Numerical Solutions of the Diffusion Equation

Larry Caretto
Mechanical Engineering 501AB

Seminar in Engineering Analysis

March 18, 2009

California State University Northridge

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

California State University Northridge 2

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

California State University Northridge 3

Review Finite Difference Grids

- 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

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

California State University Northridge 4

Review 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)

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

California State University Northridge 5

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^{th} order error by a^n

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

California State University Northridge 6

Review Derivative Expressions

- First-order error, first derivatives

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

- Second-order error, first derivatives

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

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

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

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

California State University Northridge

7

Find f' and f'' for sin at x = 1

Second order central

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

$$f_i' = \frac{\sin(1+.1) - \sin(1-.1)}{2(.1)} \qquad f_i'' = \frac{\sin(1+.1) + \sin(1-.1) - 2\sin(1)}{(.1)^2}$$

$$f_i' = \frac{\sin(1+.01) - \sin(1-.01)}{2(.01)} \qquad f_i'' = \frac{\sin(1+.01) + \sin(1-.01) - 2\sin(1)}{(.01)^2}$$

$$f_i' = \frac{\sin(1+.001) - \sin(1-.001)}{2(.001)} \qquad f_i'' = \frac{\sin(1+.001) + \sin(1-.001) - 2\sin(1)}{(.001)^2}$$

California State University Northridge

8

Review 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

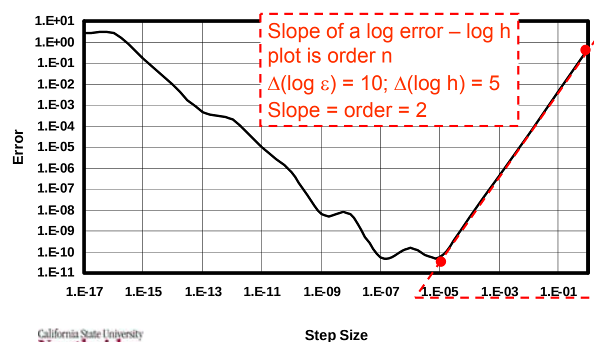
$$E = \frac{2.7185536702 - 2.7180100139}{2(0.0001)} - 2.718281828459 = 4.5x10^{-9}$$

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

California State University Northridge

9

Figure 2-1. Effect of Step Size on Error



California State University Northridge

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

California State University Northridge

11

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

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

California State University Northridge

12

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

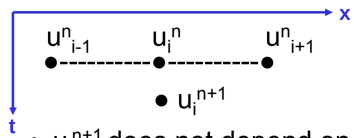
California State University Northridge 13

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)

California State University Northridge 14

Explicit Method Example

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

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

$$u_1^1 = f\left[u_0^0 + u_2^0\right] + (1-2f)u_1^0 = 0.16[0 + 1000] + 0.68[1000] = 840$$
$$u_2^1 = f\left[u_1^0 + u_3^0\right] + (1-2f)u_2^0 = 0.16[1000 + 1000] + 0.68[1000] = 1000$$
$$u_3^1 = f\left[u_2^0 + u_4^0\right] + (1-2f)u_3^0 = 0.16[1000 + 0] + 0.68[1000] = 840$$

- Repeat for subsequent time steps

California State University Northridge 15

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

California State University Northridge 16

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

California State University Northridge 17

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

California State University Northridge 18

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

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 $f = \alpha\Delta t/(\Delta x)^2 \le 0.5$
- 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

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

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

- 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^{n+1} depends on other u^{n+1}
  - More work per step, but can take longer time steps with this method
  - Apply to diffusion equation at time n + 1/2

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

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

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

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

$$f_{i+1} + f_{i-1} = 2 f_i + 2 f_i'' \frac{h^2}{2} + 2 f_i'''' \frac{h^4}{24} + \ldots..$$

$$f_i = \frac{f_{i+1} + f_{i-1}}{2} - f_i'' \frac{h^2}{4} - f_i'''' \frac{h^4}{48} + \ldots.. = \frac{f_{i+1} + f_{i-1}}{2} + O(h^2)$$

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

- Apply average to space derivative

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

- Substitute into diffusion equation

$$\left.\frac{\partial u}{\partial t}\right|_i^{n+\frac{1}{2}} - \alpha\left.\frac{\partial^2 u}{\partial x^2}\right|_i^{n+\frac{1}{2}} = \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

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

- Introduce $f = \alpha\Delta t/(\Delta x)^2$ and rearrange

California State University Northridge

25

Crank-Nicholson Equation

- Resulting equation has three values at new time step

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

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

- Tridiagonal system of equations easily solved by special application of Gauss elimination called Thomas algorithm

$$-fu_{i-1}^{n+1} + 2(1+f)u_i^{n+1} - fu_{i+1}^{n+1} = R_i^n$$

California State University Northridge

26

Crank-Nicholson Equations

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

$$\begin{bmatrix} 2(1-f) & -f & 0 & 0 & \cdots & 0 & 0 \\ -f & 2(1-f) & -f & 0 & \cdots & 0 & 0 \\ 0 & -f & 2(1-f) & -f & \cdots & 0 & 0 \\ 0 & 0 & -f & 2(1-f) & & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2(1-f) & -f \\ 0 & 0 & 0 & 0 & \cdots & -f & 2(1-f) \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ \vdots \\ u_{N-2}^{n+1} \\ u_{N-1}^{n+1} \end{bmatrix} = \begin{bmatrix} R_1^n + fu_0^n \\ R_2^n \\ R_3^n \\ \vdots \\ \vdots \\ R_{N-2}^n \\ R_{N-1}^n + fu_N^n \end{bmatrix}$$

California State University Northridge

27

Thomas Algorithm

- General format for tridiagonal equations

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

California State University Northridge

28

Thomas Algorithm II

- Gauss elimination upper triangular form

$$\begin{bmatrix} 1 & -E_0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -E_1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -E_2 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -E_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} F_0 \\ F_1 \\ F_2 \\ \vdots \\ \vdots \\ F_{N-1} \\ F_N \end{bmatrix}$$

California State University Northridge

29

Thomas Algorithm III

- Forward computations
  - Initial: $E_0 = -C_0 / B_0$ $F_0 = D_0 / B_0$
  - For i = 1,… N-1:

$$E_i = \frac{-C_i}{B_i + A_i E_{i-1}} \qquad F_i = \frac{D_i - A_i F_{i-1}}{B_i + A_i E_{i-1}}$$

- Get last x value first $x_N = F_N = \dfrac{D_N - A_N F_{N-1}}{B_N + A_N E_{N-1}}$
- Back substitute: $x_i = F_i + E_i x_{i+1}$

California State University Northridge

30

Crank Nicholson Results

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

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
	t = 0	1000	1000	1000	1000	1000
n = 0	t = 0+	0	1000	1000	1000	1000
n = 1	t = 0.0005	0	-73.35	423.96	690.85	834.09
n = 2	t = 0.001	0	352.75	305.27	440.73	599.81
n = 3	t = 0.0015	0	25.7	320.81	439.19	533.34
n = 4	t = 0.002	0	203.86	209.57	347.52	473.02
n = 5	t = 0.0025	0	56.79	252.91	334.12	422.43
n = 6	t = 0.003	0	141.46	177.47	298.2	397.48

California State University Northridge 31

Crank Nicholson Results II

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
n = 7	t = 0.0035	0	66.73	209.02	279.22	363.26
n = 8	t = 0.004	0	109.4	160.3	263.81	347.29
n = 9	t = 0.0045	0	68.71	179.63	245.68	324.49
n = 10	t = 0.005	0	90.79	148.2	237.92	311.75
n = 11	t = 0.0055	0	67.5	159.07	222.68	296.08
n = 12	t = 0.006	0	78.99	138.51	217.76	285.25
n = 13	t = 0.0065	0	65.08	144.07	205.56	273.92
n = 14	t = 0.007	0	70.94	130.31	201.68	264.62
n = 15	t = 0.0075	0	62.29	132.69	192.04	255.97
n = 16	t = 0.008	0	65.1	123.21	188.58	247.99
n = 17	t = 0.0085	0	59.5	123.75	180.95	241.06

California State University Northridge 32

Crank Nicholson Results III

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
n = 18	t = 0.009	0	60.65	117	177.71	234.21
n = 19	t = 0.0095	0	56.86	116.5	171.59	228.43
n = 20	t = 0.01	0	57.1	111.53	168.52	222.53
n = 21	t = 0.0105	0	54.43	110.47	163.53	217.57
n = 22	t = 0.011	0	54.19	106.68	160.64	212.45
n = 23	t = 0.0115	0	52.22	105.35	156.49	208.11
n = 24	t = 0.012	0	51.73	102.36	153.78	203.64
n = 25	t = 0.0125	0	50.21	100.93	150.27	199.78
Exact	t = 0.0125	0	50.43	100.66	150.48	199.72
Error	t = 0.0125	0	0.216	0.272	0.212	0.061

California State University Northridge 33

Fully Implicit Method

- Discretize diffusion equation at t_{n+1}

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

$$\left.\frac{\partial u}{\partial t}\right|_i^{n+1} - \alpha \left.\frac{\partial^2 T}{\partial x^2}\right|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} - \alpha \frac{u_{i+1}^{n+1} + u_{i-1}^{n+1} - 2u_i^{n+1}}{(\Delta x)^2} + O[(\Delta t), (\Delta x)^2] = 0$$

$$-fu_{i-1}^{n+1} + (1 + 2f)u_i^{n+1} - fT_{i+1}^{n+1} = u_i^n$$

- Tridiagonal system of equations
- Almost same work as CN and no spurious oscillations, but less accuracy

California State University Northridge 34

Fully Implicit Results

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

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
	t = 0	1000	1000	1000	1000	1000
n = 0	t = 0+	0	1000	1000	1000	1000
n = 1	t = 0.0005	0	358.26	588.17	735.71	830.39
n = 2	t = 0.001	0	218.22	408.43	562.69	682.35
n = 3	t = 0.0015	0	166.26	322.13	460.74	578.96
n = 4	t = 0.002	0	139.05	272.65	396.35	507.18
n = 5	t = 0.0025	0	121.84	240.25	352.17	455.26
n = 6	t = 0.003	0	109.75	217.08	319.77	415.99

California State University Northridge 35

Fully Implicit Results II

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
n = 7	t = 0.0035	0	100.65	199.49	294.81	385.13
n = 8	t = 0.004	0	93.50	185.57	274.85	360.14
n = 9	t = 0.0045	0	87.68	174.19	258.43	339.38
n = 10	t = 0.005	0	82.82	164.67	244.62	321.81
n = 11	t = 0.0055	0	78.69	156.56	232.81	306.69
n = 12	t = 0.006	0	75.13	149.54	222.55	293.50
n = 13	t = 0.0065	0	72.00	143.38	213.53	281.87
n = 14	t = 0.007	0	69.24	137.93	205.52	271.52
n = 15	t = 0.0075	0	66.77	133.05	198.35	262.22
n = 16	t = 0.008	0	64.55	128.66	191.88	253.82
n = 17	t = 0.0085	0	62.54	124.67	186.01	246.17

California State University Northridge 36

Fully Implicit Results III

		i = 0	i = 1	i = 2	i = 3	i = 4
		x = 0	x = .01	x = .02	x = .03	x = .04
n = 18	t = 0.009	0	60.70	121.03	180.64	239.17
n = 19	t = 0.0095	0	59.02	117.70	175.71	232.74
n = 20	t = 0.01	0	57.47	114.62	171.16	226.79
n = 21	t = 0.0105	0	56.03	111.78	166.95	221.28
n = 22	t = 0.011	0	54.70	109.13	163.04	216.16
n = 23	t = 0.0115	0	53.46	106.67	159.38	211.37
n = 24	t = 0.012	0	52.30	104.36	155.96	206.88
n = 25	t = 0.0125	0	51.21	102.20	152.76	202.67
Exact	t = 0.0125	0	50.43	100.66	150.48	199.72
Error	t = 0.0125	0	0.779	1.542	2.273	2.956

California State University Northridge 37

Richardson/Leapfrog

- Use two time step central differences

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

- Result is explicit with second order accuracy in time

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

- However result is unstable for any f and cannot be used

California State University Northridge 38

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

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

$$2u_i^n = u_i^{n+1} + u_i^{n-1} + O[(\Delta t)^2]$$

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

California State University Northridge 39

DuFort Frankel

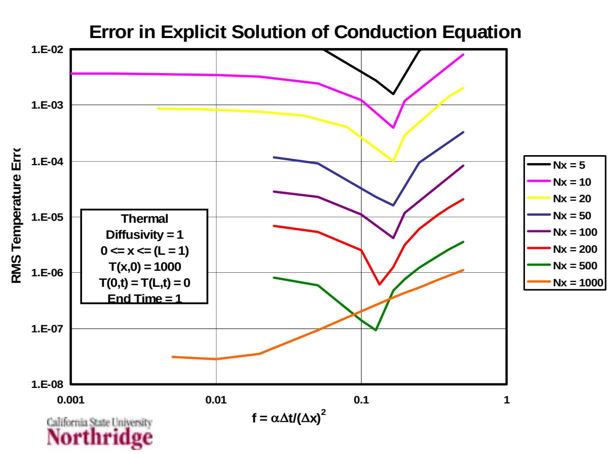
- Rearrange and introduce $f = \alpha\Delta t/(\Delta x)^2$

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

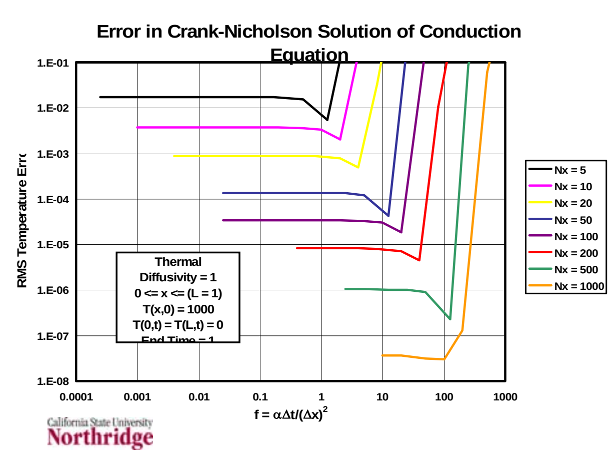
$$(1 + 2f)u_i^{n+1} = u_i^{n-1}(1 - 2f) + 2f\left(u_{i+1}^n + u_{i-1}^n\right)$$

- Result is explicit for values at time n+1
- Explicit start required to get first set of values at time n-1

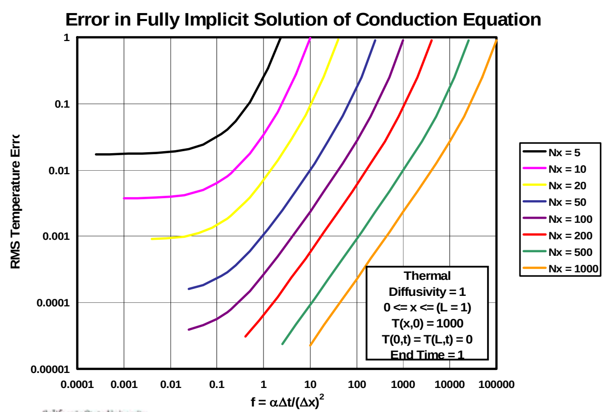
California State University Northridge 40



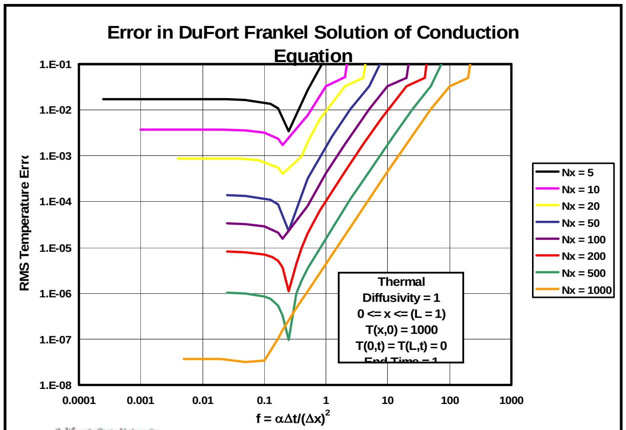
California State University Northridge



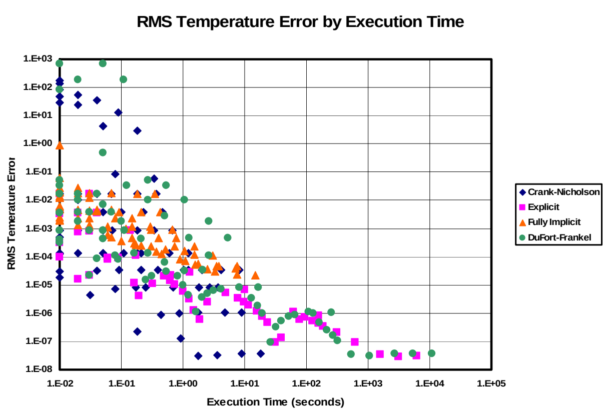
California State University Northridge



California State University Northridge



California State University Northridge



California State University Northridge

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

California State University Northridge 46

Explicit Method Example

- How many values can you compute for initial conditions below with f = 0.25

$$u_i^{n+1} = f\left(u_{i+1}^n + u_{i-1}^n\right) + (1 - 2f)u_i^n = \frac{u_{i+1}^n + u_{i-1}^n}{4} + \frac{u_i^n}{2}$$

?	70	80	90	100	90	80	70	?
?	?	80	90	95	90	80	?	?
?	?	?	88.75	92.5	88.75	?	?	?
?	?	?	?	90.625	?	?	?	?

California State University Northridge 47