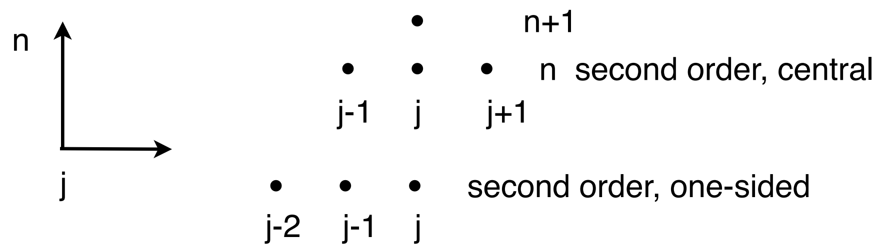
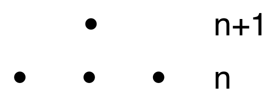
D. Some terminology

Stencil = set of points in the finite-difference scheme: refer to Euler Explicit

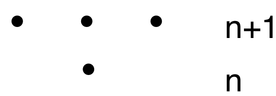


FTCS = Forward time centered space



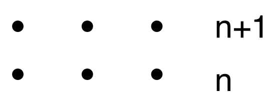
Euler explicit

BTCS = Backward time centered space



Euler implicit

CTCS = Centered time centered space



Crank-Nicholson Implicit

Euler implicit $$T_j^{n+1} - T_j^n = \alpha(T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1})$$

First order in time: $$T_j^{n+1} = T_j^n + \Delta t \partial_t T + O(\Delta t)^2$$

$$T_j^{n+1} = T_j^n + \frac{\kappa \Delta t}{\Delta x^2}(T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1}) + O(\Delta t)^2$$

E. Crank-Nicholson: Implicit, second order in time -- trapezoidal rule

Euler-explicit $$\frac{T_j^{n+1} - T_j^n}{\Delta t} = F(T^n) \quad \text{not centered in time} \Rightarrow \text{first order}$$

One idea, leap frog $$\frac{T_i^{n+1} - T_i^{n-1}}{2\Delta t} = F(T^n)$$ tends to be unstable.

Crank-Nicholson: $$\frac{T_j^{n+1} - T_j^n}{\Delta t} = F(T^{n+1/2}) = ½\left[F(T^n) + F(T^{n+1})\right]$$

For diffusion equation:

$$T_j^{n+1} - T_j^n = \frac{\alpha}{2}\left[(T_{j+1}^n - 2T_j^n + T_{j-1}^n) + (T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1})\right]$$

or $$(1+\alpha)T_j^{n+1} - \frac{\alpha}{2}T_{j+1}^{n+1} - \frac{\alpha}{2}T_{j-1}^{n+1} = (1-\alpha)T_j^n + \frac{\alpha}{2}T_{j+1}^n + \frac{\alpha}{2}T_{j-1}^n$$

L.h.s. is unknown, r.h.s. is known from previous time step. Linear algebra of the form

$\mathbf{A} \cdot \mathbf{T}^{n+1} = \mathbf{b}^n$

where **A** is the tri-diagonal matrix *Tridiag* {... α/2, (1+ α), α/2 ...}. Solve by Thomas algorithm.

Pseudo code
```
FOR t=Δt to NΔt
 DO 2,N-1
   A(i,1)=-α/2
   A(i,2)=1+α
   A(i,3)=-α/2
   b(i)=T_i + (α/2)(T_{j+1} + T_{j-1} - 2T_j)
 ENDDO
 Set A(1,:), A(N,:) to boundary conditions
 CALL THOMAS(A,b[rhs↓,ans↑])
T(:) = b(:) ; t=t+Δt  ! print
END FOR
```

Comments

1. Simple test:

   Constant wall temperature T(0)=Twall --> A(1,2)=1, A(1,3)=0, b(1)=T_{wall}

   T(1)=0

   Steady state solution

   $\partial_t T=\kappa\partial_x^2 T \rightarrow \partial_x^2 T$ so T=a+bx $\rightarrow$ T= T_{wall}(1-x)

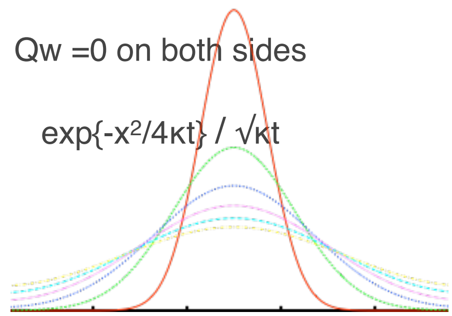
   T(x,t)=T_{wall} F(x,t). Long time T $\rightarrow$ T_{wall}(1-x)

   Or $\kappa\partial_x T_{wall} = Q_w$ for heat flux; T_{wall} floats.

   T(0)=0 and heat flux contition at x=1 has a solution: T=Q_w x/κ

   But can't have one heat flux and one insulated wall ($\kappa\partial_x T=0$).

2. Conservation of heat:



$$\int \partial_t T dx = \int \kappa\partial_x^2 T dx = \kappa(\partial_x T_1 - \partial_x T_0)$$
$$= Q_1 - Q_0 = 0$$

C.f. energy conserving schemes

3. Non-uniform diffusivity or grid.

$\int\kappa\partial^2 T/\partial x^2\, dx = -\int\partial\kappa/\partial x\, \partial T/\partial x\, dx \neq 0$ does not conserve heat

$$\int_0^L \partial_t T dx = \int_0^L \partial_x(\kappa\partial_x T)dx$$
$$= \kappa\partial_x T dx|_0^L = flux\ through\ walls$$

Discretization that is consistent (finite volume):

$$\delta_x(\kappa\delta_x T)_j = \frac{(\kappa\delta_x T)_{j+1/2} - (\kappa\delta_x T)_{j-1/2}}{x_{j+1/2} - x_{j-1/2}}$$

$$\delta_x(\kappa\delta_x T) = \frac{1}{x_{j+1/2} - x_{j-1/2}}\left[\frac{\kappa_{j+1/2}(T^n_{j+1} - T^n_j)}{x_{j+1} - x_j} - \frac{\kappa_{j-1/2}(T^n_j - T^n_{j-1})}{x_j - x_{j-1}}\right]$$
$$= \frac{2}{x_{j+1} - x_{j-1}}\left[\frac{\kappa_{j+1} + \kappa_j}{2}\frac{(T^n_{j+1} - T^n_j)}{x_{j+1} - x_j} - \frac{\kappa_j + \kappa_{j-1}}{2}\frac{(T^n_j - T^n_{j-1})}{x_j - x_{j-1}}\right]$$

F. Stability analysis

Recall o..d.e's: if $|x_{n+1}/x_n| > 1$ unstable, $\dot{x}=\alpha x$, $\alpha_r < 0$. Same idea for p.d.e. solvers

1. NB: Question is whether *error*, $\varepsilon(t)$, grows.
2. Stability of p.d.e. algorithms. Let $T = T_{exact} + \varepsilon(x,t)$. T_{exact} satisfies full equations and boundary conditions:

   $\delta_t T_{exact} = \kappa\, \delta^2_x T_{exact}$ + Source *and* non-homogeneous b.c.s

   $\delta_t\, \varepsilon = \kappa\, \delta^2_x\, \varepsilon$ *and* homogeneous boundary conditions (generally linearized eqn.)
3. Von Neuman (Fourier) analysis

   a. Representation of error = Σ sine waves. For linear problem can consider a single wave, with wavelength as a parameter: is any wavelength unstable?
   $\cos(n\pi x/L) = \cos(n\pi j/J) = \cos(j\Theta)$ *i.e.,* $\Theta = n\pi/J$, n=1,2,3...J

   NB: $e^{i\Theta} = \cos\Theta + i \sin\Theta$ where $i=\sqrt{-1}$

   proof: $F= e^{i\Theta}$; $F' = iF \Rightarrow F'' = -F$ with $F(0)=1$, $F'(0)=i$ $\therefore$ $F= A\cos\Theta + B\sin\Theta$, A=1, B=i

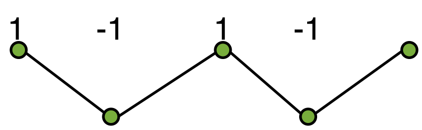
   Assume

   $$\varepsilon = a_n e^{i\Theta j}, \quad j=0,1,2,...J.. \quad \pi/J \approx 0 \le \Theta \le \pi$$

   Θ is phase change per grid point. Stability in unbounded domain (b.c.'s are difficult).

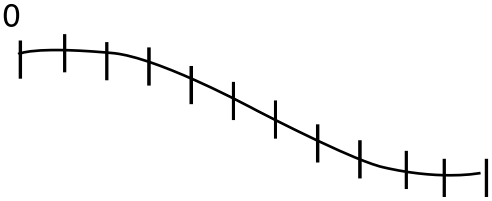
   Shortest wavelength, n=1; oscillation over three grid points or phase change of π per grid point.

   $\Theta = \pi$



   Longest wave, n = J; 1/2 wavelength across domain

   $\Theta = \pi/J$ j = 0



b. Euler Explicit (FTCS) for heat equation

$\varepsilon_j^{n+1} - \varepsilon_j^n = \alpha\,(\varepsilon_{j+1}^n + \varepsilon_{j-1}^n - 2\varepsilon_j^n)$

Assume $\varepsilon_j = a_n e^{i\Theta j}$; $\varepsilon_{j+1} = e^{i\Theta}\varepsilon_j$

$a_{n+1}\varepsilon_j = a^n\varepsilon_j + \alpha\, a^n\varepsilon_j(e^{i\Theta} + e^{-i\Theta} - 2)$

using $e^{i\Theta} + e^{-i\Theta} - 2 = (e^{i\Theta/2} - e^{-i\Theta/2})^2 = [2i \sin(\Theta/2)]^2 = -4\sin^2(\Theta/2)$ this becomes

$a_{n+1} = a_n(1 - 4\alpha \sin^2(\Theta/2))$ so the amplification factor is

$$\boxed{\mathrm{G} \equiv \left|\frac{a^{n+1}}{a^n}\right| = |1 - 4\alpha\sin^2(\theta/2)|}$$

c. If G < 1 *errors* damp, method is stable. Instability can occur if $4\alpha \sin^2(\Theta/2) > 2$. That gives $\alpha > 1/(2 \sin^2(\Theta/2))$. But $\sin^2(\Theta/2) \le 1$ so max is at $\Theta = \pi$ and unstable if $\alpha > 1/2$: dominant instability 

(see comment, good idea $1-2\alpha > 0$ from a previous lecture)

or $\alpha = \kappa\Delta t / \Delta x^2 < 1/2 \rightarrow \Delta t < \Delta x^2/2\kappa$ is stability condition. Small grid spacing requires small time-step

$$\boxed{\Delta t < \frac{\Delta x^2}{2\kappa}}$$

d. Euler Implicit (BTCS) unconditionally stable (review VonNeuman)

$\varepsilon_j^{n+1} - \varepsilon_j^n = \alpha\,(\varepsilon_{j+1}^{n+1} + \varepsilon_{j-1}^{n+1} - 2\varepsilon_j^{n+1})$

$a^{n+1} - \alpha\, a^{n+1} (e^{i\Theta} + e^{-i\Theta} - 2) = a^{n+1}(1 + 4\alpha \sin^2(\Theta/2)) = a^n$

Having used $e^{i\Theta} + e^{-i\Theta} - 2 = (e^{i\Theta/2} - e^{-i\Theta/2})^2 = -4 \sin^2(\Theta/2)$. The gain is

$$G = \left|\frac{a^{n+1}}{a^n}\right| = \left|\frac{1}{1 + 4\alpha\sin^2(\theta/2)}\right| < 1$$

Hence Euler *Implicit* is stable for all Δt; a.k.a., *unconditionally stable*

e. Crank-Nicholson (CTCS)

$\varepsilon_j^{n+1} - \alpha/2\ (\varepsilon_{j+1}^{n+1} + \varepsilon_{j-1}^{n+1} - 2\varepsilon_j^{n+1}) = \varepsilon_j^n + \alpha/2\ (\varepsilon_{j+1}^n + \varepsilon_{j-1}^n - 2\varepsilon_j^n)$

$a^{n+1}[1 - \alpha/2\ (e^{i\Theta} + e^{-i\Theta} - 2)] = a^n[1+ \alpha/2\ (e^{i\Theta} + e^{-i\Theta} - 2)]$

$$\left|\frac{a^{n+1}}{a^n}\right| = \left|\frac{1 - 2\alpha\sin^2(\theta/2)}{1 + 2\alpha\sin^2(\theta/2)}\right| \le 1$$

- Unconditionally stable (stable for all Δt). But for $\alpha > 1/2$ the sign of a^{n+1}/ a^n oscillates
- Stable, but Δt is constrained by accuracy.
- Large Δt can be useful for getting to steady state. But for C-N, $\Theta \rightarrow 0$ and $G \rightarrow 1$ when Δt is large; long wavelength errors damp slowly. Euler Implicit is better for getting to steady state: C-N errors oscillate; E-I errors damp.
- Relative merits

Implicit	**Explicit**
more work/time step	requires smaller Δt
C-N $O(\Delta t)^2$	Euler is $O(\Delta t)$; but can use A-B, R-K, or 3-point backward $(-T_n+4T_{n-1}-3T_{n-2})/2\Delta t$
Better stability (unconditional)	Stable for small Δt (conditional)

Trade off of work/time step versus stability (larger time-step)