Numerical Solutions of the Diffusion Equation
Larry Caretto
Mechanical Engineering 501AB
Seminar in Engineering Analysis
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Outline
• Review last class
• Numerical solutions of the diffusion equation in one space dimension
  – Explicit algorithm
  – Stability of algorithms
  – Crank-Nicholson algorithm
  – (Fully) implicit algorithm
  – DuFort-Frankel algorithm

Review Numerical Analysis
• Transform differential equation into a system of algebraic equations
• Obtain solution for discrete points in domain
• Two basic approaches: finite differences and finite elements
• Start with finite elements
• Get expressions for derivatives and measure of error with their use

Review Finite Difference Grids
• Grid notation for four independent variables: x, y, z, and t
  
  \[ \begin{align*}
  x_0 &= x_{\text{min}} & x_N &= x_{\text{max}} & x_i - x_{i-1} &= \Delta x_i \\
  y_0 &= y_{\text{min}} & y_M &= y_{\text{max}} & y_j - y_{j-1} &= \Delta y_j \\
  z_0 &= z_{\text{min}} & z_K &= z_{\text{max}} & z_k - z_{k-1} &= \Delta z_k \\
  t_0 &= t_{\text{min}} & t_L &= t_{\text{max}} & t_n - t_{n-1} &= \Delta t_n 
  \end{align*} \]

• 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 \( u \)
  
  \[ u_{ijk}^n = u(x_i, y_j, z_k, t_n) \]

Review Truncation Error
• If we truncate series after \( m \) terms
  
  \[ f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^nf}{dx^n}(x-a)^n \]

  Terms used
  Truncation error, \( \varepsilon_m \)

  Can write truncation error as single term at unknown location (derivation based on the theorem of the mean)
  
  \[ \varepsilon_n = \sum_{n=0}^{m} \frac{1}{n!} \frac{d^nf}{dx^n}(x-a)^n = \frac{1}{(m+1)!} \frac{d^{m+1}f}{dx^{m+1}}(x-a)^{m+1} \]

Review Order of the Error
• Derivative expressions have error that is proportional to \( h^n \)
• This power, \( n \), is called the order of the error
• Use notation \( O(h^n) \) to indicate this error
• Reducing step size by a factor of \( a \) reduces \( n^{\text{th}} \) order error by \( a^n \)
  
  \[ \varepsilon_z \approx \varepsilon \left( \frac{h_z}{h_1} \right)^n \]
Review Derivative Expressions

- First-order error, first derivatives
  \[ f'_i = \frac{f_{i+1} - f_i}{h} + O(h) \]
  \[ f'_i = \frac{f_i - f_{i-1}}{h} + O(h) \]

- Second-order error, first derivatives
  \[ f'_i = -\frac{f_{i+2} - 4f_{i+1} + 3f_i}{2h} + O(h^2) \]
  \[ f'_i = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2) \]

- Second derivative
  \[ f''_i = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} + O(h^2) \]

Find \( f' \) and \( f'' \) for \( \sin(1) \)

Second order central

\[ f'_i = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2) \]
\[ f''_i = \frac{\sin(1.01) - \sin(0.99)}{0.02} + O(h^4) \]

Review Roundoff Error

- Possible in derivative expressions from subtracting close differences
- Example \( f(x) = e^x \):
  \[ f'(x) \approx \frac{(e^{x+h} - e^{x-h})}{2h} \]
  and error at \( x = 1 \) is \( \frac{(e^{1+h} - e^{1-h})}{2h} - e \)

\[ E = \frac{3.004166 - 2.722815}{2(0.01)} - 2.718282 = 4.5 \times 10^{-3} \]

\[ E = \frac{2.7185536702 - 2.7180100139}{2(0.00001)} - 2.718281828459 = 4.5 \times 10^{-3} \]

\[ E = \frac{2.71828210028724 - 2.71828155660388}{2(0.00000001)} - 2.718281828 = 5.9 \times 10^{-5} \]

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

Diffusion Equation

- Apply difference formulas derived for ordinary derivatives to partial derivatives
- Use notation to consider different coordinate directions
- Apply to diffusion equation
- 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

\[ \frac{\partial u}{\partial t} = \frac{u_{i+1}^{n+1} - u_i^n}{\Delta t} + O(\Delta t) \]
\[ \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^{n+1} + 2u_i^n - u_{i-1}^{n+1}}{(\Delta x)^2} + O((\Delta x)^2) \]
Diffusion Equation II

- Substitute finite difference expressions into differential equation
\[ \frac{u^{n+1}_i - u^n_i}{\Delta t} = \alpha \frac{u^n_{i+1} + u^n_{i-1} - 2u^n_i}{(\Delta x)^2} + O(\Delta t, (\Delta x)^2) \]

- Ignore truncation error, solve for \( u^{n+1}_i \)
\[ u^{n+1}_i = \alpha \frac{\Delta t}{(\Delta x)^2} (u^n_{i+1} + u^n_{i-1} + (1 - 2f)u^n_i) \]

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

Explicit Method Example

- Pick \( \alpha = 1 \), \( \Delta x = 0.25 \), \( N_x = 4 \), \( \Delta t = 0.01 \)
- \( f = \alpha \Delta t/(\Delta x)^2 = 1.01/0.25^2 = 0.16 \)
- Pick initial \( u^0_i = 1000 \) and boundaries, \( u^n_0 = u^n_{N_x} = 0 \) for \( n \geq 0 \)
- Apply \( u^{n+1}_i = f(u^n_{i+1} + u^n_{i-1}) + (1 - 2f)u^n_i \)
- \( u'_i = f(u^n_{i+1} + u^n_{i-1}) + (1 - 2f)u^n_i = 0.16(0 + 1000) + 0.68(1000) = 1000 \)
- \( u'_i = f(u^n_{i+1} + u^n_{i-1}) + (1 - 2f)u^n_i = 0.16(1000 + 1000) + 0.68(1000) = 1000 \)
- \( u'_i = f(u^n_{i+1} + u^n_{i-1}) + (1 - 2f)u^n_i = 0.16(1000 + 0) + 0.68(1000) = 1000 \)
- Repeat for subsequent time steps

Explicit Method Results \( f = 0.16 \)

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<th>( i = 0 )</th>
<th>( i = 1 )</th>
<th>( i = 2 )</th>
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Explicit Results \( f = 0.16 \)

<table>
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<tr>
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Explicit Method Results \( f = 0.32 \)

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Explicit Results $f = 0.64$

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<td>125.1</td>
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<td>Error</td>
<td>t = 0.20</td>
<td>385.9</td>
<td>422.5</td>
<td>385.9</td>
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</table>

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

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

FTCS Truncation Error

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

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

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

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

Crank-Nicholson Method

- Seek more accurate time derivative
- Provides implicit method
  - Value of $u_{i+1}^{n+1}$ depends on other $u_{i+1}^{n+1}$
  - More work per step, but can take longer time steps with this method
  - Apply to diffusion equation at time $n + 1/2$

$$\frac{\partial u_i^{n+1}}{\partial t} = \frac{u_i^{n+1} - u_i^n}{2 \Delta t} + O((\Delta t)^2) = u_i^{n+1} - u_i^n + O((\Delta t)^2) = \alpha \frac{\partial^2 u_i}{\partial x^2}$$

Space Derivative at $t_{n+1/2}$

- Take average of space derivative at time steps $n$ and $n + 1$
- Show average is second order accurate

$$f_{i+1} = f_i + f_{i+1} - f_i^h = \frac{h^2}{2} + f_i^h$$

$$f_{i-1} = f_i - f_{i-1} = \frac{h^2}{2} - f_i^h$$

$$f_{i+1} + f_{i-1} = 2 f_i + 2 f_i^h = \frac{h^2}{2} + 2 f_i^h + \cdots$$

$$f_i = f_{i+1} + f_{i-1} = \frac{h^2}{4} - f_i^h = \frac{h^2}{4} \cdots = \frac{f_{i+1} + f_{i-1}}{2} + O(h^2)$$
Using Space Derivative at \( t_{n+1/2} \)

- Apply average to space derivative
  \[
  \frac{\partial^2 u}{\partial x^2} \bigg|_{n+1/2} = \frac{1}{2} \left[ \frac{\partial^2 u}{\partial x^2} \bigg|_n + \frac{\partial^2 u}{\partial x^2} \bigg|_{n+1} \right] + O(\Delta t^2)
  \]
- Substitute into diffusion equation
  \[
  \frac{\partial^2 u}{\partial t^2} \bigg|_{n+1/2} - \frac{\partial^2 u}{\partial x^2} = \frac{u_{n+1} - u_n}{\Delta t} + \frac{u_{n+1} - 2u_n + u_{n-1}}{2(\Delta x)^2} + O(\Delta t^2)
  \]
- Introduce \( f = \alpha \Delta t / (\Delta x)^2 \) and rearrange

Crank-Nicholson Equation

- Resulting equation has three values at new time step
  \[
  - \frac{f}{2} u_{i+1}^{n+1} + (1 + f) u_i^{n+1} - \frac{f}{2} u_{i-1}^{n+1} = \frac{f}{2} \left[ u_{i+1}^n + u_{i-1}^n \right] + (1 - f) u_i^n
  \]
- Tridiagonal system of equations easily solved by special application of Gauss elimination called Thomas algorithm
  \[
  - fu_{i+1}^{n+1} + 2(1 + f) u_i^{n+1} - fu_{i-1}^{n+1} = R_i
  \]

Crank-Nicholson Equations

- Consider case where boundary potentials \( u_0 \) and \( u_N \) are specified
- Rewrite equations in matrix form to show tridiagonal structure

Thomas Algorithm

- General format for tridiagonal equations

\[
\begin{bmatrix}
B_0 & C_0 & 0 & 0 & \cdots & 0 & 0 \\
A_1 & B_1 & C_1 & 0 & \cdots & 0 & 0 \\
0 & A_2 & B_2 & C_2 & \cdots & 0 & 0 \\
0 & 0 & A_3 & B_3 & \cdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & B_{N-1} & C_{N-1} \\
0 & 0 & 0 & 0 & \cdots & A_N & B_N
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
x_2 \\
\vdots \\
\vdots \\
x_{N-1} \\
x_N
\end{bmatrix}
= 
\begin{bmatrix}
D_0 \\
D_1 \\
D_2 \\
\vdots \\
\vdots \\
D_{N-1} \\
D_N
\end{bmatrix}
\]

Thomas Algorithm II

- Gauss elimination upper triangular form

\[
\begin{bmatrix}
1 & -E_0 & 0 & \cdots & 0 & 0 \\
0 & 1 & -E_0 & \cdots & 0 & 0 \\
0 & 0 & 1 & -E_2 & \cdots & 0 \\
0 & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 - E_{N-1} \\
0 & 0 & 0 & 0 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
x_2 \\
\vdots \\
\vdots \\
x_{N-1} \\
x_N
\end{bmatrix}
= 
\begin{bmatrix}
F_0 \\
F_1 \\
F_2 \\
\vdots \\
\vdots \\
F_{N-1} \\
F_N
\end{bmatrix}
\]

Thomas Algorithm III

- Forward computations
  - Initial: \( E_0 = -C_0 / B_0 \), \( F_0 = D_0 / B_0 \)
  - For \( i = 1, \ldots, N-1 \):
    \[
    E_i = \frac{-C_i}{B_i + A_i E_{i-1}} \quad F_i = \frac{D_i - A_i F_{i-1}}{B_i + A_i E_{i-1}}
    \]
- Get last \( x \) value first
  \[
  x_N = F_N = \frac{D_N - A_N F_{N-1}}{B_N + A_N E_{N-1}}
  \]
- Back substitute: \( x_i = F_i + E_i x_{i+1} \)
Crank Nicholson Results

• Results for $\alpha = 1$, $L = 1$, $\Delta x = 0.01$, $\Delta t = 0.0005$, $f = \alpha \Delta t / (\Delta x)^2 = 5$

<table>
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<tr>
<th>i = 0</th>
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<td>x = 0.04</td>
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<tr>
<td>n = 0</td>
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<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>n = 1</td>
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<td>588.17</td>
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<td>n = 6</td>
<td>t = 0.003</td>
<td>105.75</td>
<td>217.08</td>
<td>319.77</td>
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</tbody>
</table>

Fully Implicit Results

• Same as CN results: $\alpha = 1$, $L = 1$, $\Delta x = 0.01$, $\Delta t = 0.0005$, $f = \alpha \Delta t / (\Delta x)^2 = 5$

<table>
<thead>
<tr>
<th>i = 0</th>
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Crank Nicholson Results II

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<td>t = 0.0085</td>
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<td>109.4</td>
<td>180.3</td>
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</table>

Fully Implicit Results II

• Discretize diffusion equation at $t_{n+1}$

\[
\frac{\partial u}{\partial t} = \frac{u_{i+1} - u_i}{\Delta t} + O(\Delta t) \quad \text{and} \quad \frac{\partial^2 u}{\partial t^2} = \frac{u_{i+1} + u_{i-1} - 2u_i}{(\Delta t)^2} + O(\Delta t)^2
\]

\[
\frac{\partial^2 u}{\partial t^2} - \alpha^2 \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1} - u_i - u_i - u_{i-1} + 2u_i}{(\Delta x)^2} + O((\Delta t), (\Delta x)^2) = 0
\]

- $f(t_{i+1}) = f(t_i)$

• Tridiagonal system of equations

• Almost same work as CN and no spurious oscillations, but less accuracy

Crank Nicholson Results III

Fully Implicit Method

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<tr>
<th>i = 0</th>
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### Fully Implicit Results III

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### Richardson/Leapfrog

- Use two time step central differences
  \[ \frac{\partial u}{\partial t} = \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta} + O(\Delta t^2) \]
- Result is explicit with second order accuracy in time
  \[ u_{i+1}^{n+1} = u_{i}^{n+1} + \alpha \frac{u_{i+1}^{n} + u_{i-1}^{n} - 2u_{i}^{n}}{(\Delta x)^2} \]
- However result is unstable for any \( f \) and cannot be used

### DuFort Frankel

- Modification of Richardson method to provide stability
- Replace \( 2u_{i}^{n} \) in second derivative by average at time steps \( n+1 \) and \( n-1 \)
- Introduces another \( O(\Delta t^2) \) error

\[ \frac{\partial u}{\partial t} = \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta} + O(\Delta t^2) \]

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

\[ v = \alpha \frac{\Delta t}{(\Delta x)^2} \]

- Result is explicit for values at time \( n+1 \)
- Explicit start required to get first set of values at time \( n-1 \)
**This Week’s Homework**

- Download assignment from web
  - Find first and second derivative of \( \sin x \) at \( x = 1 \) for \( h = .1, .01, \) and \( .001 \) using second-order central-difference expressions
  - Repeat for \( x = 0.01 \) with \( h = .001 \) and \( .0001 \)
  - Do problems 5, 23, and 28 on pp 646-647 of Hoffman (diffusion equation solutions)
  - Computer assignment due after midterm
- Download and run program used to get charts just shown for one of the suggested assignments

**Explicit Method Example**

- How many values can you compute for initial conditions below with \( f = 0.25 \)
  
  \[
  u_i^{n+1} = f(u_{i+1}^n + u_{i-1}^n) + (1 - 2f)u_i^n = \frac{u_{i+1}^n + u_{i-1}^n}{4} + \frac{u_i^n}{2}
  \]
  
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