent Prandtl number, $\sigma_t^{(\phi)}$, is empirical constant in turbulence models

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Model Guidance

- Choosing a model
  - Previous work at your organization or from literature research
  - User's manual for code
  - Use default constants
  - Unusual features: non-equilibrium turbulence, high strain rates, adverse pressure gradients, rotating machinery, compressible flows
  - Check y^+ values for correct spacing with wall functions or laminar sublayer

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More Guidance

- Common models
  - k-ε standard model and variants for internal simple flows
    - Solve two PDEs
  - Spalart-Allmaras for aerospace applications with wall-bounded flows
    - Only one PDE
  - Reynolds stress model for complex flows
    - Requires solution of seven PDEs
  - Several other models
    - No one right model for all applications

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Numerical Analysis

- Want to express derivatives and integrals in terms of discrete data points
- Use different methods
  - Develop interpolation polynomial and integrate or differentiate this result
  - Use Taylor series to get expressions for derivatives
- Want expressions and measure of error with their use

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Finite Difference Grids

- Subdivide region into discrete points
- Spacing between the points may be uniform or non-uniform
- Example: grid for $x_{min} \leq x \leq x_{max}$ with N+1 nodes numbered from zero to N
- Initial node value, $x_0 = x_{min}$
- Final grid node value, $x_N = x_{max}$
- Node spacing between $\Delta x_i = x_i$ and x_{i-1}
- Uniform spacing, $h = \Delta x_i = (x_{min} - x_{max})/N$
- N+1 nodes give N spaces

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Finite Difference Grids II

- Non-uniform grid illustrated below

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x_0 x_1 x_2 x_3 x_{N-2} x_{N-1} x_N

- Two space dimensions require x and y grids (M+1 y nodes)

  $x_0 = x_{min}$ $x_N = x_{max}$ $x_i - x_{i-1} = \Delta x_i$

  $y_0 = y_{mjn}$ $y_M = y_{max}$ $y_j - y_{j-1} = \Delta y_j$
- Most general case has three space dimensions (x, y, z, and time)

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Finite Difference Grids III

- Grid notation for four independent variables: x, y, z and t

  $x_0 = x_{min}$ $x_N = x_{max}$ $x_i - x_{i-1} = \Delta x_i$

  $y_0 = y_{mjn}$ $y_M = y_{max}$ $y_j - y_{j-1} = \Delta y_j$

  $z_0 = z_{mkn}$ $z_K = z_{max}$ $z_k - z_{k-1} = \Delta z_k$

  $t_0 = t_{min}$ $t_L = t_{max}$ $t_n - t_{n-1} = \Delta t_n$
- Dependent variable u(x,y,z,t) at discrete points $u(x_i, y_j, z_k, t_n)$
- Use notation below for this value of u

$$u_{ijk}^n = u(x_i, y_j, z_k, t_n)$$

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Derivative Expressions

- Obtain from differentiating interpolation polynomials or from Taylor series
- Series expansion for f(x) about x = a

$$f(x) = f(a) + \left.\frac{df}{dx}\right|_{x=a}(x-a) + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=a}(x-a)^2 + \frac{1}{3!}\left.\frac{d^3 f}{dx^3}\right|_{x=a}(x-a)^3 + \ldots$$

- Note: $d^0f/dx^0 = f$ and $0! = 1$

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=a}(x-a)^n$$

- What is error from truncating series?

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Truncation Error

- If we truncate series after m terms

$$f(x) = \underbrace{\boxed{\sum_{n=0}^{m} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=a}(x-a)^n}}_{\text{Terms used}} + \underbrace{\boxed{\sum_{n=m+1}^{\infty} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=a}(x-a)^n}}_{\text{Truncation error, } \varepsilon_m}$$

- Can write truncation error as single term at unknown location (derivation based on the theorem of the mean)

$$\varepsilon_m = \sum_{n=m+1}^{\infty} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=a}(x-a)^n = \frac{1}{(m+1)!}\left.\frac{d^{m+1} f}{dx^{m+1}}\right|_{x=\xi}(x-a)^{m+1}$$

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Derivative Expressions

- Look at finite-difference grid with equal spacing: $h = \Delta x$ so $x_i = x_0 + ih$
- Taylor series about $x = x_i$ gives $f(x_i + kh) = f[x_0 + (i+k)h] = f_{i+k}$ in terms of $f(x_i) = f_i$

$$f(x_i + kh) = f(x_i) + \left.\frac{df}{dx}\right|_{x=x_i} kh + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=x_i} (kh)^2 + \frac{1}{3!}\left.\frac{d^3 f}{dx^3}\right|_{x=x_i} (kh)^3 + \ldots..$$

- Compact derivative notation

$$f_i' = \left.\frac{df}{dx}\right|_{x=x_i} \qquad f_i'' = \left.\frac{d^2 f}{dx^2}\right|_{x=x_i} \qquad \cdots \qquad f_i^n = \left.\frac{d^n f}{dx^n}\right|_{x=x_i}$$

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Derivative Expressions II

- Combine all definitions for compact series notation

$$f(x_i + kh) = f(x_i) + \left.\frac{df}{dx}\right|_{x=x_i} kh + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=x_i} (kh)^2 + \frac{1}{3!}\left.\frac{d^3 f}{dx^3}\right|_{x=x_i} (kh)^3 + \ldots..$$

$$f_{i+k} = f_i + f_i' kh + \frac{f_i''(kh)^2}{2!} + \frac{f_i'''(kh)^3}{3!} + \ldots..$$

- Use this formula to get expansions for various grid locations about $x = x_i$ and use results to get derivative expressions

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Derivative Expressions III

- Apply general equation for k = 1 and k = –1

$$f_{i+k} = f_i + f_i' kh + \frac{f_i''(kh)^2}{2!} + \frac{f_i'''(kh)^3}{3!} + \ldots$$

$$f_{i+1} = f_i + f_i' h + \frac{f_i'' h^2}{2!} + \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_{i-1} = f_i - f_i' h + \frac{f_i'' h^2}{2!} - \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_i' = \frac{f_{i+1} - f_i}{h} - \frac{f_i'' h}{2!} - \frac{f_i''' h}{3!} - \ldots.. = \frac{f_{i+1} - f_i}{h} + Ah \qquad \text{Forward}$$

$$f_i' = \frac{f_i - f_{i-1}}{h} + \frac{f_i'' h}{2!} - \frac{f_i''' h}{3!} - \ldots.. = \frac{f_i - f_{i-1}}{h} + Ah \qquad \text{Backward}$$

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Derivative Expressions IV

- Subtract f_{i+1} and f_{i-1} expressions

$$f_{i+1} = f_i + f_i' h + \frac{f_i'' h^2}{2!} + \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_{i-1} = f_i - f_i' h + \frac{f_i'' h^2}{2!} - \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_{i+1} - f_{i-1} = 2 f_i' h + \frac{2 f_i''' h^3}{3!} + \frac{2 f_i''''' h^5}{5!} + \ldots..$$

Solve this result for f_i'

$$f_i' = \frac{f_{i+1} - f_{i-1}}{h} + \frac{f_i''' h^2}{3!} + \frac{f_i''''' h^4}{5!} - \ldots.. = \frac{f_{i+1} - f_{i-1}}{2h} + Ah^2$$

- Result called central difference expression

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Error in Arithmetic Mean

- Add f_{i+1} and f_{i-1} expressions

$$f_{i+1} = f_i + f_i' h + \frac{f_i'' h^2}{2!} + \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_{i-1} = f_i - f_i' h + \frac{f_i'' h^2}{2!} - \frac{f_i''' h^3}{3!} + \ldots..$$

$$f_{i+1} + f_{i-1} = 2 f_i + \frac{2 f_i'' h^2}{2!} + \frac{2 f_i'''' h^4}{4!} + \ldots..$$

Solve this result for f_i

$$f_i = \frac{f_{i+1} + f_{i-1}}{2} + \frac{f_i'' h^2}{2!} + \frac{f_i'''' h^4}{4!} - \ldots.. = \frac{f_{i+1} + f_{i-1}}{2} + Ah^2$$

- Shows error in use of arithmetic mean

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Order of the Error

- Forward and backward derivative have error term that is proportional to h
- Central difference error is proportional to h^2
- Error proportional to h^n called n^{th} order
- Reducing step size by a factor of a reduces n^{th} order error by a^n

$$\varepsilon_2 \approx \varepsilon_1 \left(\frac{h_2}{h_1}\right)^n$$

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Order of the Error Notation

- Write the error term for n^{th} error term as $O(h^n)$
  - Big oh notation, O, denotes order
  - Recognizes that factor multiplying h^n may change slightly with h

First order forward $f_i' = \frac{f_{i+1} - f_i}{h} + O(h)$

First order backward $f_i' = \frac{f_i - f_{i-1}}{h} + O(h)$

Second order central $f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$

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Higher Order Derivatives

- Add f_{i+1} and f_{i-1} expressions

$$f_{i+1} = f_i + f_i' h + \frac{f_i'' h^2}{2!} + \frac{f_i''' h^3}{3!} + ...$$

$$f_{i-1} = f_i - f_i' h + \frac{f_i'' h^2}{2!} - \frac{f_i''' h^3}{3!} + ...$$

$$f_{i+1} + f_{i-1} = 2 f_i + 2\frac{f_i'' h^2}{2!} + \frac{2 f_i'''' h^4}{4!} + \frac{2 f_i'''''' h^6}{6!} + ...$$

$$f_i'' = \frac{f_{i+1} + f_{i-1} - 2 f_i}{h^2} + \frac{f_i''' h^2}{3!} + \frac{f_i'''' h^4}{5!} - ..... = \frac{f_{i+1} + f_{i-1} - 2 f_i}{h^2} + O\left(h^2\right)$$

- f'' is second-order, central difference

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Higher Order Directional

- We can get higher order derivative expressions at the expense of more computations
- Get second order forward and backward derivative expressions from f_{i+2} and f_{i-2}, respectively
- Combine with previous expressions for f_{i+1} and f_{i-1} to eliminate first order error term

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Specific Taylor Series

- General equation $f_{i+k} = f_i + f_i' kh + \frac{f_i''(kh)^2}{2!} + \frac{f_i'''(kh)^3}{3!} + ...$
- k = 2 $f_{i+2} = f_i + 2 f_i' h + 4\frac{f_i'' h^2}{2!} + 8\frac{f_i''' h^3}{3!} + ...$
- k = -2 $f_{i-2} = f_i - 2 f_i' h + 4\frac{f_i'' h^2}{2!} - 8\frac{f_i''' h^3}{3!} + ...$
- k = 3 $f_{i+3} = f_i + 3 f_i' h + 9\frac{f_i'' h^2}{2!} + 27\frac{f_i''' h^3}{3!} + ...$
- k = -3 $f_{i-3} = f_i - 3 f_i' h + 9\frac{f_i'' h^2}{2!} - 27\frac{f_i''' h^3}{3!} + ...$

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Second Order Forward

- Subtract $4f_{i+1}$ from f_{i+2} to eliminate h^2 term

$$f_{i+2} - 4 f_{i+1} = \left[f_i + 2 f_i' h + 4 f_i'' \frac{h^2}{2} + 8 f_i''' \frac{h^3}{6} + ... \right]$$

$$-4\left[f_i + f_i' h + f_i'' \frac{h^2}{2} + f_i''' \frac{h^3}{6} + .. \right]$$

$$f_{i+2} - 4 f_{i+1} + 3 f_i = -2h f_i' + 4 f_i''' \frac{h^3}{6} + ...$$

Second order error

$$f_i' = \frac{- f_{i+2} + 4 f_{i+1} - 3 f_i}{2h} + f_i''' \frac{h^2}{3} + ...$$

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Second Order Backwards

- Add $4f_{i-1}$ to $-f_{i-2}$ to eliminate h^2 term

$$- f_{i-2} + 4 f_{i-1} = -\left[f_i - 2 f_i' h + 4 f_i'' \frac{h^2}{2} - 8 f_i''' \frac{h^3}{6} + ... \right]$$

$$+4\left[f_i - f_i' h + f_i'' \frac{h^2}{2} - f_i''' \frac{h^3}{6} + .. \right]$$

$$- f_{i-2} + 4 f_{i-1} - 3 f_i = -2h f_i' + 4 f_i''' \frac{h^3}{6} + ...$$

Second order error

$$f_i' = \frac{f_{i+2} - 4 f_{i+1} + 3 f_i}{2h} + f_i''' \frac{h^2}{3} + ...$$

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Other Derivative Expressions

- Can continue in this fashion
  - Write Taylor series for f_{i+1}, f_{i-1}, f_{i+2}, f_{i-2}, f_{i+3}, f_{i-3}, etc.
  - Create linear combinations with factors that eliminate desired terms
  - Eliminate f_i term to obtain central difference
  - Keep only terms in f_k with $k \geq i$ for forward difference expressions
  - Keep only terms in f_k with $k \leq i$ for forward difference expressions
  - See results for different expressions in common numerical analysis texts

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Order of Error Examples

- Table 2-1 in notes shows error in first derivative for e^x around x = 1
  - Using first- and second-order forward and second-order central differences
  - Step h = 0.4, 0.2, and 0.1
  - Error ratio for doubling step size
    - 4.01 to 4.02 for central differences
    - 2.07 to 2.15 for first-order forward differences
    - 4.32 to 4.69 for second-order forward

$$n \approx \frac{\log\left(\varepsilon_2 / \varepsilon_1\right)}{\log\left(h_2 / h_1\right)} = \frac{\log(\varepsilon_2) - \log(\varepsilon_1)}{\log(h_2) - \log(h_1)}$$

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Roundoff Error

- Possible in derivative expressions from subtracting close differences
- Example f(x) = e^x: f'(x) ≈ (e^{x+h} – e^{x-h})/(2h) and error at x = 1 is (e^{1+h} – e^{1-h})/(2h) - e

$$E = \frac{3.004166 - 2.722815}{2(0.1)} - 2.718282 = 4.5x10^{-3}$$

Second order error

$$E = \frac{2.7185536702 - 2.7180100139}{2(0.0001)} - 2.718281828459 = 4.5x10^{-9}$$

$$E = \frac{2.71828210028724 - 2.71828155660388}{2(0.0000001)} - 2.718281828 = 5.9x10^{-9}$$

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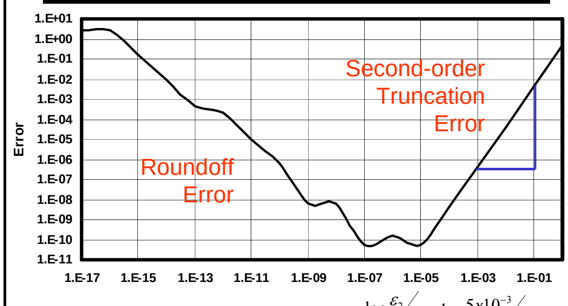
Figure 2-1. Effect of Step Size on Error



$$n = \frac{\log \varepsilon_2 / \varepsilon_1}{\log h_2 / h_1} = \frac{\log 5x10^{-3} / 5x10^{-7}}{\log 100} = 2$$

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Uneven Step Sizes

- Apply general Taylor series for $f_k = f(x_k)$ in terms of $f_i = f(x_i)$ for k = i + 1 and i – 1

$$f_k = f_i + f_i'(x_k - x_i) + \frac{f_i''}{2!}(x_k - x_i)^2 + \frac{f_i'''}{3!}(x_k - x_i)^3 + ...$$

$$f_{i+1} = f_i + f_i'(x_{i+1} - x_i) + \frac{f_i''}{2!}(x_{i+1} - x_i)^2 + \frac{f_i'''}{3!}(x_{i+1} - x_i)^3 + ...$$

$$f_{i-1} = f_i + f_i'(x_{i-1} - x_i) + \frac{f_i''}{2!}(x_{i-1} - x_i)^2 + \frac{f_i'''}{3!}(x_{i-1} - x_i)^3 + ...$$

- Subtract (or add) the last two equations to get an expression for f_i' (or f_i)

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First Derivative

- Solve subtraction for f_i' and rearrange

$$f_{i+1} - f_{i-1} = f_i'\left[(x_{i+1} - x_i) - (x_{i-1} - x_i)\right] + \frac{f_i''}{2!}\left[(x_{i+1} - x_i)^2 - (x_{i-1} - x_i)^2\right] + \frac{f_i'''}{3!}\left[(x_{i+1} - x_i)^3 - (x_{i-1} - x_i)^3\right] + ...$$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}} - \frac{f_i''}{2!}\frac{(x_{i+1} - x_i)^2 - (x_{i-1} - x_i)^2}{x_{i+1} - x_{i-1}} - \frac{f_i'''}{3!}\frac{(x_{i+1} - x_i)^3 - (x_{i-1} - x_i)^3}{x_{i+1} - x_{i-1}} + ...$$

- If $x_{i+1} - x_i = x_i - x_{i-1} = h$, we have second order central difference
- Uneven step size gives first order error of $f_i''[(x_{i+1} - x_i) - (x_i - x_{i-1})]/[2(x_{i+1} - x_{i-1})]$

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Arithmetic Mean

- Solve addition for f_i and rearrange

$$f_{i+1}+f_{i-1}=2f_i+f_i'[(x_{i+1}-x_i)+(x_{i-1}-x_i)]+\frac{f_i''}{2!}\left[(x_{i+1}-x_i)^2+(x_{i-1}-x_i)^2\right]+\frac{f_i'''}{3!}\left[(x_{i+1}-x_i)^3+(x_{i-1}-x_i)^3\right]+.....$$

$$f_i=\frac{f_{i+1}+f_{i-1}}{2}-f_i'\frac{x_{i+1}+x_{i-1}-2x_i}{2}-\frac{f_i''}{2!}\frac{(x_{i+1}-x_i)^2+(x_{i-1}-x_i)^2}{2}+.....$$

- If $x_{i+1} - x_i = x_i - x_{i-1} = h$, we have second order error
- Uneven step size gives first order error of f_i' $(x_{i+1} + x_{i-1} - 2x_i)/2$

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Second Derivative

- Start with same equations; subtract $(x_{i+1} - x_i)$ times second equation from $(x_{i-1} - x_i)$ times first equation to eliminate f_i' term

$$f_{i+1}=f_i+f_i'(x_{i+1}-x_i)+\frac{f_i''}{2!}(x_{i+1}-x_i)^2+\frac{f_i'''}{3!}(x_{i+1}-x_i)^3+.....$$

$$f_{i-1}=f_i+f_i'(x_{i-1}-x_i)+\frac{f_i''}{2!}(x_{i-1}-x_i)^2+\frac{f_i'''}{3!}(x_{i-1}-x_i)^3+.....$$

$$(x_{i-1}-x_i)f_{i+1}-(x_{i+1}-x_i)f_{i-1}=(x_{i-1}-x_i)f_i-(x_{i+1}-x_i)f_i$$
$$+\frac{f_i''}{2!}\left[(x_{i-1}-x_i)(x_{i+1}-x_i)^2-(x_{i+1}-x_i)(x_{i-1}-x_i)^2\right]$$
$$+\frac{f_i'''}{3!}\left[(x_{i-1}-x_i)(x_{i+1}-x_i)^3-(x_{i+1}-x_i)(x_{i-1}-x_i)^3\right]+\cdots$$

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Second Derivative II

- Divide by $x_{i-1} - x_i$ and define $r_i = (x_{i+1} - x_i)/(x_i - x_{i-1})$ (r_i = 1 for uniform grid)

$$f_{i+1}+r_if_{i-1}=f_i+r_if_i+\frac{f_i''}{2!}\left[(x_{i+1}-x_i)^2-(x_{i+1}-x_i)(x_{i-1}-x_i)\right]$$
$$+\frac{f_i'''}{3!}\left[(x_{i+1}-x_i)^3-(x_{i+1}-x_i)(x_{i-1}-x_i)^2\right]+\cdots$$

$$f_i''=2\frac{f_{i+1}+r_if_{i-1}-(1+r_i)f_i}{(x_{i+1}-x_i)^2-(x_{i+1}-x_i)(x_{i-1}-x_i)}$$
$$-\frac{f_i'''}{3}\frac{(x_{i+1}-x_i)^3-(x_{i+1}-x_i)(x_{i-1}-x_i)^2}{(x_{i+1}-x_i)^2-(x_{i+1}-x_i)(x_{i-1}-x_i)}+\cdots$$

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Second Derivative III

- Rearrange individual terms

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

$$\frac{(x_{i+1}-x_i)^3-(x_{i+1}-x_i)(x_{i-1}-x_i)^2}{(x_{i+1}-x_i)^2-(x_{i+1}-x_i)(x_{i-1}-x_i)}=\frac{(x_{i+1}-x_i)\left(1-r_i^{-2}\right)}{1+r_i^{-1}}$$

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Second Derivative IV

- Result shows first-order truncation error that is zero for equal step sizes (r_i – 1)

$$f_i''=\frac{f_{i+1}+r_if_{i-1}-(1+r_i)f_i}{(x_i-x_{i-1})^2\frac{r_i^2+r_i}{2}}-\frac{f_i'''}{3}\frac{(x_{i+1}-x_i)\left(1-r_i^{-2}\right)}{1+r_i^{-1}}+\cdots$$

- Alternative approach second derivative is first derivative of first derivative
- Apply unequal difference equation for first derivative $\quad f_i'=\frac{f_{i+1}-f_{i-1}}{x_{i+1}-x_{i-1}}+\cdots$

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Second Derivative V

$$f_i''=\frac{\left.\frac{df}{dx}\right|_{i+1/2}-\left.\frac{df}{dx}\right|_{i-1/2}}{x_{i+1/2}-x_{i-1/2}}+.....=\frac{\left.\frac{df}{dx}\right|_{i+1/2}-\left.\frac{df}{dx}\right|_{i-1/2}}{x_{i+1/2}-x_{i-1/2}}+.....$$

$$=\frac{\frac{f_{i+1}-f_i}{x_{i+1}-x_i}-\frac{f_i-f_{i-1}}{x_i-x_{i-1}}}{\frac{x_{i+1}+x_i}{2}-\frac{x_i+x_{i-1}}{2}}+.....=2\frac{\frac{f_{i+1}-f_i}{x_{i+1}-x_i}-\frac{f_i-f_{i-1}}{x_i-x_{i-1}}}{x_{i+1}-x_{i-1}}+.....$$

- Can rearrange to show that this gives same result as Taylor series approach

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Proof of Same Result

$$f_i'' = 2\frac{\frac{f_{i+1}-f_i}{x_{i+1}-x_i} - \frac{f_i - f_{i-1}}{x_i - x_{i-1}}}{x_{i+1}-x_{i-1}} = 2\frac{\frac{f_{i+1}-f_i}{\Delta x_{i+1}} - \frac{f_i - f_{i-1}}{\Delta x_i}}{\Delta x_{i+1}+\Delta x_i} \bullet \frac{\Delta x_{i+1}}{\Delta x_{i+1}}$$

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

$$f_i'' = \frac{f_{i+1} + r_i f_{i-1} - \left(1+r_i\right) f_i}{\left(\Delta x_i\right)^2 \frac{r_i^2 + r_i}{2}}$$

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Finite-volume Approach

- Integrate PDE over a small volume
- Where derivatives occur, replace them by finite-difference expressions
- Where source terms occur, replace terms like $\int_{\Delta V} S dV$ by $S_{avg}\Delta V$
  - S_{avg} is average S for control volume
- Finite Volume grid notation

Variables defined at Nodes

Volume boundaries at Faces

●--------------|--------------●---------------|---------------●

$x_W = x_{i-1}$ $x_w = x_{i-1/2}$ $x_P = x_i$ $x_e = x_{i+1/2}$ $x_E = x_{i+1}$

$\delta x_{WP} = x_P - x_W$, $\delta x_{wP} = x_P - x_w$, $\delta x_{Pe} = x_e - x_P$, $\delta x_{PE} = x_E - x_P$

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Finite Volume Example

- Consider 1D diffusion and source only

$$\frac{d}{dx}\Gamma\frac{d\varphi}{dx} + S = 0 \qquad \int\left(\frac{d}{dx}\Gamma\frac{d\varphi}{dx} + S\right)dV = \int\left(\frac{d}{dx}\Gamma\frac{d\varphi}{dx} + S\right)Adx = 0$$

- Integrate over finite-volume grid

●--------------|--------------●---------------|---------------●

$x_W = x_{i-1}$ $x_w = x_{i-1/2}$ $x_P = x_i$ $x_e = x_{i+1/2}$ $x_E = x_{i+1}$

$\delta x_{WP} = x_P - x_W$, $\delta x_{wP} = x_P - x_w$, $\delta x_{Pe} = x_e - x_P$, $\delta x_{PE} = x_E - x_P$

$$A\int\frac{d}{dx}\Gamma\frac{d\varphi}{dx}dx + \int S dV = A\int_{x_w}^{x_e} d\left(\Gamma\frac{d\varphi}{dx}\right) + \bar{S}\Delta V = \left(\Gamma A\frac{d\varphi}{dx}\right)_e - \left(\Gamma A\frac{d\varphi}{dx}\right)_w + \bar{S}\Delta V = 0$$

- What are Γ and $d\phi/dx$ at w and e faces?

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Finite Volume Example II

- Use mean value for coefficient
  - $\Gamma_e = (\Gamma_P + \Gamma_E)/2$ and $\Gamma_w = (\Gamma_W + \Gamma_P)/2$
- Use central difference for $d\phi/dx$
  - $d\phi/dx|_e = (\phi_E - \phi_P)/\delta x$ $d\phi/dx|_w = (\phi_P - \phi_W)/\delta x$
- Substitute into $\left(\Gamma A\frac{d\varphi}{dx}\right)_e - \left(\Gamma A\frac{d\varphi}{dx}\right)_w + \bar{S}\Delta V = 0$
  - Define $\bar{S}\Delta V = S_u + S_p\varphi_P$

$$\Gamma_e A_e\frac{\varphi_E - \varphi_P}{\delta x_{PE}} - \Gamma_w A_w\frac{\varphi_P - \varphi_W}{\delta x_{WP}} + S_u + S_p\varphi_P = \frac{\Gamma_e A_e\varphi_E}{\delta x_{PE}} + \frac{\Gamma_w A_w\varphi_W}{\delta x_{WP}} + S_u - \left(\frac{\Gamma_e A_e}{\delta x_{PE}} + \frac{\Gamma_w A_w}{\delta x_{WP}} + S_p\right)\varphi_P = 0$$

  - Define $a_E = \frac{\Gamma_e A_e}{\delta x_{PE}}$ $a_W = \frac{\Gamma_w A_w}{\delta x_{WP}}$ $a_P = \frac{\Gamma_e A_e}{\delta x_{PE}} + \frac{\Gamma_w A_w}{\delta x_{WP}} - S_p = a_E + a_W - S_p$

$$a_E\varphi_E + a_W\varphi_W + S_u - a_P\varphi_P = 0 \qquad a_E\varphi_E + a_W\varphi_W - a_P\varphi_P = -S_u$$

$$a_P\varphi_P = a_E\varphi_E + a_W\varphi_W + S_u$$

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Finite-Volume Example III

- This represents equation for one node
  - Need to write equations for all nodes
  - Simple for one-dimensional problem
  - Here is where i, i+1, i-1 notation is easier
    - $a_{W,i}\phi_{i-1} - a_{p,i}\phi_i + a_{E,i}\phi_{i+1} = -S_{u,i}$
    - Apply this result for nodes from i = 1 to i = N – 1
    - Nodes i = 0 and i = N are boundary conditions
    - Look at constant Γ, A, and δx such that $\Gamma A = 1$
    - Let $S_u = 0$ and $S_p = -10\delta x$ for all nodes

$$a_E = \frac{\Gamma_e A_e}{\delta x_{PE}} = \frac{1}{\delta x} \quad a_W = \frac{\Gamma_w A_w}{\delta x_{WP}} = \frac{1}{\delta x} \quad a_P = a_E + a_W - S_p = \frac{2}{\delta x} + 10\delta x$$

$$a_E\varphi_E + a_W\varphi_W - a_P\varphi_P = \frac{\varphi_{i-1}}{\delta x} - \left(\frac{2}{\delta x} + 10\delta x\right)\varphi_i - \frac{\varphi_{i+1}}{\delta x} = S_{u,i} = 0$$

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Finite-Volume Example IV

$$\frac{\varphi_{i-1}}{\delta x} - \left(\frac{2}{\delta x} + 10\delta x\right)\varphi_i - \frac{\varphi_{i+1}}{\delta x} = 0 \quad \Rightarrow \quad \varphi_{i-1} - \left[2 + 10(\delta x)^2\right]\varphi_i + \varphi_{i+1} = 0$$

- Need to handle boundary conditions
  - Assume $\phi = 2$ at x = 0 and $\phi = 3$ at x = L = 1
  - Nodes numbered from 0 to N
    - $x_0 = 0$ and $x_N = L = 1$ (assumed); $\phi_0 = 2$ and $\phi_N = 3$
    - At i = 1 (1 node in from left boundary) $\phi_0 - [2 + (\delta x)^2]\phi_1 + \phi_2 = 0$ with $\phi_0 = 2$ gives $-[2 + (\delta x)^2]\phi_1 + \phi_2 = -2$
    - At i = N – 1 (1 node in from right boundary) $\phi_{N-2} - (2 + \delta x)\phi_{N-1} + \phi_N = 0$ with $\phi_N = 3$ gives $\phi_{N-2} - [2 + (\delta x)^2]\phi_{N-1} = -3$

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Finite-Volume Example V

- System of equations to solve

$$
\begin{aligned}
-2.4\phi_1 + \phi_2 &= -2\\
\phi_1 - 2.4\phi_2 + \phi_3 &= 0\\
\phi_2 - 2.4\phi_3 + \phi_4 &= 0\\
\phi_3 - 2.4\phi_4 &= -3
\end{aligned}
$$

- Matrix form

$$
\begin{bmatrix} -2.4 & 1 & 0 & 0 \\ 1 & -2.4 & 1 & 0 \\ 0 & 1 & -2.4 & 1 \\ 0 & 0 & 1 & -2.4 \end{bmatrix}
\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix}
=
\begin{bmatrix} -2 \\ 0 \\ 0 \\ -3 \end{bmatrix}
$$

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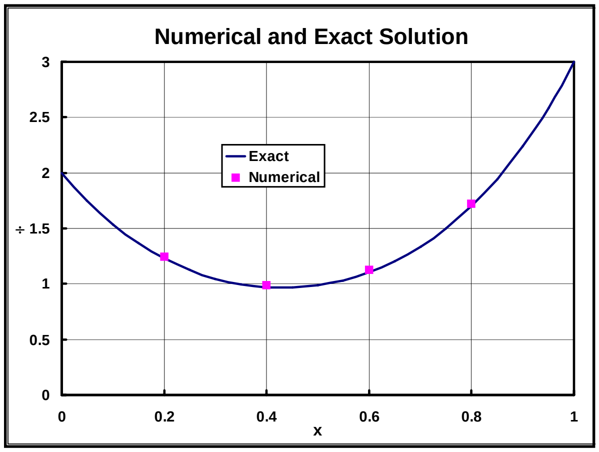

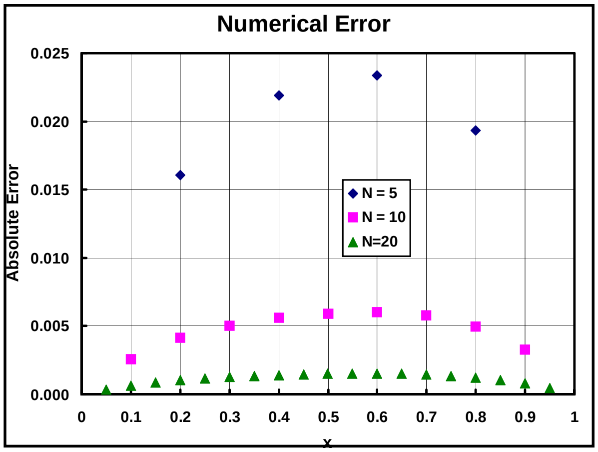

Error in Gradient

Exact dH/dx at x = 0 is -5.54268				
	Second order		First Order	
	dH/dx	Error	dH/dx	Error
N = 5	-5.0175	0.5252	-3.7719	1.7708
N = 10	-5.3713	0.1713	-4.6014	0.9413
N = 20	-5.5024	0.0403	-5.0648	0.4779
Exact dH/dx at x = L is 8.98450				
	Second order		First Order	
	dH/dx	Error	dH/dx	Error
N = 5	8.1181	0.8664	6.3976	2.5869
N = 10	8.7104	0.2741	7.5899	1.3946
N = 20	8.9184	0.0661	8.2704	0.7141

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