Numerical Methods for PDEs

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Outline

- Review midterm solutions
- Review basic material on numerical calculus
  - Expressions for derivatives, error and error order
- Numerical methods for the diffusion equation
  - Explicit and Implicit
  - First and second order time derivatives

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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 $x_{min} \le x \le x_{max}$ with N+1 nodes numbered from zero to N
- Initial node value, $x_0 = x_{min}$
- Final grid node value, $x_N = x_{max}$
- Nodal spacing $\Delta x_i = x_i - x_{i-1}$ (i = 1, N)
- 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

Δx_1 Δx_2 Δx_3 Δx_{N-1} Δx_N
●----●-------●-----------●---~ ~---●------●------●
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
  $x_0 = x_{min}$ $x_N = x_{max}$ $x_i - x_{i-1} = \Delta x_i$
  $y_0 = y_{mjn}$ $y_M = y_{max}$ $y_j - y_{j-1} = \Delta y_j$
  $z_0 = z_{min}$ $z_K = z_{max}$ $z_k - z_{k-1} = \Delta z_k$
  $t_0 = t_{min}$ $t_L = t_{max}$ $t_n - t_{n-1} = \Delta t_n$
- 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

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

- 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 $x_i = x_0 + ih$
- Want Taylor series for $f_{i+k} = f(x_{i+k})$ in terms of $f_i = f(x_i)$ and derivatives at $x = x_i$

$x_{i+k} - x_i = [x_0 + (i + k)h] - [x_0 + ih] = kh$

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

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

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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

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

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

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

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

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

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Derivative Expressions IV

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

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

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

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

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

- Result called central difference expression

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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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Other Derivatives

- Second-order, central-difference, second derivative

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

- Second-order, forward and backward difference, first derivatives

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

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

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Other Derivative Expressions

- Can derive various finite-difference expressions for derivatives
  – Derivative order, first, second, etc.
  – Order of the error (typically second although higher orders used)
  – Forward, backwards and central difference expressions (typically use central except at boundaries)
  – Derive by Taylor series manipulations
  – See results on page 271 of Hoffman

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Order of Error Examples

- Table 1 in “introduction” notes shows first derivative error 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 $f(x) = e^x$: $f'(x) \approx (e^{x+h} - e^{x-h})/(2h)$ 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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Error *vs*. Step Size Plot

- Plot the log of the error versus the log of the step size
- For regions where there is no roundoff error this will be a straight line whose slope is the order of the error

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

$$\log \varepsilon_2 - \log \varepsilon_1 \approx n(\log h_2 \approx \log h_1) \quad \Rightarrow \quad n \approx \frac{\log \varepsilon_2 - \log \varepsilon_1}{\log h_2 \approx \log h_1}$$

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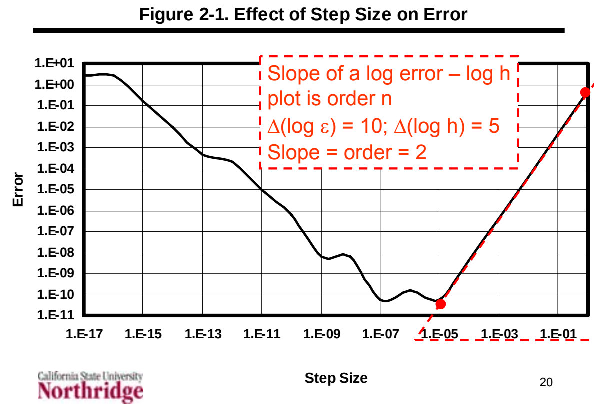

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Numerical PDE Solutions

- Define a finite-difference grid in the independent variables (x, y, z, t)
- Place grid points on region boundary whose values are found from boundary conditions for the problem
- At some grid location convert differential equation into a finite difference equation
  - Observe truncation error in process
  - Neglect truncation error to get set of algebraic equations to solve

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Diffusion Equation

- Apply difference formulas derived for ordinary derivatives to partial derivatives
- Use notation to consider different coordinate directions
- Apply to diffusion equation $\left[\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}\right]_i^n$
- Grids $x_i = x_0 + i\Delta x$ and $t_n = t_0 + n\Delta t$
- Try finite difference expressions below to get simple finite-difference equation

$$\left.\frac{\partial u}{\partial t}\right|_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t) \quad and \quad \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n = \frac{u_{i+1}^n + u_{i-1}^n - 2u_i^n}{(\Delta x)^2} + O[(\Delta x)^2]$$

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Diffusion Equation II

- Substitute finite difference expressions into differential equation

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n + u_{i-1}^n - 2u_i^n}{(\Delta x)^2} + O[\Delta t, (\Delta x)^2]$$

- Ignore truncation error, solve for u_i^{n+1}

$$u_i^{n+1} = \frac{\alpha \Delta t}{(\Delta x)^2}\left(u_{i+1}^n + u_{i-1}^n\right) + \left(1 - \frac{2\alpha\Delta t}{(\Delta x)^2}\right)u_i^n$$

- Obtain potential at $x = x_i$ and $t = t_{n+1}$ in terms of u values at old time step

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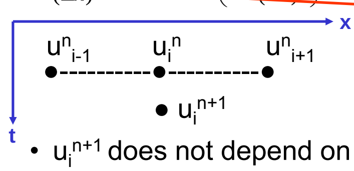
Explicit (FTCS) Method

- Method just derived is called explicit method; can solve one equation at a time

$$u_i^{n+1} = \frac{\alpha \Delta t}{(\Delta x)^2}\left(u_{i+1}^n + u_{i-1}^n\right) + \left(1 - \frac{2\alpha\Delta t}{(\Delta x)^2}\right)u_i^n = f\left(u_{i+1}^n + u_{i-1}^n\right) + (1 - 2f)u_i^n$$

$$f \equiv \frac{\alpha \Delta t}{(\Delta x)^2}$$



- u_i^{n+1} does not depend on other u values at the new time step (n+1)

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Explicit Method Example

- Pick α = 1, Δx = 0.25, N_x = 4, Δt = 0.01
- f = $\alpha\Delta t/(\Delta x)^2$ = 1(.01)/(.25)^2 = 0.16
- Pick initial u_i^0 = 1000 and boundaries, u^n_0 = u^n_4 = 0 for time > 0 (n ≥ 0)

$$Apply\ u_i^{n+1} = f\left(u_{i+1}^n + u_{i-1}^n\right) + \left(1-2f\right)u_i^n$$

$$u_1^1 = f\left[u_0^0 + u_2^0\right] + (1-2f)u_1^0 = 0.16[0+1000] + 0.68[1000] = 840$$

$$u_2^1 = f\left[u_1^0 + u_3^0\right] + (1-2f)u_2^0 = 0.16[1000+1000] + 0.68[1000] = 1000$$

$$u_3^1 = f\left[u_2^0 + u_4^0\right] + (1-2f)u_3^0 = 0.16[1000+0] + 0.68[1000] = 840$$

- Repeat for subsequent time steps

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Explicit Method Results f = 0.16

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0.00	x = 0.25	x = 0.50	x = 0.75	x = 1.00
	t = 0	1000	1000	1000	1000	1000
n = 0	t = 0+	0	1000	1000	1000	0
n = 1	t = 0.01	0	840	1000	840	0
n = 2	t = 0.02	0	731.2	948.8	731.2	0
n = 3	t = 0.03	0	649	879.2	649	0
n = 4	t = 0.04	0	582	805.5	582	0
n = 5	t = 0.05	0	524.6	734	524.6	0
n = 6	t = 0.06	0	474.2	667	474.2	0
n = 7	t = 0.07	0	429.2	605.3	429.2	0
n = 8	t = 0.08	0	388.7	548.9	388.7	0

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Explicit Method Results f = 0.16

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0.00	x = 0.25	x = 0.50	x = 0.75	x = 1.00
n = 12	t = 0.12	0	262	370.5	262	0
n = 13	t = 0.13	0	237.5	335.8	237.5	0
n = 14	t = 0.14	0	215.2	304.4	215.2	0
n = 15	t = 0.15	0	195	275.8	195	0
n = 16	t = 0.16	0	176.8	250	176.8	0
n = 17	t = 0.17	0	160.2	226.5	160.2	0
n = 18	t = 0.18	0	145.2	205.3	145.2	0
n = 19	t = 0.19	0	131.6	186.1	131.6	0
n = 20	t = 0.20	0	119.2	168.6	119.2	0
Exact	t = 0.20	0	125.1	176.9	125.1	0
Error	t = 0.20	0	5.8	8.2	5.8	0

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Explicit Results f = 0.32

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0.00	x = 0.25	x = 0.50	x = 0.75	x = 1.00
	t = 0	1000	1000	1000	1000	1000
n = 0	t = 0+	0	1000	1000	1000	0
n = 1	t = 0.02	0	680	1000	680	0
n = 2	t = 0.04	0	564.8	795.2	564.8	0
n = 3	t = 0.06	0	457.9	647.7	457.9	0
n = 8	t = 0.16	0	162.2	229.4	162.2	0
n = 9	t = 0.18	0	131.8	186.4	131.8	0
n = 10	t = 0.20	0	107.1	151.4	107.1	0
Exact	t = 0.20	0	125.1	176.9	125.1	0
Error	t = 0.20	0	18	25.4	18	0

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Explicit Results f = 0.64

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0.00	x = 0.25	x = 0.50	x = 0.75	x = 1.00
	t = 0	1000	1000	1000	1000	1000
n = 0	t = 0+	0	1000	1000	1000	0
n = 1	t = 0.04	0	360	1000	360	0
n = 2	t = 0.08	0	539.2	180.8	539.2	0
n = 3	t = 0.12	0	-35.3	639.6	-35.3	0
n = 4	t = 0.16	0	419.2	-224.2	419.2	0
n = 5	t = 0.20	0	-260.9	599.3	-260.9	0
Exact	t = 0.20	0	125.1	176.9	125.1	0
Error	t = 0.20	0	385.9	422.5	385.9	0

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What Happened?

- We are seeing effects of instability
- Difference equations may not converge
  - Unstable equations grow without bound
  - May have stable equations that produce incorrect results
  - Conditional stability requires step size less than that needed for accuracy
  - Goal of absolute stability not always possible
  - Discussions of stability complex, can sometimes use physical arguments

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Stability of Explicit Method

- If the values of u_{i+1} and u_{i-1} are fixed an increase in u_i^n should increase u_i^{n+1}
- If f is greater than 0.5, an increase in u_i^n will cause a decrease in u_i^{n+1}
- We can avoid this incorrect result by keeping $f = \alpha\Delta t/(\Delta x)^2 \leq 0.5$
- This imposes a time step limit that may be less than the limit required for accuracy in the solution

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FTCS Truncation Error

- Derivation in appendix for notes on solving PDEs gives this equation

$$TE_i^n = \alpha\sum_{k=2}^{\infty}(\Delta x)^{2k-2}\left[\frac{2}{(2k)!} - \frac{f^{k-1}}{k!}\right]\frac{\partial^{2k}T}{\partial x^{2k}}\bigg|_i^n$$

$$TE_i^n = \frac{\alpha(\Delta x)^2}{2}\left(\frac{1}{6} - f\right)\frac{\partial^4 T}{\partial x^4}\bigg|_i^n + \frac{\alpha(\Delta x)^4}{6}\left(\frac{1}{60} - f^2\right)\frac{\partial^6 T}{\partial x^6}\bigg|_i^n + \cdots$$

- Setting $f = \alpha\Delta t/(\Delta x)^2 = 1/6$ eliminates first term in the truncation error

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Alternative Methods

- Next class will show how to avoid stability limit by using explicit methods
  - Solution for u_i^{n+1} depends on other u values at new time step
  - Requires solution of simultaneous equations for all u_i^{n+1}
  - Crank-Nicholson uses values for old and new time steps in space derivatives
  - Fully implicit uses new time values only

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