

Schrödinger equation:

$$i\hbar \frac{d}{dt} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x, t)$$

Finite differences:

$$\frac{d}{dt} f(t) \approx \frac{f(t + \Delta t) - f(t)}{\Delta t} = f_t$$

$$\frac{d^2}{dx^2} f(x) \approx \frac{f(x - \Delta x) - 2f(x) + f(x + \Delta x)}{\Delta x^2} = f_{xx}$$

Use the finite difference approximation of the Schrödinger equation:

$$i\hbar \Psi_t = -\frac{\hbar^2}{2m} \Psi_{xx}$$

Explicit:

$$i\hbar \frac{\Psi(x, t + \Delta t) - \Psi(x, t)}{\Delta t} = -\frac{\hbar^2}{2m} \frac{\Psi(x - \Delta x, t) - 2\Psi(x, t) + \Psi(x + \Delta x, t)}{\Delta x^2}$$

Implicit:

$$i\hbar \frac{\Psi(x, t + \Delta t) - \Psi(x, t)}{\Delta t} = -\frac{\hbar^2}{2m} \frac{\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)}{\Delta x^2}$$

$$i\hbar [\Psi(x, t + \Delta t) - \Psi(x, t)] = -\frac{\hbar^2}{2m} \frac{\Delta t}{\Delta x^2} [\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)]$$

$$-i\hbar \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\Delta t}{\Delta x^2} [\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)] - i\hbar \Psi(x, t + \Delta t)$$

$$\hbar \Psi(x, t) = -i \frac{\hbar^2}{2m} \frac{\Delta t}{\Delta x^2} [\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)] + \hbar \Psi(x, t + \Delta t)$$

$$\Psi(x, t) = -i \frac{\hbar}{2m} \frac{\Delta t}{\Delta x^2} [\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)] + \Psi(x, t + \Delta t)$$

$$r = -i \frac{\hbar}{2m} \frac{\Delta t}{\Delta x^2}$$

$$\Psi(x, t) = r [\Psi(x - \Delta x, t + \Delta t) - 2\Psi(x, t + \Delta t) + \Psi(x + \Delta x, t + \Delta t)] + \Psi(x, t + \Delta t)$$

$$\Psi(x, t) = r \Psi(x - \Delta x, t + \Delta t) + (1 - 2r) \Psi(x, t + \Delta t) + r \Psi(x + \Delta x, t + \Delta t)$$

Stencil:

$$\Psi(t) = \begin{bmatrix} r & (1 - 2r) & r \end{bmatrix} \Psi(t + \Delta t)$$

Jacobi method:

$$Ax = b$$

$$A\Psi(t + \Delta t) = \Psi(t)$$

$$x_i^{k+1} = \frac{1}{A_{ii}} \left( b_i - \sum_{i \neq j} A_{ij} x_j^k \right)$$

Intuition for why it works:

$$A_{ii} x_i^{k+1} = b_i - \sum_{i \neq j} A_{ij} x_j^k$$

$$A_{ii} x_i^{k+1} + \sum_{i \neq j} A_{ij} x_j^k = b_i$$

$$Ax = b$$

Application to our FDM:

$$\Psi(x, t + \Delta t)^{k+1} = \frac{1}{1 - 2r} \left[ \Psi(x, t) - r\Psi(x - \Delta x, t + \Delta t)^k - r\Psi(x + \Delta x, t + \Delta t)^k \right]$$