

## Finite Diff Approach 1.2)

$$\text{equation: } \frac{d^2y}{dx^2} + \alpha \frac{dy}{dx} + \beta y = f(x)$$

$$\text{BC: } y(a) = y_a \quad y(b) = y_b$$

finite diff.

$$\frac{dy}{dx}\Big|_i = \frac{y_{i+1} - y_{i-1}}{2h}$$

$$\frac{d^2y}{dx^2}\Big|_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

$$\Rightarrow \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \alpha \cdot \frac{y_{i+1} - y_{i-1}}{2h} + \beta y_i = f(x_i)$$

rearrange and multiply by  $h^2$

$$y_{i+1} \left(1 - \frac{h}{2}\alpha\right) + y_i \left(h^2\beta - 2\right) + y_{i-1} \left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_i)$$

In case of the assignment:

Question 1.2:

$$\frac{d^2\phi^*}{dx^{*2}} = \phi^*(x^*)$$

$$\text{domain: } 0 < y < 10$$

Boundary condition:

$$\begin{aligned} -\phi^*(0) &= \frac{\phi_0}{v_T} \\ -\frac{d\phi^*}{dx^*}(x^* = 10) &= 0 \end{aligned} \quad \text{where } \phi^* = \frac{\phi}{v_T} \quad \text{with } \phi = \phi_0 \cdot \exp\left(-\frac{x}{\lambda}\right)$$

Centraal Diff method:

$$\frac{1 \cdot \phi^*[i+1] - 2 \cdot \phi^*[i] + 1 \cdot \phi^*[i-1]}{h^2} = \phi^*(x^*) f_i$$

$$\text{rearrange: } 1 \cdot \phi^*[i+1] - 2 \cdot \phi^*[i] + 1 \cdot \phi^*[i-1] = 0 \quad \text{notice it is in range } [1, N-2]$$

$$\phi^*[i+1] - (2+h^2)\phi^*[i] + \phi^*[i-1] = 0$$

Constructing matrix A:  $(A y = b)$

$$\text{case } i=1 : \phi^*_{i-1} = \phi^*(0) = \frac{\phi_0}{v_T}$$

$$1 \cdot \phi^*(0) - (2+h^2)\phi^*[i] + \phi^*[i-1] = 0$$

$$-(2+h^2)\phi^*[i] + \phi^*[i-1] = 0 - 1 \cdot \phi^*(0)$$

case  $2 \leq i \leq N-3$

$$1 \cdot \phi^*[i-1] - (2+h^2)\phi^*[i] + \phi^*[i-1] = 0$$

case  $i = N-2$  : (far right case)

Neumann boundary:

$$\frac{d\phi^*}{dx^2} = 0 \\ \Rightarrow \frac{\phi_{i+1} - \phi_{i-1}}{2h} = 0 \Rightarrow \phi_{i+1} = \phi_{i-1}$$

in matrix A:

$$1 \cdot \phi_{i-1} - (2 + h^2) \phi_{i-1} + 1 \cdot \phi_{i+1} = 0$$

plug in for  $\phi_{i+1} = \phi_{i-1}$

$$\Rightarrow 2 \phi_{i-1} - (2 + h^2) \phi_{i-1} = 0$$

Question 2:

$$\frac{d^2\phi}{dx^2} = \frac{k_B T}{\epsilon} \sinh\left(\frac{e\phi(x)}{k_B T}\right)$$

$$\frac{d^2\phi^*}{dx^2} = \sinh(\phi^*(x^*)) \\ x^* = \frac{x}{\lambda} \quad \phi^* = \frac{\phi}{U_T} \quad U_T = \frac{k_B T}{\epsilon}$$

$$\frac{1 \cdot \phi^*_{i-1} - 2 \cdot \phi^*_{i-1} + 1 \cdot \phi^*_{i+1}}{h^2} = \sin(\phi^*(x^*))$$

$$1 \cdot \phi^*_{i-1} - 2 \cdot \phi^*_{i-1} - \underbrace{h^2 \sin(\phi^*_{i-1})}_{f(x)} + 1 \cdot \phi^*_{i+1} = 0 \\ f(x) \rightarrow \text{can be solved with Newton Raphson}$$

where Newton Raphson will guess for the value of  $\phi^*$ . It does so by expanding F around an estimate  $\phi_{i-1}$  using Taylor series:

$$F(\phi_{i-1} + s\phi) \approx F(\phi_{i-1}) + J(\phi_{i-1}) \cdot s\phi$$

$\epsilon$  Jacobian

$$F_{i-1} = \phi_{i-1} - 2\phi_{i-1} - h^2 \cdot \sinh(\phi_{i-1}) + \phi_{i+1}$$

Term:

$$\frac{dF_i}{d\phi_{i-1}} = 1 \quad \begin{array}{l} \text{Derivative} \\ \text{note any other derivative = 0} \end{array} \\ \Rightarrow \text{only diagonal has values}$$

$$\phi_{i-1} \quad \frac{dF_i}{d\phi_{i-1}} = -2 - h^2 \cosh(\phi_{i-1})$$

$$\phi_{i+1} \quad \frac{dF_i}{d\phi_{i+1}} = 1$$

note only Neumann conditions must be applied to the Jacobian

the Dirichlet boundary  $\phi[0] = \frac{ph=0}{U_T}$  will be defined in solution

however Neumann must be defined

$$\therefore @ N = -1 \quad \frac{d\phi^*}{dx^2} = 0 \Rightarrow$$

$$F_{N-1} = 2\phi_{i-1} - 2\phi_{i-1} - h^2 \cdot \cosh(\phi_{i-1})$$