• Muddiest Points from Class 02/15

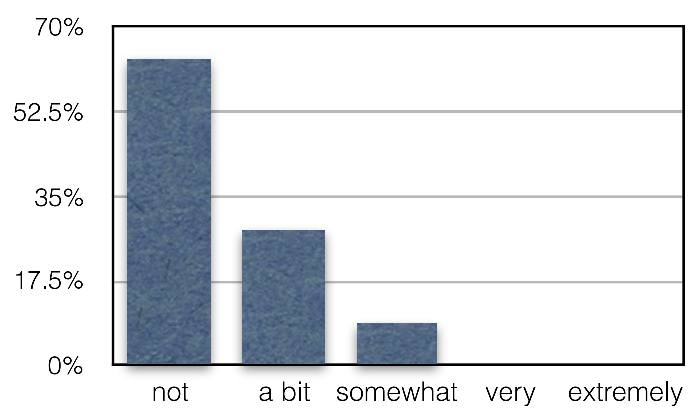
- *"In what cases would a cell centered mesh be important to implement?"*
  - cell centered meshes are perhaps the most common mesh type in CFD solvers
  - quantities like pressure, temperature, density are typically computed at cell centers

- *"Will there be many more opportunities to get the core course outcome #1?"*
  - yes, for example in homeworks 4, 5, 8, and bonus homework 11

- *"Is it possible to use multiple rows of ghost boxes for find a more accurate answer? If it is, how is that possible if the ghost boxes are estimates themselves?"*
  - yes, multiple layers of ghost cells are quite common.
  - all that is required is that the discrete formulas used to determine the ghost values are of the same or higher order than the discrete formulas used to solve the PDE

- *"On slide 12, you say discretize time and and show an eqtn t^n=n*delta_t. Why is time now an exponential? Or is that just a counter…?"*
  - the n is an index counter

- *"Should we code separate routines for node centered and cell centered meshes or should we combine things into one routine? Which is recommended?"*
  - code separate routines



Second Model Problem: Parabolic Equations

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Step 7: Solve (but how?)

- substitute into ODE

$$\left.\frac{d\varphi}{dt}\right|_i = \frac{\alpha}{h^2}\left(\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}\right) \qquad \left.\frac{d\varphi}{dt}\right|_i^n = \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right)$$

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$

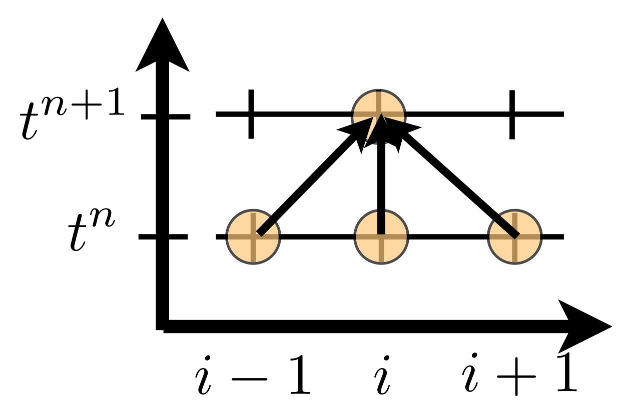
$$\boxed{\varphi_i^{n+1} = \varphi_i^n + \frac{\alpha \Delta t}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)}$$

FTCS <u>F</u>orward <u>T</u>ime <u>C</u>entral <u>S</u>pace

- FTCS expresses a single unknown, φ_i^{n+1}, as a function of only knowns!

  ⇒ feature of **explicit** methods

  solution at t^{n+1} depends only on solution at t^n

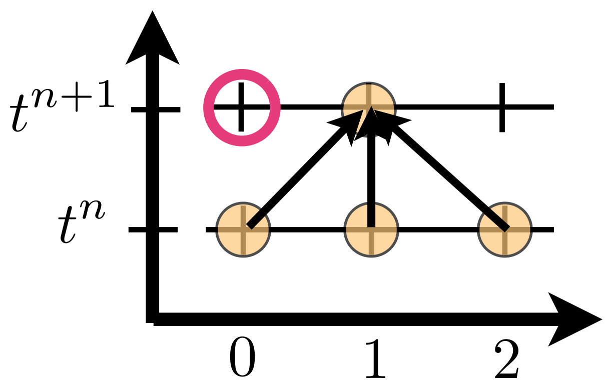


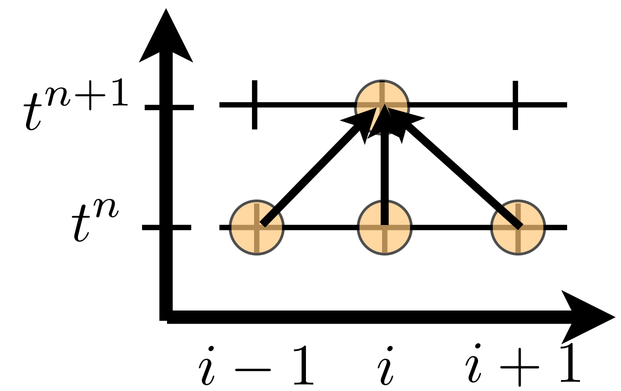
Second Model Problem: Parabolic Equations

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Step 7: Solve (but how?)

- BUT: problem at boundary





boundary point (bc) does not influence the solution at same t !

- boundaries lag by one time step
- this violates characteristics of parabolic equations

Second Model Problem: Parabolic Equations

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Step 7: Solve (but how?)

- Alternative: use backwards time difference: **Laasonen Method (BTCS)**

$$\left.\frac{d\varphi}{dt}\right|_i^{n+1} = \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right) \qquad \left.\frac{d\varphi}{dt}\right|_i = \frac{\alpha}{h^2}\left(\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}\right)$$

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}\right)$$

Problem: no longer explicit, but now implicit

- gather all *n+1* terms on left hand side

$$\boxed{\frac{\alpha \Delta t}{h^2}\varphi_{i-1}^{n+1} - \left(1 + 2\frac{\alpha \Delta t}{h^2}\right)\varphi_i^{n+1} + \frac{\alpha \Delta t}{h^2}\varphi_{i+1}^{n+1} = -\varphi_i^n}$$

$$\Rightarrow \quad a_i^n \varphi_{i-1}^{n+1} + b_i^n \varphi_i^{n+1} + c_i^n \varphi_{i+1}^{n+1} = d_i^n$$

$\Rightarrow$ tri-diagonal system

$\Rightarrow$ solve directly using Gauss (see Class 5)

$\Rightarrow$ much more work than FTCS! So, what's the benefit?

$\Rightarrow$ need to discuss accuracy, stability, and consistency

- Definitions:

1. **Consistency**: numerical approximation approaches PDE as $\Delta x, \Delta y, \Delta t \to 0$

2. **Stability**: numerical solution remains bounded

3. **Convergence**: numerical solution approaches PDE solution as $\Delta x, \Delta y, \Delta t \to 0$

turns out if 1. and 2. are true, then 3. is true for linear, well posed initial value problems

Accuracy

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

- both FTCS and BTCS use

$$\left.\frac{d\varphi}{dt}\right|_i^n \approx \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right) \qquad \left.\frac{d\varphi}{dt}\right|_i^{n+1} \approx \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right)$$

Taylor series:

$$\varphi_i^{n+1} = \varphi_i^n + \Delta t \left.\frac{\partial \varphi_i}{\partial t}\right|^n + O(\Delta t^2) \qquad \varphi_i^n = \varphi_i^{n+1} - \Delta t \left.\frac{\partial \varphi_i}{\partial t}\right|^{n+1} + O(\Delta t^2)$$

$$\left.\frac{d\varphi}{dt}\right|_i^n = \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right) + O(\Delta t) \qquad \left.\frac{d\varphi}{dt}\right|_i^{n+1} = \frac{1}{\Delta t}\left(\varphi_i^{n+1} - \varphi_i^n\right) + O(\Delta t)$$

both are first order in time

Consistency

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Consistency ≜ numerical approximation approaches PDE

<u>Example: FTCS</u>

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

- Question: Does this approach the PDE, as $\Delta x, \Delta t \to 0$?

Consistency

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

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

Need Taylor series for each term in FTCS

$$\varphi_i^{n+1} = \varphi_i^n + \Delta t \left.\frac{\partial \varphi}{\partial t}\right|^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 \varphi}{\partial t^2}\right|^n + O(\Delta t^3)$$

$$\varphi_{i+1}^n = \varphi_i^n + \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i + \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + \frac{\Delta x^4}{24}\left.\frac{\partial^4 \varphi}{\partial x^4}\right|_i + O(\Delta x^5)$$

$$\varphi_{i-1}^n = \varphi_i^n - \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i - \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + \frac{\Delta x^4}{24}\left.\frac{\partial^4 \varphi}{\partial x^4}\right|_i + O(\Delta x^5)$$

Substitute Taylor series into FTCS

$$\frac{1}{\Delta t}\left(\varphi_i^n + \Delta t \left.\frac{\partial \varphi}{\partial t}\right|^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 \varphi}{\partial t^2}\right|^n + O(\Delta t^3) - \varphi_i^n\right) = \frac{\alpha}{\Delta x^2}\left(\varphi_i^n + \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i + \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i\right.$$

$$\left. + \frac{\Delta x^4}{24}\left.\frac{\partial^4 \varphi}{\partial x^4}\right|_i + O(\Delta x^5) - 2\varphi_i^n + \varphi_i^n - \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i - \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + \frac{\Delta x^4}{24}\left.\frac{\partial^4 \varphi}{\partial x^4}\right|_i + O(\Delta x^5)\right)$$

$$\frac{\partial \varphi}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} + O(\Delta t^2) = \alpha\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 \varphi}{\partial x^4} + O(\Delta x)^3\right)$$

Consistency

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Consistency ≜ numerical approximation approaches PDE

<u>Example: FTCS</u>

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

Modified equation:

$$\frac{\partial \varphi}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} + O(\Delta t^2) = \alpha\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 \varphi}{\partial x^4} + O(\Delta x)^3\right)$$

- Question: Does this approach the PDE, as $\Delta x, \Delta t \rightarrow 0$?

as $\Delta x, \Delta t \rightarrow 0$: $\quad \frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$ ⇒ original PDE ⇒ FTCS is consistent

- Similar analysis shows that BTCS is consistent, too

- Definitions:

1. **Consistency**: numerical approximation approaches PDE as $\Delta x, \Delta y, \Delta t \rightarrow 0$

2. **Stability**: numerical solution remains bounded

3. **Convergence**: numerical solution approaches PDE solution as $\Delta x, \Delta y, \Delta t \rightarrow 0$

turns out if 1. and 2. are true, then 3. is true for linear, well posed initial value problems

Stability

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Consistency is not enough. We also need stability!

Stability:

- all methods introduce errors! What type of errors?
  - round-off errors (finite precision, ...)
  - discretization errors (truncation errors: Taylor series, method, ...)
- Question is what happens with these error?
  - if the errors grow ⇒ **unstable solution**

⇒ We need to understand and control errors ⇒ **stability analysis**

- Two options:
  - discrete perturbation analysis
  - von Neumann stability analys
- these are doable for model equations, but for full equations often too cumbersome ⇒ numerical experiments

Discrete Perturbation Analysis

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Idea: Introduce a perturbation (error) at one point and study its effect on its neighbors

- if perturbation decreases ⇒ stable
- if perturbation increases ⇒ unstable

Example: FTCS

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$

- introduce at point *i* a perturbation (error) *ε* at t^n: $\varphi_i^n \to \varphi_i^n + \varepsilon$

$$\frac{\varphi_i^{n+1} - (\varphi_i^n + \varepsilon)}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2(\varphi_i^n + \varepsilon) + \varphi_{i-1}^n\right)$$

- for simplicity, let's assume all $\varphi^n = 0$

$$\frac{\varphi_i^{n+1} - \varepsilon}{\Delta t} = -2\frac{\alpha}{h^2}\varepsilon \quad \Leftrightarrow \quad \varphi_i^{n+1} = \varepsilon\left(1 - 2\frac{\alpha \Delta t}{h^2}\right) \quad \Leftrightarrow \quad \boxed{\frac{\varphi_i^{n+1}}{\varepsilon} = (1 - 2B)}$$

$$B = \frac{\alpha \Delta t}{h^2}$$

Discrete Perturbation Analysis

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

This was of course a bit simplistic, because in general $\varphi^n \neq 0$

- let's drop this simplification
- Question: if we introduce a perturbation ε_i^n, what's the perturbation ε_i^{n+1}?

$$\frac{\varphi_i^{n+1} + \varepsilon_i^{n+1} - (\varphi_i^n + \varepsilon_i^n)}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2(\varphi_i^n + \varepsilon_i^n) + \varphi_{i-1}^n\right)$$

subtract FTCS from this

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$

$$\frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = -2\frac{\alpha}{h^2}\varepsilon_i^n \quad \Leftrightarrow \quad \varepsilon_i^{n+1} = \varepsilon_i^n\left(1 - 2\frac{\alpha \Delta t}{h^2}\right) \quad \Leftrightarrow \quad \boxed{\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n} = (1 - 2B)}$$

- exact same as before! $\frac{\varphi_i^{n+1}}{\varepsilon} = (1 - 2B)$

Discrete Perturbation Analysis

$$\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n} = (1 - 2B)$$

For stability, the error must not grow $\Rightarrow \left| \dfrac{\varepsilon_i^{n+1}}{\varepsilon_i^n} \right| \leq 1$

$$\Leftrightarrow \quad |1 - 2B| \leq 1 \quad \Leftrightarrow \quad -1 \leq 1 - 2B \leq 1$$

right limit:

$$1 - 2B \leq 1 \quad | -1 \quad \Leftrightarrow \quad -2B \leq 0 \quad \Leftrightarrow \quad B \geq 0 \quad \Leftrightarrow \quad \frac{\alpha \Delta t}{h^2} \geq 0 \quad ✓$$

left limit:

$$-1 \leq 1 - 2B \quad | -1 \quad \Leftrightarrow \quad -2 \leq -2B \quad | : (-2) \quad \Leftrightarrow \quad \boxed{B \leq 1} \quad \Leftrightarrow \quad \frac{\alpha \Delta t}{h^2} \leq 1$$

$$\boxed{\Delta t \leq \frac{h^2}{\alpha}}$$

Discrete Perturbation Analysis

$$\varphi_i^{n+1} = (1-2B)\varepsilon \qquad B = \frac{\alpha \Delta t}{h^2}$$

But this tells us only how the perturbation propagates in time.
What about space?

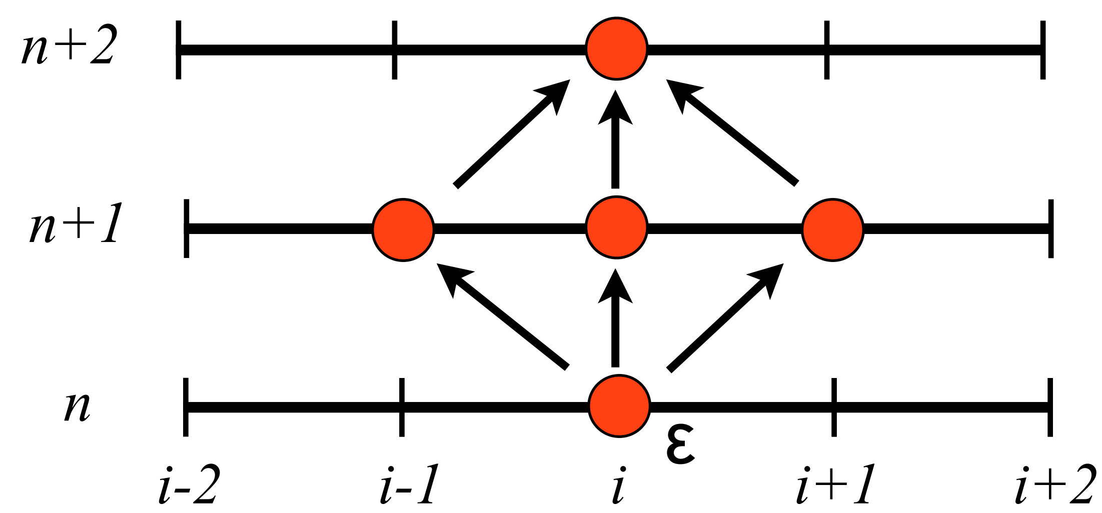
Q: What's the impact on i+1 (at n+1)?

$$\frac{\varphi_{i+1}^{n+1} - \varphi_{i+1}^{n}}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+2}^{n} - 2\varphi_{i+1}^{n} + (\varphi_i^n + \varepsilon_i^n)\right)$$

for simplicity, again $\varphi^n = 0$

$$\varphi_{i+1}^{n+1} = B\varepsilon \qquad \varphi_{i-1}^{n+1} = B\varepsilon$$

error spreads in space!



Q: What's the impact on i (at n+2)?

$$\frac{\varphi_i^{n+2} - \varphi_i^{n+1}}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}\right) \Leftrightarrow \quad \varphi_i^{n+2} = \varphi_i^{n+1} + B\left(\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}\right)$$

$$\varphi_i^{n+2} = (1-2B)\varepsilon + B\left(B\varepsilon - 2(1-2B)\varepsilon + B\varepsilon\right)$$

$$\varphi_i^{n+2} = \varepsilon\left(1 - 4B + 6B^2\right)$$

Discrete Perturbation Analysis

$$\varphi_i^{n+1} = (1-2B)\varepsilon \qquad B = \frac{\alpha\Delta t}{h^2}$$

$$\varphi_{i+1}^{n+1} = B\varepsilon \qquad \varphi_{i-1}^{n+1} = B\varepsilon$$

$$B \leq 1$$

Q: What's the impact on i (at n+2)?

$$\varphi_i^{n+2} = \varepsilon\left(1-4B+6B^2\right)$$

for stability, we must have $\left|\frac{\varphi_i^{n+2}}{\varepsilon}\right| \leq 1$

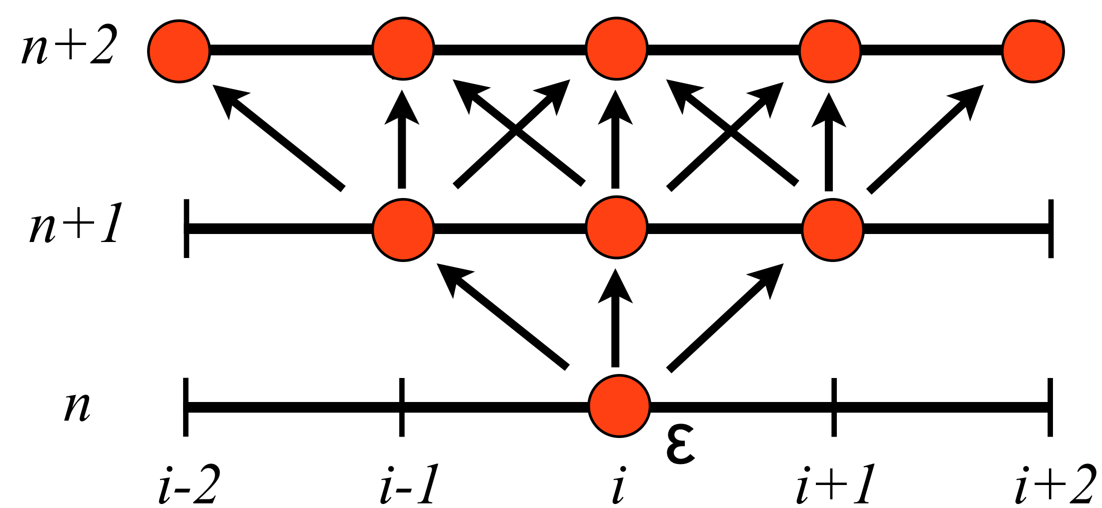
$$\left|1-4B+6B^2\right| \leq 1$$

$$1-4B+6B^2 \leq 1 \quad \wedge \quad 1-4B+6B^2 \geq -1$$

$$-4B+6B^2 \leq 0 \quad \wedge \quad -4B+6B^2 \geq -2$$

$$-4+6B \leq 0 \quad \wedge \quad 2B-3B^2 \leq 1$$

$$\boxed{B \leq \frac{2}{3}} \quad \wedge \quad B(2-3B) \leq 1 \;\checkmark$$



Q: What's the impact on i+1 (at n+2)?

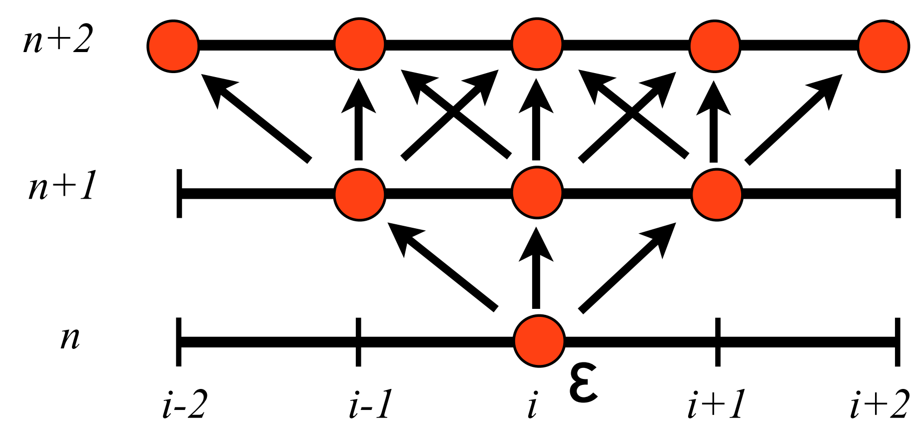
$$\varphi_{i+1}^{n+2} = 2B(1-2B)\varepsilon$$

Q: What's the impact on i+2 (at n+2)?

$$\varphi_{i+2}^{n+2} = B^2\varepsilon$$

etc.

Discrete Perturbation Analysis



In the end, the error will reach every grid point with approximately the **same magnitude**

⇒ 2 cases:

- case 1: error has same sign everywhere

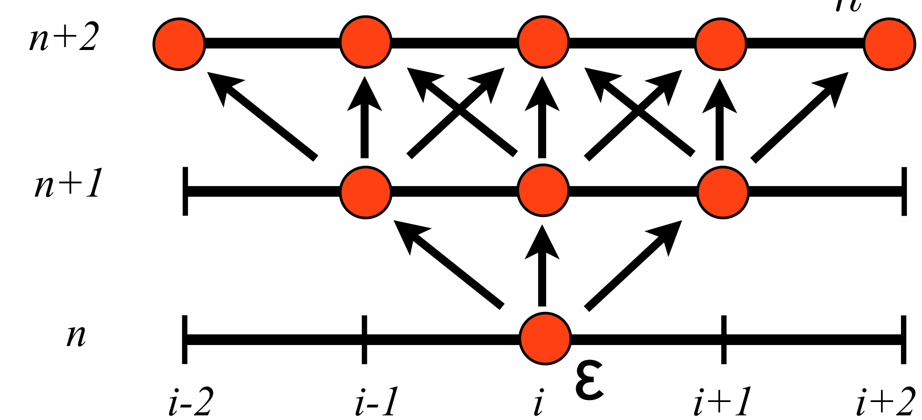
$$\varphi_{i-1}^m = \varepsilon^m \qquad \varphi_i^m = \varepsilon^m \qquad \varphi_{i+1}^m = \varepsilon^m$$

substitute into FTCS: $$\frac{\varphi_i^{m+1} - \varphi_i^m}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^m - 2\varphi_i^m + \varphi_{i-1}^m\right)$$

$$\frac{\varphi_i^{m+1} - \varepsilon^m}{\Delta t} = \frac{\alpha}{h^2}\left(\varepsilon^m - 2\varepsilon^m + \varepsilon^m\right) \quad \Rightarrow \quad \varphi_i^{m+1} = \varepsilon^m$$

Discrete Perturbation Analysis

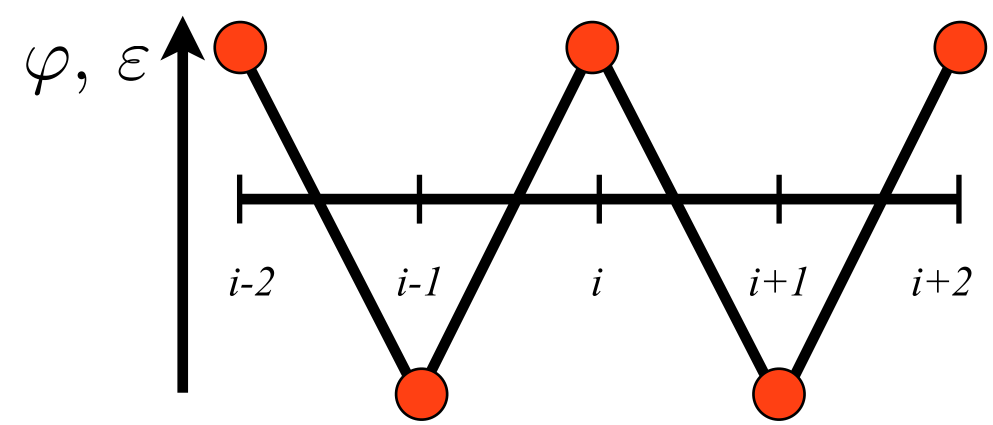
$$B = \frac{\alpha \Delta t}{h^2}$$



In the end, the error will reach every grid point with approximately the **same magnitude**

⇒ 2 cases:

- case 2: error alternates sign



$$\varphi_{i-1}^m = -\varepsilon^m \qquad \varphi_i^m = \varepsilon^m \qquad \varphi_{i+1}^m = -\varepsilon^m$$

substitute into FTCS:

$$\frac{\varphi_i^{m+1} - \varphi_i^m}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^m - 2\varphi_i^m + \varphi_{i-1}^m\right)$$

$$\frac{\varphi_i^{m+1} - \varepsilon^m}{\Delta t} = \frac{\alpha}{h^2}\left(-\varepsilon^m - 2\varepsilon^m - \varepsilon^m\right) \qquad \varphi_i^{m+1} = \varepsilon^m - 4B\varepsilon^m = \varepsilon^m(1-4B)$$

stable, if $\left|\frac{\varphi_i^{m+1}}{\varepsilon^m}\right| \leq 1$ $\qquad |1-4B| \leq 1$

$$1 - 4B \leq 1 \quad \wedge \quad 1 - 4B \geq -1$$

$$-4B \leq 0 \;\checkmark \quad \wedge \quad B \leq \frac{1}{2}$$

$$\boxed{\Delta t \leq \frac{1}{2}\frac{h^2}{\alpha}}$$

but quite tedious on paper.
Useful numerically!
Alternative: von Neumann