Partial diff equation

- Huge topic!
- Diff. eqs with der. of more than one variable
- Often both space and time (but can be other things!)
- Examples from physics

  - Wave eq.: 1D $$\frac{\partial^2 u}{\partial x^2} = A \frac{\partial^2 u}{\partial t^2}$$

    2D $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = A \frac{\partial^2 u}{\partial t^2}$$

  - Diffusion eq. 1D $$\frac{\partial^2 u}{\partial x^2} = A \frac{\partial u}{\partial t}$$

  - Maxwell's eq. ...

  - Poisson's eq. 2D $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)$$

  - Schrödinger eq. 2D $$i \frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + f(x,y,t)\, u$$

- Classification of PDEs (here of two variables)

General 2nd order, linear PDE:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + f\left(u, x, y, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = G(x, y)$$

- Discriminant: $Q = B^2 - 4AC$
- Classification:

$Q < 0$: Elliptic

$Q = 0$: Parabolic (*) (analogy with class. of conic sections)

$Q > 0$: Hyperbolic

Examples:

- Poisson eq.: Elliptic
- Diffusion eq: Parabolic
- Wave eq: Hyperbolic

- Our focus:

Three methods:

- Forward diff.s (explicit)
- Backward diff (implicit)
- Crank-Nicolson (— " —)

- Partial diff eqs. (PDEs) cont

- Will look at

  1) Forward difference scheme

  2) Backward diff. scheme

  3) Crank-Nicolson

- Discretized partial derivatives:

- Example: 2 vars. $u(x,y) \longrightarrow u_{ij}$

- First derivatives:

$$\frac{\partial u}{\partial x} \approx \begin{cases} \dfrac{u_{i+1,j} - u_{ij}}{\Delta x} + \mathcal{O}(\Delta x) & \text{Forward diff.} \\[2ex] \dfrac{u_{ij} - u_{i-1,j}}{\Delta x} + \mathcal{O}(\Delta x) & \text{Backward diff.} \\[2ex] \dfrac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + \mathcal{O}(\Delta x^2) & \text{Central diff.} \end{cases}$$

(Similarly for $\frac{\partial u}{\partial y}$, keeping index i fixed.)

Notation: $\Delta x^2 = (\Delta x)^2$

- Second derivatives:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{(\Delta x)^2} + \mathcal{O}(\Delta x^2)$$

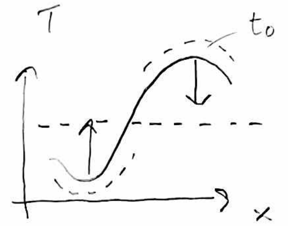
$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) \approx \frac{\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j}}{2\Delta x}$$

Using central difference for each derivative

We won't need this

$$\approx \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4\Delta x \Delta y} + \mathcal{O}(\Delta x^2, \Delta y^2)$$

- Example: 1D diffusion eq. (heat eq.)



Evolves towards equilibrium state

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \qquad D \text{ constant}$$

- We'll take $D=1$
- Will use notation that dist. space and time indices: $u(x,t) \rightarrow u_i^n$ (n ← time, i ← space)

1) Forward difference, a.k.a "the explicit scheme"

- Discretize + approximate, using F.D. for $\frac{\partial u}{\partial t}$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

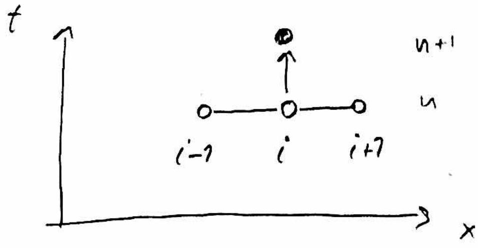
$$u_i^{n+1} = u_i^n + \frac{\Delta t}{\Delta x^2}\left[u_{i+1}^n - 2u_i^n + u_{i-1}^n\right]$$

- Define $\alpha \equiv \frac{\Delta t}{\Delta x^2}$

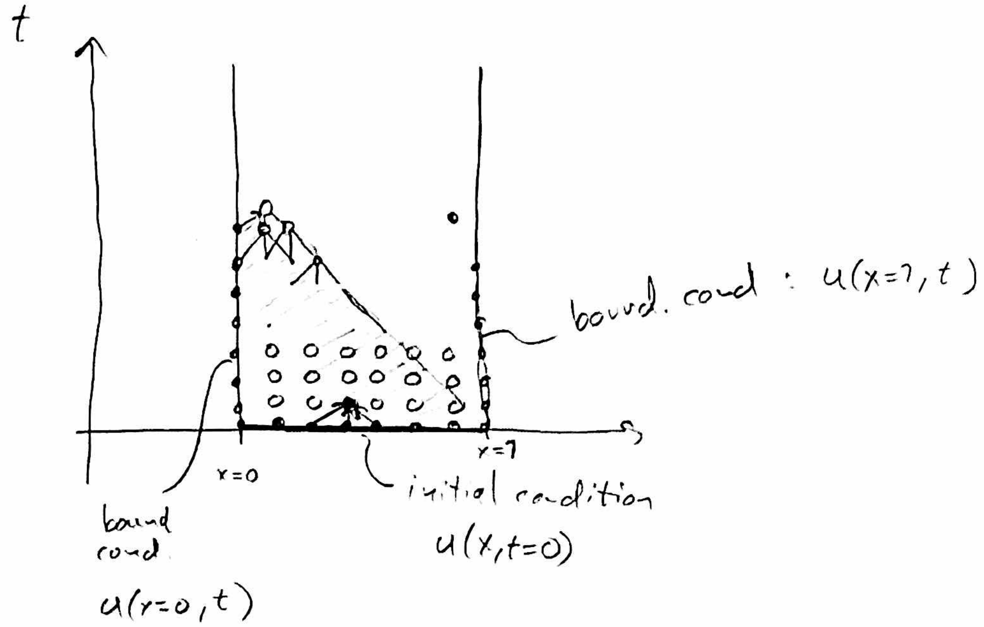
$$\boxed{u_i^{n+1} = (1-2\alpha)u_i^n + \alpha\left[u_{i+1}^n + u_{i-1}^n\right]} \qquad (*)$$

- <u>Explicit</u>: Can obtain u_i^{n+1} (next time step) using <u>only</u> solution at current time step (n)

[And no need to solve a system of eqs.]



"calculational molecule"



- Can express (*) as

$$\underline{\bar{u}^{n+1} = A\,\bar{u}^{n}}$$

[Just matrix multiplication, no need to solve a system of equations.]

where

$$A = \mathbb{1} - \alpha B$$

and $B = \text{tridiag}(-1, 2, -1)$

[But no need to perform the full matrix-vector multiplication here, since A is a simple tridiag (Avoid a bunch of 0-multiplic.)]

- Criterion for <u>stability</u>:

$$\boxed{\alpha = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}}$$

[With constant $D \neq 1$: $\alpha = \dfrac{D\,\Delta t}{\Delta x^2} \leq \dfrac{1}{2}$]

$$\Delta t \leq \tfrac{1}{2}\Delta x^2$$

To get high spatial resolution, need <u>tiny</u> time steps...

$\Delta x = 0.1 \Rightarrow \Delta t \leq \frac{1}{2}(0.1)^2 = 0.005$

$\Delta x = 0.01 \Rightarrow \Delta t \leq 0.00005$

[Shown in Morten's lecture notes. Based on "spectral radius" of matrix A, req. that $\rho(A) < 1$.]

[We'll look at this later]

- Accuracy : Global error from truncation is $O(\Delta x^2) + O(\Delta t)$

- Make sure to dist accuracy and stability.
  A method can be inaccurate but in a stable way,
  In and unstable case the solution eventually "blows up"

2) Backward difference scheme (An implicit scheme)

- Now use $\dfrac{\partial u}{\partial t} \approx \dfrac{u_i^n - u_i^{n-1}}{\Delta t}$

- So diffusion eq. becomes

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

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

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

- Three unknowns: $u_{i-1}^n, u_i^n, u_{i+1}^n$

- Cannot solve one such eq. in isolation, need the full sytem of eqs. to have N eqs. w/ N unknowns

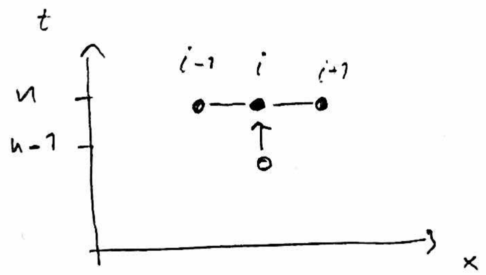
[Implicit scheme]

- Try inserting $n=1$, $n-1=0$
  $n=2$, $n-1=1$
  ⋮

$\Rightarrow$ Get familiar tridiagonal system of equations

$$\boxed{A\bar{u}^n = \underbrace{\bar{u}^{n-1}}_{\text{known}}} \quad \text{with } A = \text{tridiag}(-\alpha, 1+2\alpha, -\alpha)$$

or $$\boxed{\left[\mathbb{1} + \alpha B\right]\bar{u}^n = \bar{u}^{n-1}} \quad \text{with } B = \text{tridiag}(-1, 2, -1)$$



← calc. molecule

- We can solve $A\bar{u}^n = \bar{u}^{n-1}$ at every time step using e.g. a tridiagonal solver algo. (Proj. 1)
  for $\bar{u}^n$

- Stable for all choices of Δt, Δx, i.e. no requirement on $\alpha = \frac{\Delta t}{\Delta x^2}$ for stability. [But more work to implement than F.D.]

- Accuracy $\sim \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2)$ (Same as F.D.)

[Ended here.]

- Looking at diffusion eq. $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$, $D=1$
- FD method (a.k.a. Forward Time Centered Space, FTCS) and BD method (aka Backward Time Centered Space, BTCS) have accuracy $O(\Delta t) + O(\Delta x^2)$

7.5

- Want method with accuracy $O(\Delta t^2) + O(\Delta x^2)$

- Richardson scheme (1910): Use $\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t}$ (central difference)

  ↪ Get $O(\Delta t^2)$ accuracy, but scheme is <u>unstable</u>

$$\boxed{u_i^{n+1} = u_i^{n-1} + 2\alpha\left[u_{i+1}^n - 2u_i^n + u_{i-1}^n\right]}$$

- Dufort-Frankel scheme: Makes Richardson scheme stable by replacing

$$u_i^n \rightarrow \frac{1}{2}\left[u_i^{n+1} + u_i^{n-1}\right]$$

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

- <u>Explicit</u>, <u>stable</u>, <u>second-order accuracy</u> in space & time
- But "leapfrogs" in time, since u_i^n is absent. Requires three timesteps: $n+1$, n, $n-1$

→ Next: Crank Nicolson

John Crank
Phyllis Nicolson ~1947

3) Crank-Nicolson scheme (implicit)

- Consider the different time derivatives, $\boxed{\frac{\partial u}{\partial t} = F(x,t)}$

  - F.D. : $$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^n \qquad (1)$$

  - B.D., written with $\underline{n+1}$ and $\underline{n}$:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^{n+1}$$ ← Note

  - A linear combination of F.D. and B.D. is

$$\boxed{\frac{u_i^{n+1} - u_i^n}{\Delta t} = \theta F_i^{n+1} + (1-\theta) F_i^n} \quad , \theta \in [0,1]$$

"The θ rule"

$\theta = 1 \Leftrightarrow$ ~~F.D~~ B.D.
$\theta = 0 \Leftrightarrow$ ~~B.D.~~ F.D.

- Take $\theta = \frac{1}{2}$ to get Crank-Nicolson:

$$\boxed{\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left[F_i^{n+1} + F_i^n\right]}$$

F

- Apply to case of the diffusion eq.: $\boxed{\dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2}}$

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

- Collect (n+1) terms on LHS and n terms on the RHS
- Define $\alpha \equiv \dfrac{\Delta t}{\Delta x^2}$

$$\Rightarrow \quad \underline{-\alpha u_{i-1}^{n+1} + (2+2\alpha)u_i^{n+1} - \alpha u_{i+1}^{n+1} = \alpha u_{i-1}^n + (2-2\alpha)u_i^n + \alpha u_{i+1}^n}$$

Same type of expr. that you'll derive for the case of Schr. eq.

- Since we here only have 1+1 dim, nothing fancy req to put this into matrix form

[Just start writing out eqs. from n=0, n=1, ... to see pattern]

$$\boxed{A\bar{u}^{n+1} = B\bar{u}^n}$$

where $A = 2\cdot\mathbb{I} + \alpha T$, $T = \text{tridiag}(-1,2,-1)$

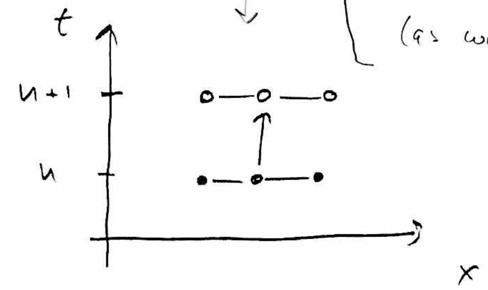
$B = 2\mathbb{I} - \alpha T$

- Solve in two steps:

1) Multiply $B\bar{u}^n \equiv \bar{b}$

2) Solve $A\bar{u}^{n+1} = \bar{b}$ for $\bar{u}^{n+1}$

- Accuracy $\sim O(\Delta t^2) + O(\Delta x^2)$
- Stable for all $\Delta x, \Delta t$
- Calc. molecule :



More computations per timestep, but gain higher accuracy, and keeps stability (as with B.D.)

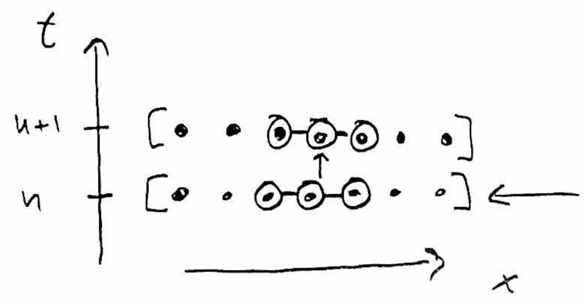
Summary of schemes :

Scheme	Accuracy	Stability req.
Forward diff (explicit)	$O(\Delta t) + O(\Delta x^2)$	$\Delta t \leq \frac{1}{2} \Delta x^2$
Backward diff (implicit)	$O(\Delta t) + O(\Delta x^2)$	any $\Delta t, \Delta x$
Crank-Nicolson	$O(\Delta t^2) + O(\Delta x^2)$	any $\Delta t, \Delta x$

... Many other methods / variations exist...

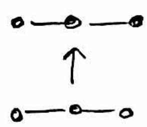
- Why is the formulation in terms of a matrix eq. more complicated with 2 (or more) space dim.?

- Consider C-N in 1+1 dim (x and t)



State of entire system at timestep n is already organized as a vector.

Comp. molecule:



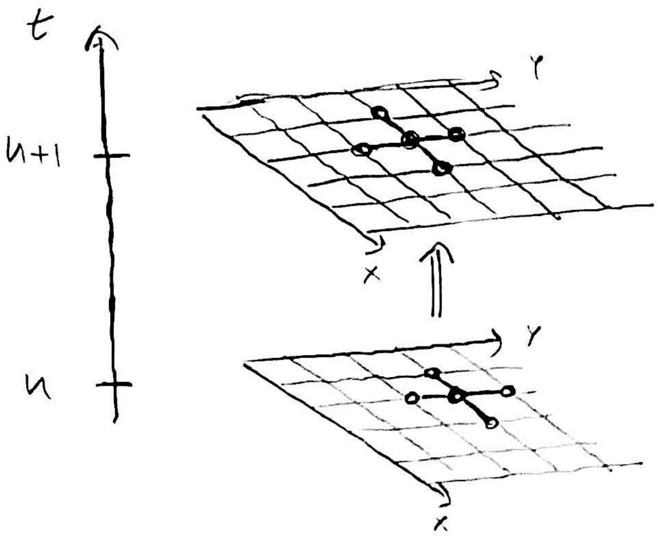
The points at a given timestep are only neighbours along one dimension

$\Rightarrow$ Gave rise to simple tridiag. structure for matrices A, B in

$$A\bar{u}^{n+1} = B\bar{u}^{n}$$

- Now look at 2+1 dim (x, y and t)

- Calc. molecule for C-N.

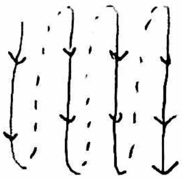


- Want to express update as matrix eq. (since implicit method)

$$A\bar{u}^{n+1} = B\bar{u}^{n}$$

- But any way to organize 2D xy grid in a 1D vector "breaks apart" some neighbours in the calc. molecule

Example:



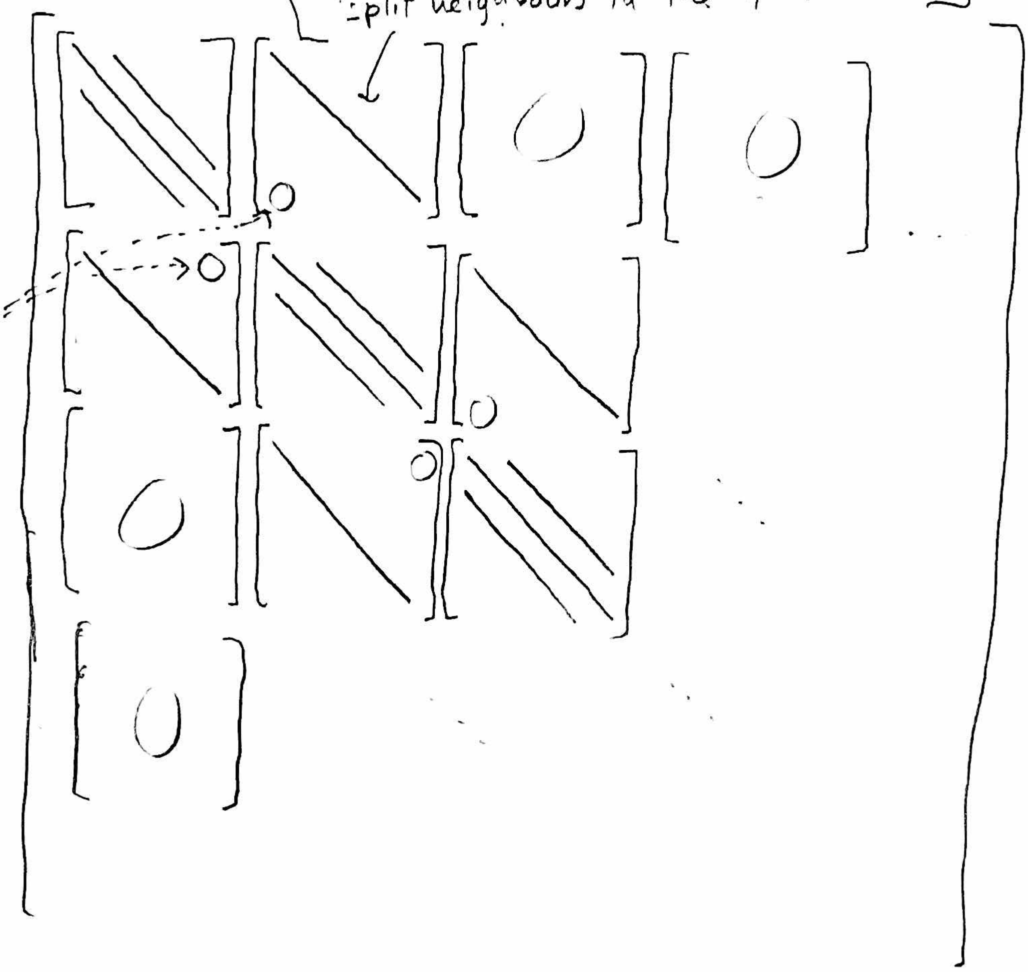
$$\begin{bmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{bmatrix} \longrightarrow \begin{array}{c} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \end{bmatrix} \end{array} \begin{array}{l} \\ \\ i,j-1 \\ \\ \\ i-1,j \\ ij \\ i+1,j \\ \\ \\ i,j+1 \\ \\ \\ \\ \\ \\ \end{array}$$

- Points in a single molecule gets pulled apart $\Rightarrow$ matrices A, B deviate from tridiag. structure (get additional diagonals, and inner band is no longer tridiag.)

[Get non-zero diagonals away from main diag., due to the split neighbours in the y-direction]

- Example

$A, B =$



Points where we hit boundary conditions

- Even higher dimensions

$\Downarrow$

more complicated matrix structure

(e.g. more off-diagonals.)