Numerical Scheme: The Diffusion Equation

$$\boxed{\frac{\partial \psi}{\partial t} = D\nabla^2\psi \equiv D\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right)}$$ generally in 3 spatial dimensions.

$\psi(x,y,z,t) \rightarrow$ Scalar function, $D \rightarrow$ Diffusion Coefficient

Consider only $\boxed{\psi = \psi(x,t)}$ (1-dimensional in space)

$$\therefore \boxed{\frac{\partial \psi}{\partial t} = D\frac{\partial^2\psi}{\partial x^2}} \rightarrow$$ Parabolic second-order partial differential equation.

Requires one initial condition in t, and two boundary conditions in x. The constant step sizes are $\boxed{\Delta x \text{ and } \Delta t}$. Discretizing, $\boxed{x = i\Delta x}$ and $\boxed{t = n\Delta t}$, i and n being integers.

To find $\boxed{\psi = \psi(x,t) \equiv \psi(i,n) \equiv \psi(i\Delta x, n\Delta t)}$.

$$\boxed{\frac{\partial \psi}{\partial t} \equiv \frac{\psi(i,n+1) - \psi(i,n)}{\Delta t}}$$ Forward numerical first derivative.

$$\boxed{\frac{\partial^2\psi}{\partial x^2} \equiv \frac{\psi(i+1,n) + \psi(i-1,n) - 2\psi(i,n)}{(\Delta x)^2}}$$

Discrete numerical second derivative.

Both derivatives are put in the one-dimensional diffusion equation. (P.T.O.)

$$\therefore \boxed{\frac{\psi(i,n+1)-\psi(i,n)}{\Delta t} = D \times \left[\frac{\psi(i+1,n)}{(\Delta x)^2} + \frac{\psi(i-1,n) - 2\psi(i,n)}{(\Delta x)^2}\right]}$$

$$\Rightarrow \boxed{\psi(i,n+1) = \psi(i,n) + \frac{D(\Delta t)}{(\Delta x)^2} \times \left[\psi(i+1,n) + \psi(i-1,n) - 2\psi(i,n)\right]}$$

ψ values at time n, give ψ at time $n+1$.

The Point-Source Solution of the diffusion equation is $\boxed{\psi(x,t) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[\frac{-x^2}{2\sigma^2}\right]}$, in which σ (the standard deviation) is $\boxed{\sigma = \sqrt{2Dt}}$.

This is a Gaussian Distribution with a spread of $\boxed{\sigma = \sqrt{2Dt}}$.

In time step Δt, spread is $\rightarrow$ $\boxed{\sigma \simeq \sqrt{2D\Delta t}}$.

For numerical stability $\boxed{\Delta x \geq \sqrt{2D\Delta t}}$ is to be maintained.