Mathematical Formulation

- The purpose of a finite difference equation is to approximate the partial differential equation (PDE) while maintaining the physical meaning.
- Example PDE:

$$\frac{\partial^2 p}{\partial x^2} = \frac{\phi \mu c_t}{k} \frac{\partial p}{\partial t} \tag{1}$$

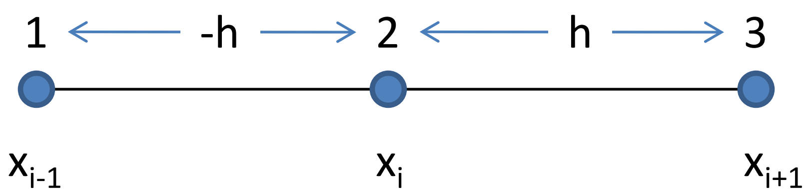
- FDEs are usually formulated by Taylor Series Expansion about a point and neglecting higher order terms

$$\psi_{(x+h)} = \psi_{(x)} + h\psi_x + \frac{h^2}{2}\psi_{xx} + \frac{h^3}{6}\psi_{xxx} + \ldots + \frac{1}{(n-1)!}h^{n-1}\psi_{x^{n-1}} \tag{2}$$

where ψ is an arbitrary function and h is distance between points.

Mathematical Formulation

- Taylor series expansion about point 2



- Define $h = x_{i+1} - x_i = \Delta x$, then

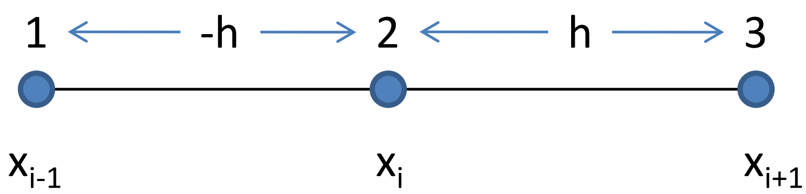
$$\psi_{(x_{i+1})} = \psi_{(x_i)} + \Delta x \psi_{x_i} + \frac{\Delta x^2}{2}\psi_{xx\,i} + \frac{\Delta x^3}{6}\psi_{xxx\,i} + \ldots \qquad (3)$$

- For point 2,

$$\psi_3 = \psi_2 + \Delta x\left(\frac{d\psi}{dx}\right)_2 + \frac{\Delta x^2}{2}\left(\frac{d^2\psi}{dx^2}\right)_2 x + \frac{\Delta x^3}{6}\left(\frac{d^3\psi}{dx^3}\right)_2 + \ldots \qquad (4)$$

Mathematical Formulation

- Taylor series expansion about point 2



- Equation 4 can be rearranged as:

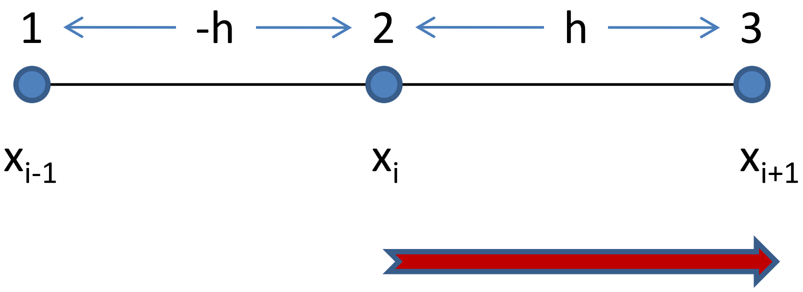
$$\left(\frac{d\psi}{dx}\right)_2 = \frac{\psi_3 - \psi_2}{\Delta x} - \underbrace{\frac{\Delta x}{2}\left(\frac{d^2\psi}{dx^2}\right)_2 - \frac{\Delta x^2}{6}\left(\frac{d^3\psi}{dx^3}\right)_2 + \ldots}_{\text{Truncation error}} \quad (5)$$

Truncation error

Known as first order accuracy O(Δx)
since Δx is the first term of TE

Mathematical Formulation

- Taylor series expansion about point 2

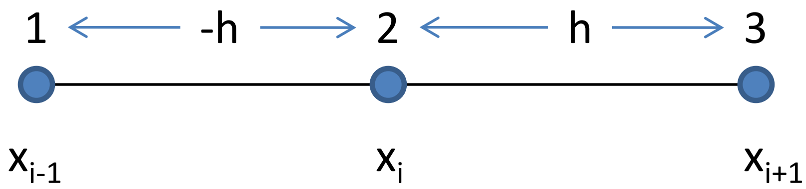


- Known as **forward difference, upwind or upstream**

$$\left(\frac{d\psi}{dx}\right)_2 = \frac{\psi_3 - \psi_2}{\Delta x} \tag{6}$$

Mathematical Formulation

- Taylor series expansion about point 2



- Define h = $x_i - x_{i-1}$ = $-\Delta x$, then

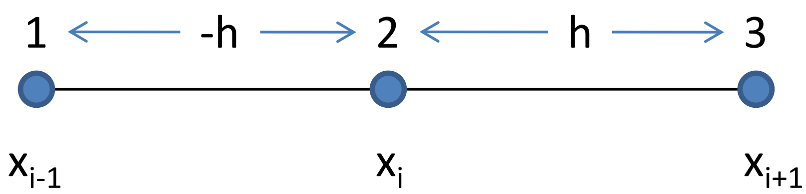
$$\psi_{(x_{i-1})} = \psi_{(x_i)} - \Delta x \psi_{x_i} + \frac{\Delta x^2}{2}\psi_{xx\,i} - \frac{\Delta x^3}{6}\psi_{xxx\,i} + \ldots \qquad (7)$$

- For point 2,

$$\psi_1 = \psi_2 - \Delta x\left(\frac{d\psi}{dx}\right)_2 + \frac{\Delta x^2}{2}\left(\frac{d^2\psi}{dx^2}\right)_2 - \frac{\Delta x^3}{6}\left(\frac{d^3\psi}{dx^3}\right)_2 + \ldots \qquad (8)$$

Mathematical Formulation

- Taylor series expansion about point 2



- Equation 4 can be rearranged as:

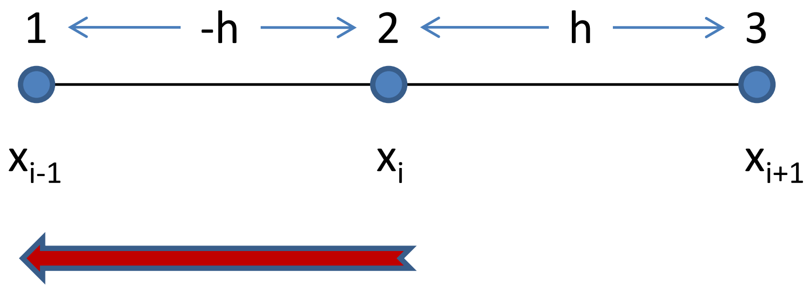
$$\left(\frac{d\psi}{dx}\right)_2 = \frac{\psi_2 - \psi_1}{\Delta x} + \frac{\Delta x}{2}\left(\frac{d^2\psi}{dx^2}\right)_2 - \frac{\Delta x^2}{6}\left(\frac{d^3\psi}{dx^3}\right)_2 + \ldots \qquad (9)$$

Truncation error

Known as first order accuracy $O(\Delta x)$
since Δx is the first term of TE

Mathematical Formulation

- Taylor series expansion about point 2



- Known as **backward difference, downwind or downstream**

$$\left(\frac{d\psi}{dx}\right)_2 = \frac{\psi_2 - \psi_1}{\Delta x} \qquad (10)$$

- Forward and backward scheme significant in both accuracy of approximation and mobility weighting scheme

Mathematical Formulation

- Since the Taylor series expansion is only valid when $\Delta x \to 0$, the desire is to have Δx small. Therefore higher order accuracy is preferred.

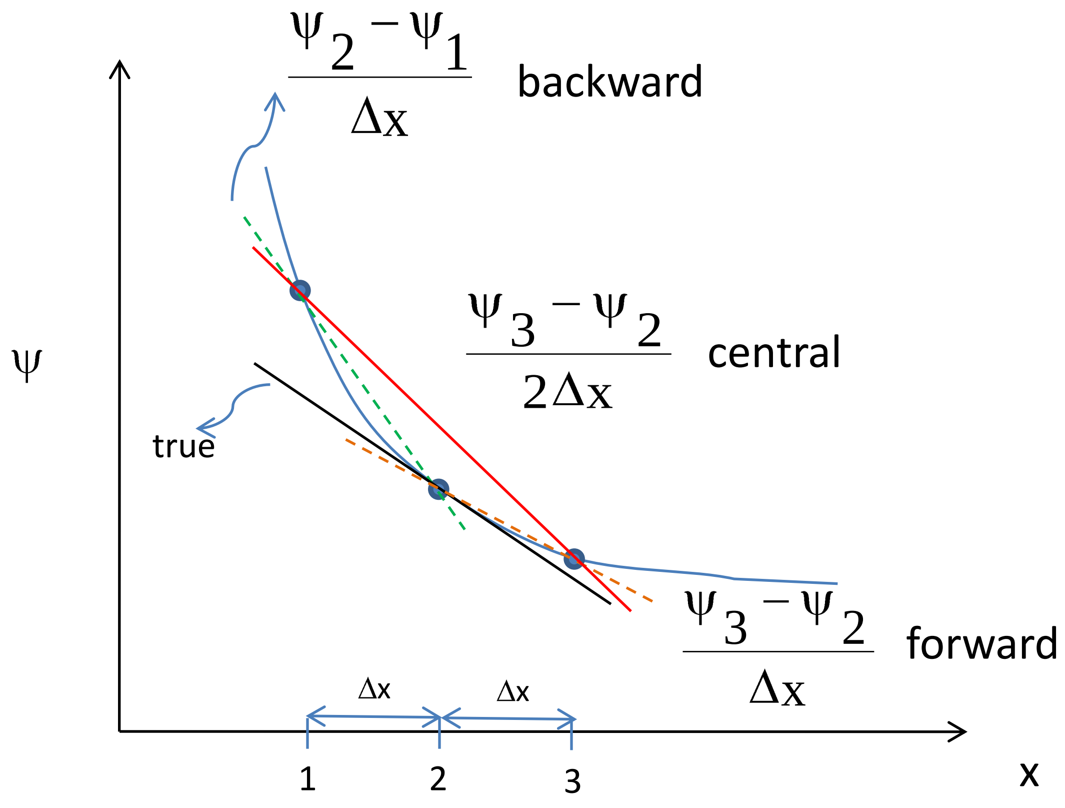
$$\Delta x > (\Delta x)^2 > (\Delta x)^3 \ldots$$

- How to increase the accuracy of FDE of $(d\psi/dx)_2$?
  - Average Equation (5) and (9)

$$\left(\frac{d\psi}{dx}\right)_2 = \frac{\psi_3 - \psi_2}{2\Delta x} - \frac{1}{6}\Delta x^2 \left(\frac{d^3\psi}{dx^3}\right)_2 + \ldots. \qquad (11)$$

- Which is 2nd order in accuracy
- Known as **central difference**

Mathematical Formulation



Comparison of forward, backward and central difference approximation for a smooth, continuous function

Mathematical Formulation

- How to approximate $(d^2\psi/dx^2)$?
  - Combine Equations (4) and (8)

$$\left(\frac{d^2\psi}{dx^2}\right)_2 = \frac{\psi_3 - 2\psi_2 + \psi_1}{\Delta x^2} - \underbrace{\frac{1}{12}\Delta x^2 \left(\frac{d^4\psi}{dx^4}\right)_2}_{\text{Truncation error}} + \ldots. \qquad (12)$$

- Which is 2nd order in accuracy…$O(\Delta x)^2$

Mathematical Formulation

- Truncation Error
  - For a function $\psi = 8x^4 + 2x + 7$ what is the truncation error, TE, of the FDE for Δx = 1 and 0.01?

$$\left(\frac{d^2\psi}{dx^2}\right)_2 = \frac{\psi_3 - 2\psi_2 + \psi_1}{\Delta x^2} - \underbrace{\frac{1}{12}\Delta x^2\left(\frac{d^4\psi}{dx^4}\right)_2}_{\text{Truncation error}} + \ldots. \qquad (12)$$

Mathematical Formulation

- Truncation Error **(Solution)**
  - For a function $\psi = 8x^4 + 2x + 7$ what is the truncation error, TE, of the FDE for Δx = 1 and 0.01?

$$\psi'_x = 32x^3 + 2$$

$$\psi''_x = 96x^2$$

$$\psi'''_x = 192x$$

$$\psi''''_x = 192$$

$$TE = -\frac{1}{12}\Delta x^2 \left(\frac{d^4\psi}{dx^4}\right)_2$$

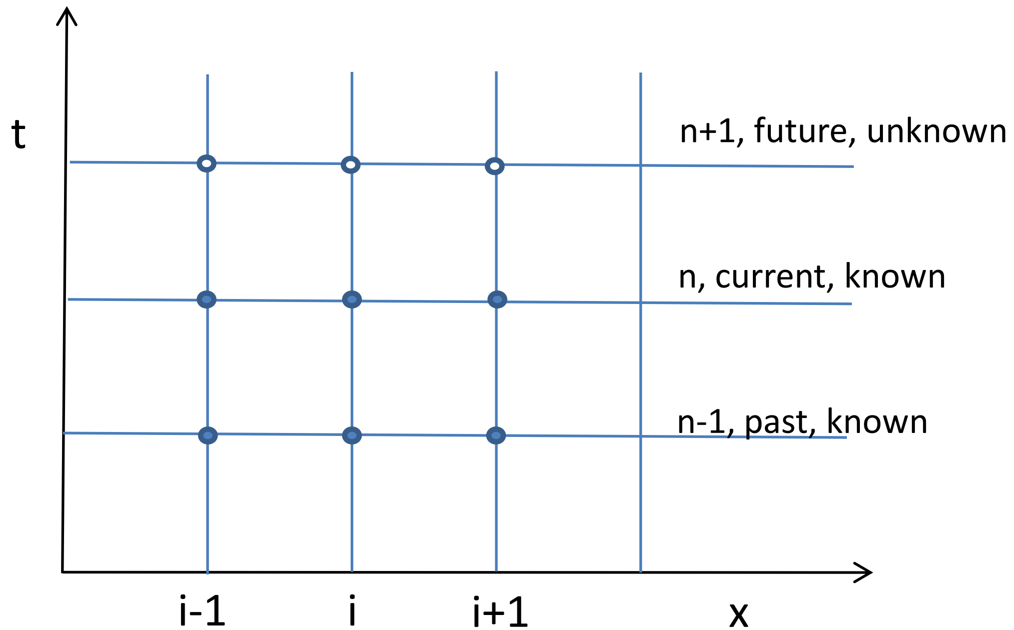
$$TE = -\frac{1}{12}\Delta x^2 * 192$$

- For Δx = 1 $\quad TE = -\frac{1}{12}(1)^2 * 192 = -16$
- For Δx = 0.01 $\quad TE = -\frac{1}{12}(0.01)^2 * 192 = -0.0016$
- Example shows that a decrease in grid size will reduce the truncation error, TE.

- Diffusivity equation is expressed by:

$$D\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \quad (13)$$

- Where D is the dispersion coefficient and C is concentration
- Its discretized field or **domain** is,



Mathematical Formulation — 1D Transient Problem

- Nomenclature

$$\psi^{n}_{i,j,k} \tag{14}$$

n: time; i: x direction; j: y direction; k: z direction

- Expand Eq. (13),

At time level, n
$$\left(\frac{\partial C}{\partial t}\right)_i^n = \left(D\frac{\partial^2 C}{\partial x^2}\right)_i^n \tag{15}$$

At time level n+1
$$\left(\frac{\partial C}{\partial t}\right)_i^{n+1} = \left(D\frac{\partial^2 C}{\partial x^2}\right)_i^{n+1} \tag{16}$$

- Eqs (15) and (16) can be expanded in space using central difference, Eq. (12)

$$\left(\frac{\partial C}{\partial t}\right)_i^n = \left(D\frac{\partial^2 C}{\partial x^2}\right)_i^n = D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} \tag{17}$$

$$\left(\frac{\partial C}{\partial t}\right)_i^{n+1} = \left(D\frac{\partial^2 C}{\partial x^2}\right)_i^{n+1} = D\frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{\Delta x^2} \tag{18}$$

- In time direction:

Can $\left(\frac{\partial C}{\partial t}\right)_i^{n+1}$ be approximated by $\frac{C_i^{n+2} - C_i^n}{2\Delta t}$?

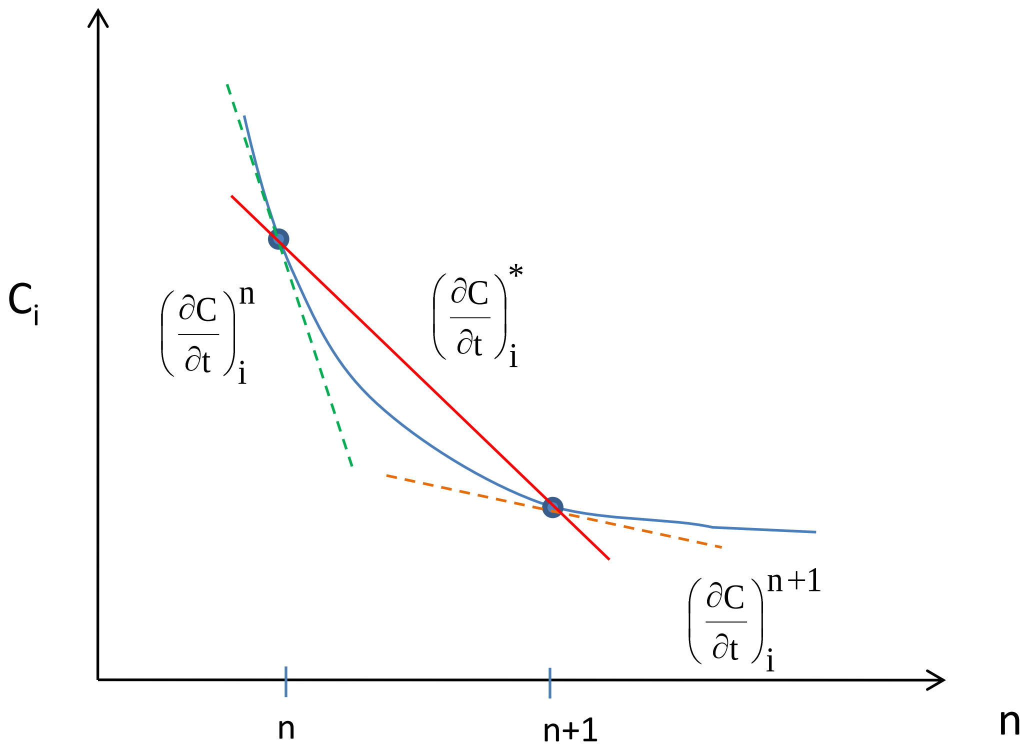
Can $\left(\frac{\partial C}{\partial t}\right)_i^{n} = \frac{C_i^{n+1} - C_i^{n-1}}{2\Delta t}$?

- One-way vs two-way coordinate
  - Does what happens at time n+1 only be affected by values at time level, n and not at time level, n+2 ?
  - Time considered a one-way coordinate
  - Space is referred to as a two-way coordinate

- In time direction, suggest between n and n+1, use

$$\left(\frac{\partial C}{\partial t}\right)_i^* = \frac{C_i^{n+1} - C_i^n}{\Delta t} \tag{19}$$

- How to relate Eq (19) with Eqs (17) and (18)?



- Let's define a weighting scheme,

$$\left(\frac{\partial C}{\partial t}\right)_i^* = \theta\left(\frac{\partial C}{\partial t}\right)^{n+1} + (1-\theta)\left(\frac{\partial C}{\partial t}\right)^{n} \tag{20}$$

- Combine Eqs (17-19), we have a complete algebraic equation,

$$\theta\left[D\,\frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{\Delta x^2}\right] + (1-\theta)\left[D\,\frac{C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n}}{\Delta x^2}\right]$$

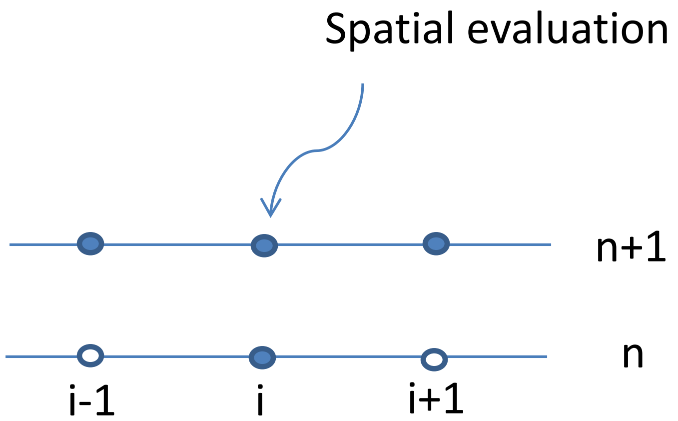
$$= \frac{C_i^{n+1} - C_i^{n}}{\Delta t} \qquad O(\Delta x^2, \Delta t) \tag{21}$$

- For θ = 1, **Fully Implicit Method**

$$\theta\left[D\frac{C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}}{\Delta x^2}\right]+(1-\theta)\left[D\frac{C_{i+1}^{n}-2C_i^{n}+C_{i-1}^{n}}{\Delta x^2}\right]$$

$$=\frac{C_i^{n+1}-C_i^{n}}{\Delta t}$$

- Need matrix solver

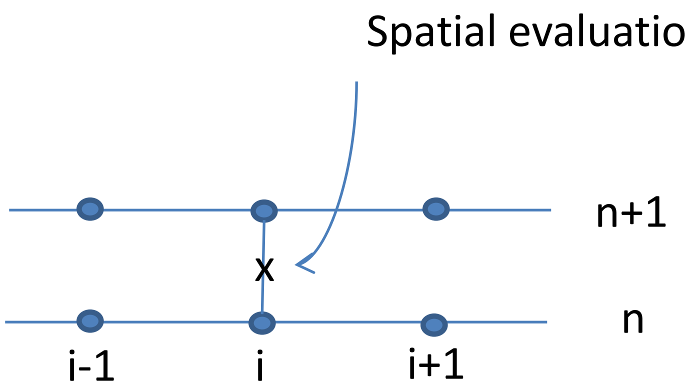


- For θ = 1/2, **Crank Nicholson Method**

$$\theta\left[D\frac{C_{i+1}^{n+1}-2C_{i}^{n+1}+C_{i-1}^{n+1}}{\Delta x^{2}}\right]+(1-\theta)\left[D\frac{C_{i+1}^{n}-2C_{i}^{n}+C_{i-1}^{n}}{\Delta x^{2}}\right]$$

$$=\frac{C_{i}^{n+1}-C_{i}^{n}}{\Delta t}$$

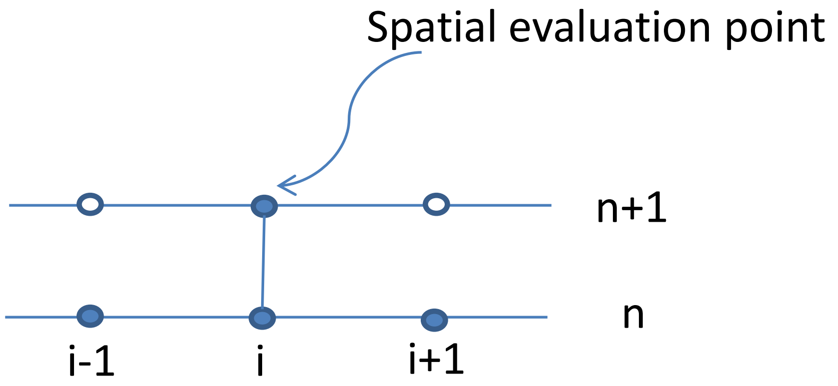
- Implicit
- Needs matrix solver



- For $\theta = 0$, **Explicit Method**

$$\theta\left[D\frac{C_{i+1}^{n+1}-2C_{i}^{n+1}+C_{i-1}^{n+1}}{\Delta x^{2}}\right]+(1-\theta)\left[D\frac{C_{i+1}^{n}-2C_{i}^{n}+C_{i-1}^{n}}{\Delta x^{2}}\right]$$

$$=\frac{C_{i}^{n+1}-C_{i}^{n}}{\Delta t}$$



- Exercise

Given $\psi = e^{-0.05t}$ at node i, what is the optimal value of θ? Use Δt = 0.1, 1.0, 10, 100 at t = 1.

Solution

$$\psi(0) = 1$$
$$\psi(0.1) = 0.995$$
$$\psi(1) = 0.951$$
$$\psi(10) = 0.607$$
$$\psi(100) = 0.00674$$

$$\frac{\partial \psi}{\partial t} = -0.05e^{-0.05t}$$
$$\left.\frac{\partial \psi}{\partial t}\right|_{\psi(0)} = -0.05$$
$$\left.\frac{\partial \psi}{\partial t}\right|_{\psi(.1)} = -0.04975$$

$$\frac{\psi_i^{n+1} - \psi_i^{n}}{\Delta t} = \theta\left(\frac{\partial \psi}{\partial t}\right)^{n+1} + (1-\theta)\left(\frac{\partial \psi}{\partial t}\right)^{n}$$

- Exercise

Given $\psi = e^{-0.05t}$ at node i, what is the optimal value of θ? Use Δt = 0.1, 1.0, 10, 100 at t = 1.

Solution

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = \theta\left(\frac{\partial \psi}{\partial t}\right)^{n+1} + (1-\theta)\left(\frac{\partial \psi}{\partial t}\right)^{n}$$

$$\frac{\psi\big|_{.1}^{n+1} - \psi\big|_{0}^{n}}{\Delta t} = \theta\left(\frac{\partial \psi}{\partial t}\right)\Bigg|_{.1}^{n+1} + (1-\theta)\left(\frac{\partial \psi}{\partial t}\right)\Bigg|_{0}^{n}$$

$$\frac{0.995 - 1}{.1} = \theta(-0.04975) + (1-\theta)(-0.05)$$

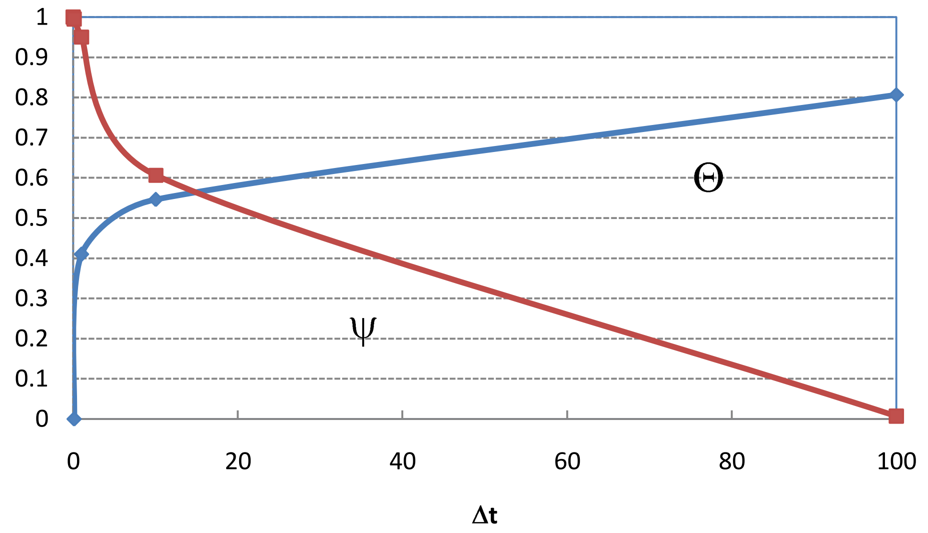
$$\theta = 0$$

- Exercise

Given $\psi = e^{-0.05t}$ at node i, what is the optimal value of θ? Use Δt = 0.1, 1.0, 10, 100 at t = 1.

Solution

- During simulation, ψ and Θ are unknown, trial and error is required.
- What is the best guess for Θ? Suppose we choose Θ = 0.75.



- Exercise

Given $\psi = at^2 + bt + c$ what is the optimal value of θ

Solution