

Modelling of transient behaviour of a diode- switching on

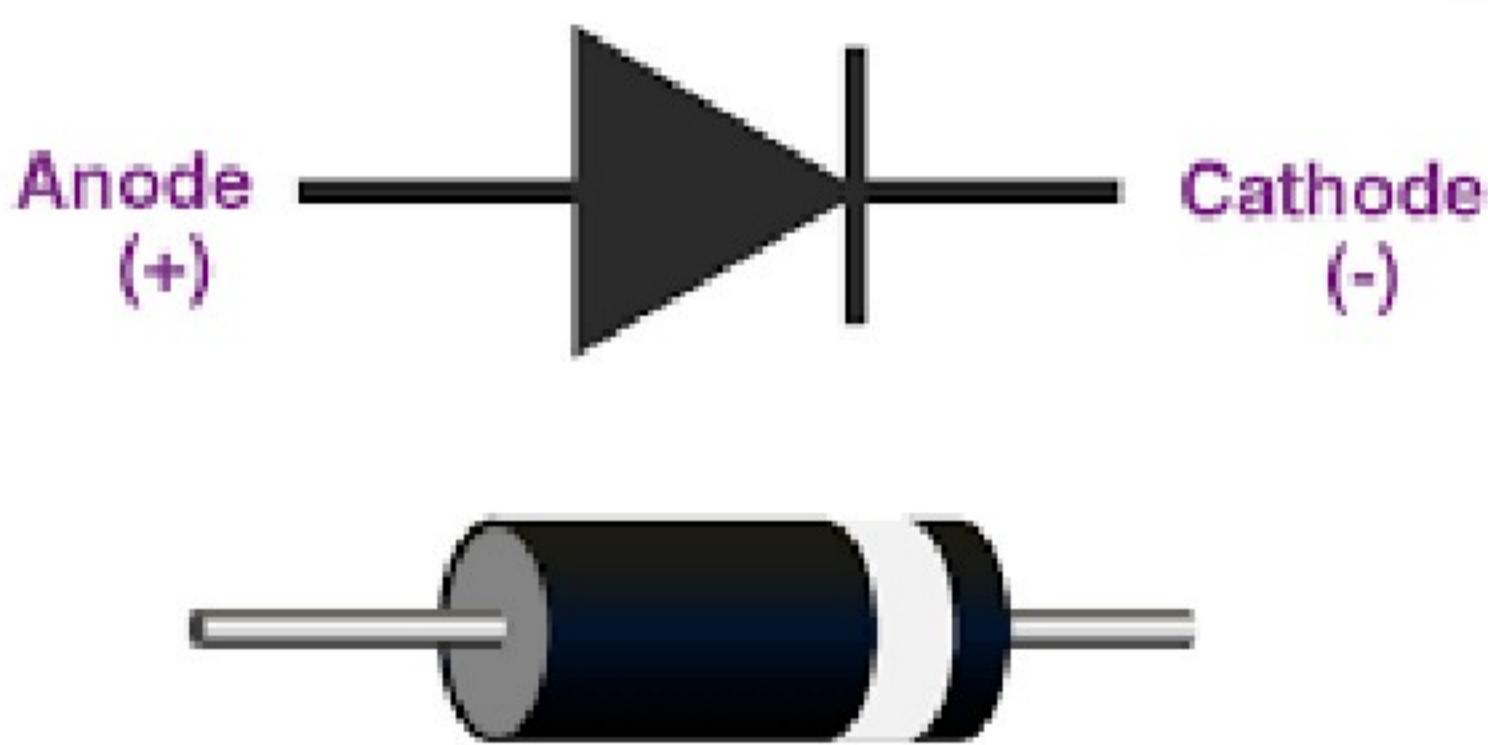
EE2503- NUMERICAL METHODS OF DEVICE MODELING

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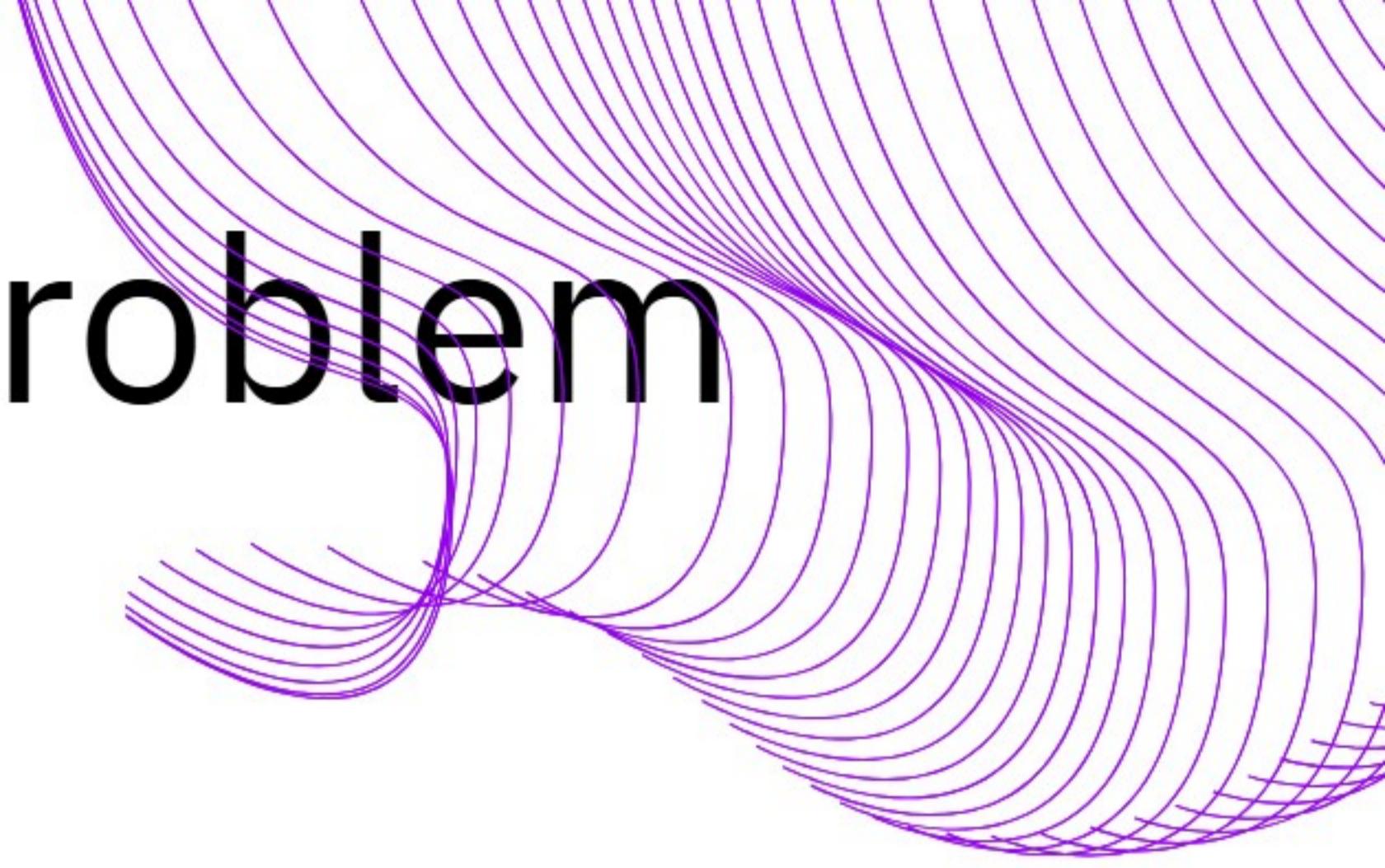
Introduction

About the project

The transient behavior of a diode during switching on refers to the brief period when the diode transitions from its off (reverse-biased) state to its on (forward-biased) state. This occurs due to factors like charge storage in the depletion region, junction capacitance, and the diode's forward recovery time. These effects cause a delay in achieving steady-state conduction, impacting the diode's performance in high-speed circuits. Understanding this behavior is crucial for optimizing diode performance in applications such as rectifiers, switching circuits, and communication systems.



Approaching the problem



- Solve Poisson's equation.
- Solve drift diffusion equation
- Carrier continuity equation (For holes and electrons)
- Implement the time-variant cases by studying the steady-state solutions
- Write a C program to simulate the above problem and calculate the properties of the diode

EQUATIONS TO BE SOLVED

Poisson's equation

$$\frac{d^2V}{dx^2} = -\frac{\rho}{\epsilon}$$

Drift diffusion equation

$$J_n = qn\mu_n E + qD_n \frac{dn}{dx}$$

$$J_p = qp\mu_p E - qD_p \frac{dp}{dx}$$

Carrier continuity equation

$$\frac{\partial n}{\partial t} = \nabla \cdot \mathbf{J}_n + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \mathbf{J}_p + G_p - R_p$$

Solving the Poisson equation

For solving the poission equation we need the boundary condition

$$V[0] = V_{\text{app}} - E_g - \frac{k_B T}{q} \ln \left(\frac{N_a}{N_v} \right)$$

$$V[N] = \frac{k_B T}{q} \ln \left(\frac{N_d}{N_c} \right)$$

now we use Jacobian matrix method to solve the system of equations to get V

Discretization of Poisson's Equation:

The Poisson equation is given as:

$$\frac{V_{i-1} - 2V_i + V_{i+1}}{\Delta x^2} = -\frac{\rho}{\epsilon}$$

Rearranging it:

$$\frac{V_{i-1} - 2V_i + V_{i+1}}{\Delta x^2} + \frac{\rho}{\epsilon} = 0$$

Solving the Poisson equation

Let's denote this equation in a more general form:

$$F_i(V_{i-1}, V_i, V_{i+1}) = 0$$

Linearization using Taylor series expansion:

$$F_i(V_{i-1}^R, V_i^R, V_{i+1}^R) = F_i(V_{i-1}^0, V_i^0, V_{i+1}^0) + \frac{\partial F_i}{\partial V_{i-1}} \Delta V_{i-1} + \frac{\partial F_i}{\partial V_i} \Delta V_i + \frac{\partial F_i}{\partial V_{i+1}} \Delta V_{i+1}$$

Neglecting higher-order terms (double differentiation terms):

$$F_i(V_{i-1}^R, V_i^R, V_{i+1}^R) = 0$$

This gives:

$$F_i(V_{i-1}, V_i, V_{i+1}) - \left(\frac{\partial F_i}{\partial V_{i-1}} \Delta V_{i-1} + \frac{\partial F_i}{\partial V_i} \Delta V_i + \frac{\partial F_i}{\partial V_{i+1}} \Delta V_{i+1} \right) = 0$$

Solving the Poisson equation

Matrix Form:

$$\begin{bmatrix} 1 & 0 & \dots & 0 \\ \frac{\partial F_2}{\partial V_1} & \frac{\partial F_2}{\partial V_2} & \frac{\partial F_2}{\partial V_3} & \dots \\ \vdots & \ddots & \vdots & \\ 0 & \dots & 1 & \end{bmatrix} \begin{bmatrix} \Delta V_1 \\ \Delta V_2 \\ \vdots \\ \Delta V_N \end{bmatrix} = \begin{bmatrix} -F_1^0 \\ -F_2^0 \\ \vdots \\ -F_N^0 \end{bmatrix}$$

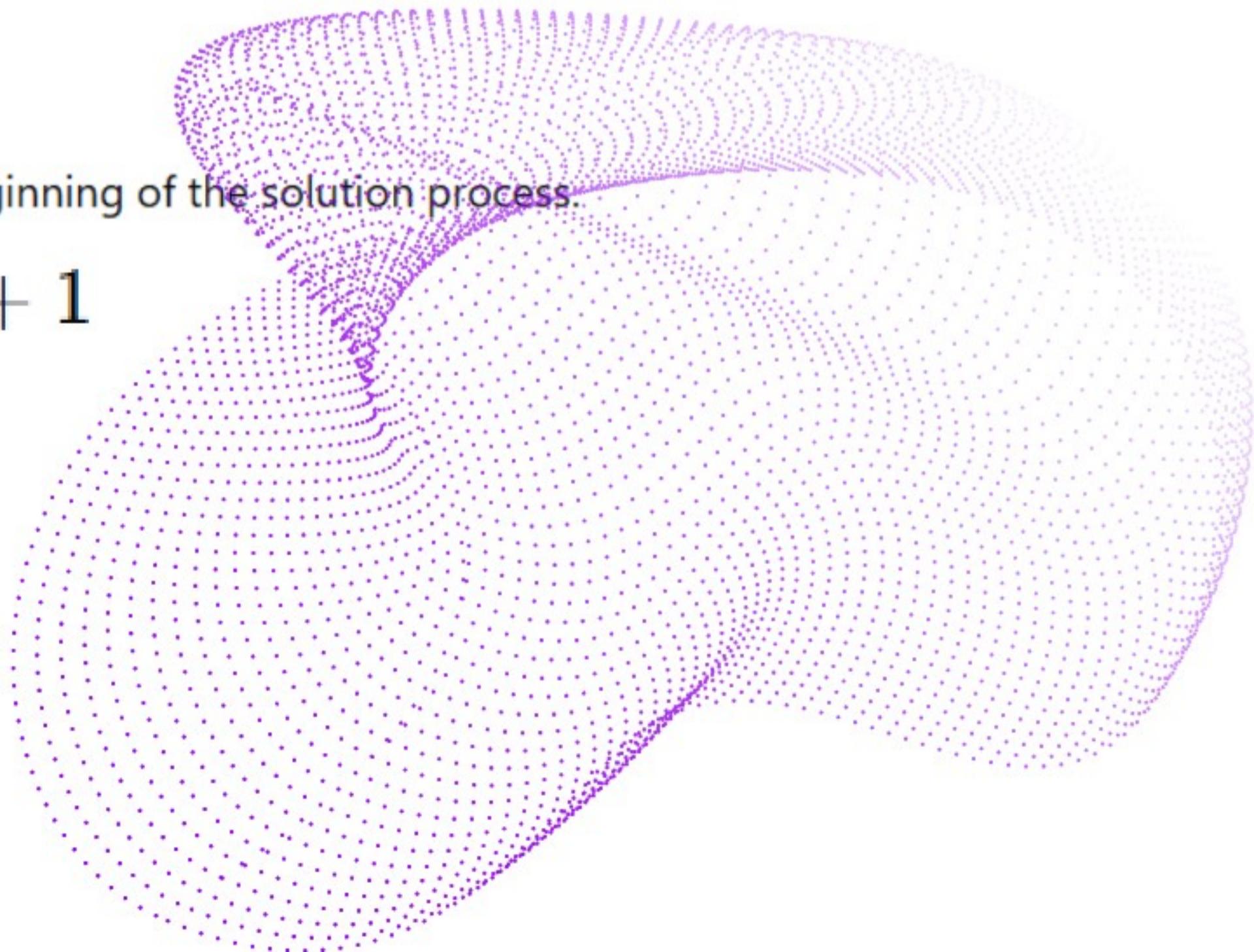
Boundary Conditions:

ΔV_1 and ΔV_N are boundary conditions that are specified at the beginning of the solution process.

$$\frac{\partial F_i}{\partial V_j} = 0 \text{ for } j \neq i, i-1, i+1$$

$$\frac{\partial F_i}{\partial V_{i-1}} = \frac{\partial F_i}{\partial V_{i+1}} = \frac{1}{\Delta x^2}$$

$$\frac{\partial F_i}{\partial V_i} = -\frac{2}{\Delta x^2} + \frac{1}{\epsilon} \frac{\partial \rho_i}{\partial V_i}$$



Solving the Poisson equation

To solve the $Ax=B$ type we use Gaussian elimination

Gaussian Elimination:

We have two steps to solve Gaussian elimination:

1. Forward Elimination

- Convert the matrix into an upper triangular form.

Example:

To make $a_{21} = 0$, perform the following operation:

$$R_2 \rightarrow R_2 - \frac{a_{21}}{a_{11}} R_1$$

2. Backward Substitution

- Solve the upper triangular matrix equation:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

Solving the Poisson equation

After forward elimination, the system becomes:

$$\begin{bmatrix} a'_{11} & a'_{12} & a'_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a'_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \end{bmatrix}$$

$$A_{33} \times X_3 = b_3$$

$$X_3 = \frac{b_3}{A_{33}}$$

Similarly, we get values of X_2 .

Solving in this method, we get values of ΔV .

and from this we will get discrete values of V

Sharfettel-Gummel discretisation

To solve the drift diffusion equation

$$J_n = qn\epsilon\mu_n + qD_n \frac{dn}{dx}$$

$$\epsilon = -\frac{dV}{dx}, \quad \phi = \frac{V}{k_B T/q}$$

$$\mathbf{J} = \left[qn\mu_n \left(-\frac{d\phi}{dx} \right) \frac{k_B T}{q} + qD_n \frac{dn}{dx} \right]$$

$$\mathbf{J} = k_B T \mu_n \left[-n \frac{d\phi}{dx} + \frac{dn}{dx} \right]$$

From Einstein equilibrium equation:

$$D_n/\mu_n = \frac{k_B T}{q}$$

$$J_{i-1/2} = k_B T \mu_{i-1/2} \left[-n_{i-1/2} \frac{d\phi}{dx} \Big|_{i-1/2} + \frac{dn}{dx} \Big|_{i-1/2} \right]$$

$$n(x) = u(x)e^\phi$$

$$J_{i-1/2} = k_B T \left[\frac{\mu_{i-1} + \mu_i}{2} \right] \left[\left(-n \frac{d\phi}{dx} + n \frac{d\phi}{dx} + e^\phi \frac{du}{dx} \right) \Big|_{i-1/2} \right]$$

$$e^{-\phi} J_{i-1/2} dx = k_B T \left(\frac{\mu_{i-1} + \mu_i}{2} \right) du$$

Integrating on both sides:

$$\int_{i-1}^i e^{-\phi} J_{i-1/2} dx = \int_{i-1}^i k_B T \left(\frac{\mu_{i-1} + \mu_i}{2} \right) du$$

$$\phi(x) = \frac{\phi_i - \phi_{i-1}}{\Delta x} (x - x_{i-1}) + \phi_{i-1}$$

$$J_{i-\frac{1}{2}} \cdot \frac{\Delta x}{\phi_i - \phi_{i-1}} [e^{-\phi_i} - e^{-\phi_{i-1}}]$$

$$= kT \mu_{\text{avg}} [n_i e^{-\phi_i} - n_{i-1} e^{-\phi_{i-1}}]$$

$$B(x) = \frac{x}{e^x - 1} \quad , \quad B(x) \cdot e^x = \frac{x}{1 - e^{-x}} = B(-x)$$

$$J_{i-\frac{1}{2}}=\frac{kT}{\Delta x}\mu_{\text{avg}}\left[n_iB(\phi_i-\phi_{i-1})-n_{i-1}B(\phi_{i-1}-\phi_i)\right]$$

$$J_{i+\frac{1}{2}}=\frac{kT}{\Delta x}\mu_{\text{avg}}\left(n_{i+1}B(\phi_{i+1}-\phi_i)-n_iB(\phi_i-\phi_{i+1})\right)$$

In Steady State since the current is uniform we equate

$$J_{i+\frac{1}{2}} = J_{i-\frac{1}{2}}$$

$$\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0$$

Whereas in transient state : using Crank Nicolson method to solve partial differentiation equation particularly diffusion problems

For transient:

$$\frac{\partial n}{\partial t} \neq 0$$

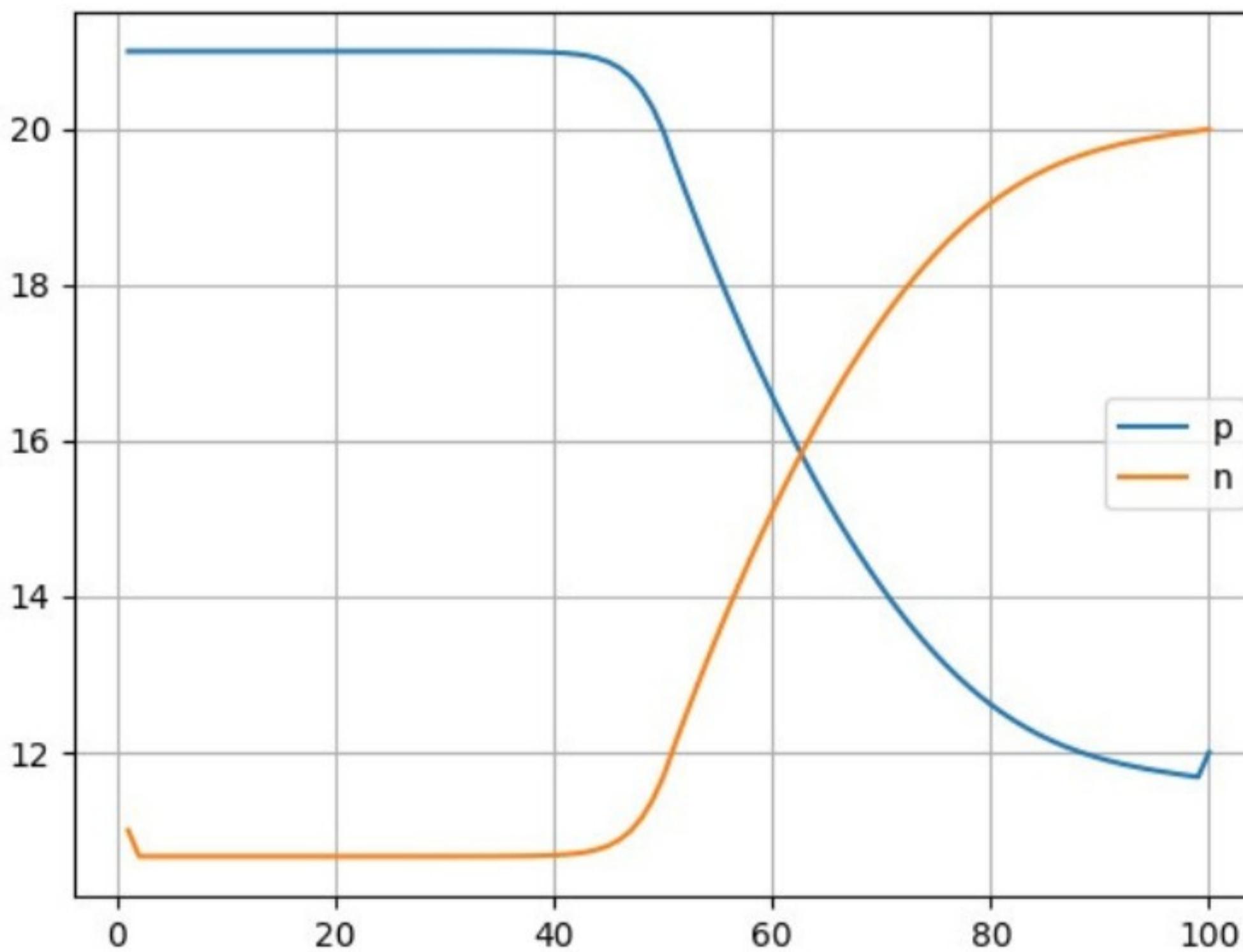
$$\frac{\partial n}{\partial t} = \frac{n[i]_{t+1} - n[i]_t}{t+1 - t}$$

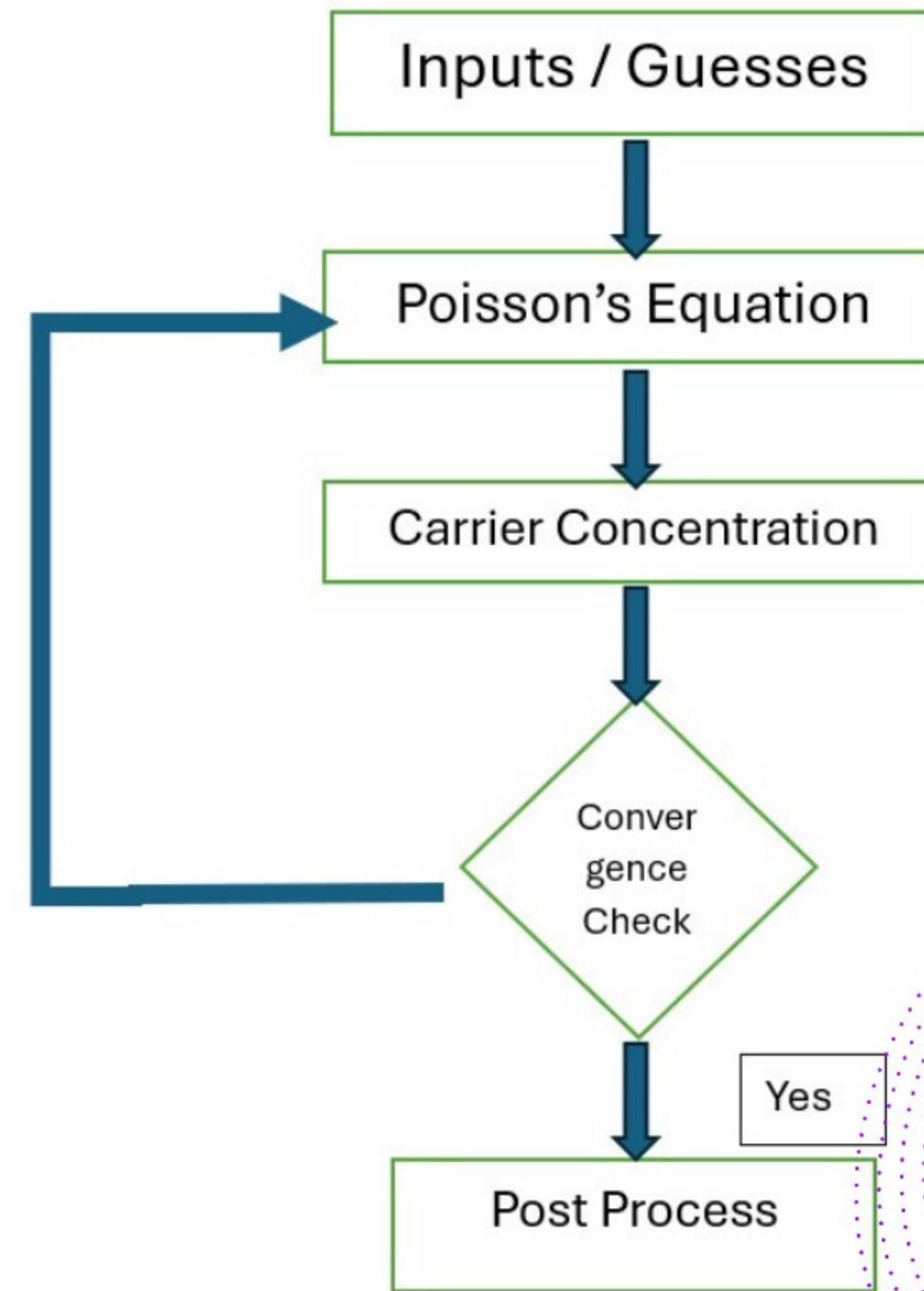
$$\nabla \cdot J_n = \frac{\partial}{\partial x} \left(\frac{J_n|_t + J_n|_{t+1}}{2} \right) \quad (\text{because } J \text{ is varying with time})$$

$$Rn[i] = \frac{1}{2} \left(\frac{n[i] - n_{eq}}{T_n} \right)_{t+1} + \frac{1}{2} \left(\frac{n[i] - n_{eq}}{T_n} \right)_t$$

$$Rn[i] = \frac{n[i]_{t+1} + n[i]_t - 2n_{eq}}{2T_n}$$

Equilibrium Condition





Our initial approach

First we started with poisons equation

to solve poisons equation, we wanted boundary conditions

How to get boundary conditions

we did Newton Raphson by taking rho at boundary = 0

$$\rho = N_D - N_A + P - n = 0$$

$$\rho = N_D - N_A + N_v * \exp[(qV + E_9) / k_B T] - N_c * \exp(qV / k_B T) = 0$$

by solving this using Newton Raphson , we will get boundary value of V

Everything we did So Far

$$\frac{d}{dx} \varepsilon \frac{dv}{dx} = -g.$$

$$N_D - N_A + P - N = 0$$

$$N_D - N_A + N_V \exp\left[\frac{q(V-E_g)}{kT}\right] - N_c \exp\left[-\frac{q(V-E_g)}{kT}\right] = 0 = f(V)$$

$T \downarrow$ $10^{16} \downarrow 2 \times 10^{16}$ \downarrow Newton rafson for V
 we get V at boundary

$$f^1(v) = 0 + N_v \exp\left[\frac{qv + Eg}{k_B T}\right] \times \frac{q}{k_B}$$

$$f'(V) = \left(\frac{q}{K_B T} \right) \left(N_V \exp\left(\frac{qV + E_g}{K_B T}\right) - N_C \exp\left(\frac{qV}{K_B T}\right) \right)$$

$$V_{new} = V_0 - \frac{f(\vartheta)}{f'(\vartheta)}$$

Poisson solver gives \rightarrow V in terms of x $V(x)$

$$N_V = 1.04 \times 10^{25} \text{ m}^{-3}$$

$$T = 300K$$

$$k_B = 1.38 \times 10^{-23}$$

$$E_g = 1.12 \times 1.6 \times 10^{-19}$$

$$q = 1.6 \times 10^{-19}$$

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continuity eq

$$\frac{\partial n}{\partial t} = -\nabla \cdot J_n + (G_n - R)$$

$$\frac{\partial P}{\partial t} = \nabla \cdot \vec{J}_P + G_P$$

Carrier Injec

$$J_n = q \mu n n E + q D n S$$

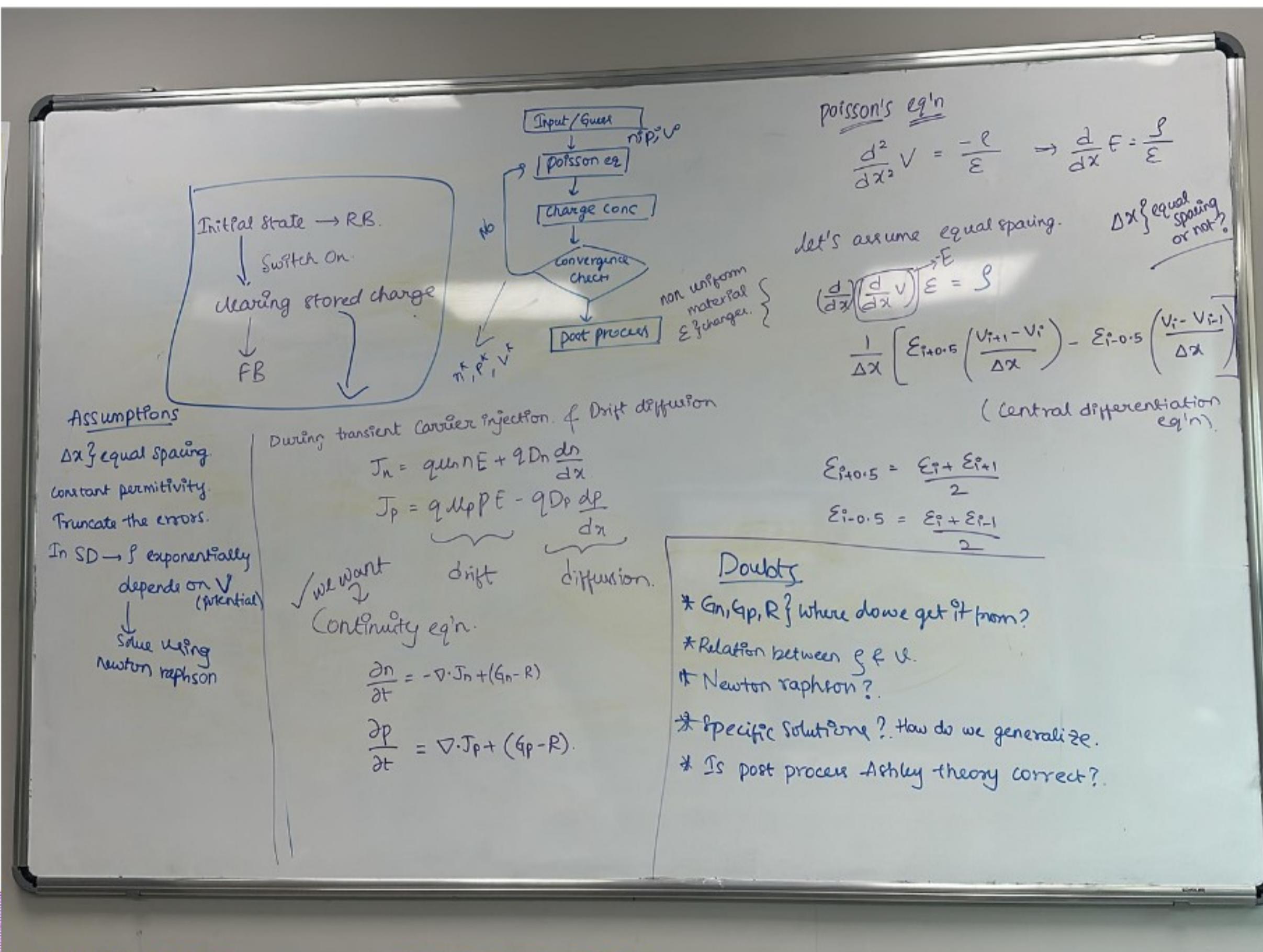
$$T_p = q_{MPPE} - q_{DP} \frac{d}{2}$$

$$n = Nv \exp\left(\frac{q\sqrt{2\pi} F q}{k_B T}\right) \quad n \rightarrow \text{terme de } q$$

dby $p \rightarrow \text{in term of } q$

$\therefore I_n$ & I_p are in terms of X

Everything we did So Far



18-10-2024

Poisson's eq'n:

$$\frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon}$$

(Discretizing)

$$\frac{V_{i+1} - 2V_i + V_{i-1}}{\Delta z^2} + \frac{P(V_i)}{\epsilon} = 0$$

Matrix Form:

$$\frac{1}{\Delta z^2} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ -2 & 1 & 0 & \dots & 0 \\ 0 & -2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_{i+1} \\ V_i \\ V_{i-1} \\ \vdots \\ V_N \end{bmatrix} = \frac{1}{\epsilon} \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_i \\ P_{i-1} \\ \vdots \\ P_N \end{bmatrix}$$

Right-hand side:

$$F_i = \frac{V_{i+1} - 2V_i + V_{i-1}}{\Delta z^2} + \frac{P(V_i)}{\epsilon} = F_i(V_{i+1}, V_i, V_{i-1})$$

$$F_i(V_{i+1}^n, V_i^n, V_{i-1}^n) = F(V_{i+1}, V_i, V_{i-1}) + \left(\frac{\partial F_i}{\partial V_{i+1}} \Delta V_{i+1} + \frac{\partial F_i}{\partial V_i} \Delta V_i + \frac{\partial F_i}{\partial V_{i-1}} \Delta V_{i-1} \right) + \text{double diff terms}$$

Matrix Equation:

$$\frac{\partial F_i}{\partial V_{i+1}} \Delta V_{i+1} + \frac{\partial F_i}{\partial V_i} \Delta V_i + \frac{\partial F_i}{\partial V_{i-1}} \Delta V_{i-1} = -F_i$$

$$\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \frac{\partial F_i}{\partial V_{i+1}} & \frac{\partial F_i}{\partial V_i} & \frac{\partial F_i}{\partial V_{i-1}} & \dots & 0 \\ \frac{\partial F_i}{\partial V_{i+1}} & \frac{\partial F_i}{\partial V_i} & \frac{\partial F_i}{\partial V_{i-1}} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_i}{\partial V_{i+1}} & \frac{\partial F_i}{\partial V_i} & \frac{\partial F_i}{\partial V_{i-1}} & \dots & 0 \end{bmatrix} \begin{bmatrix} \Delta V_{i+1} \\ \Delta V_i \\ \Delta V_{i-1} \\ \vdots \\ \Delta V_N \end{bmatrix} = -F_i$$

$$\Rightarrow J \cdot \Delta V = -F$$

$$\Delta V = J^{-1}(-F)$$

12-11-2024

Our Progress

Shockley-Gummel:

$$V = \left(\frac{qV_i}{KT} \right) \rightarrow \text{we have } J_{1/2} - J_{i+1/2} = q \Delta x R_i$$

$$\Rightarrow \phi_i = \frac{qV_i}{KT}$$

define Bernoulli $= \left(\frac{z}{e^z - 1} \right) \Rightarrow \text{Ber.}$

$$J_{i-1/2} = \frac{KT}{\Delta x} \left(\frac{\mu_{i-1} + \mu_i}{2} \right) \left(n_i \cdot \text{Ber}(\phi_i - \phi_{i-1}) - n_{i-1} \cdot \text{Ber}(\phi_{i-1} - \phi_i) \right)$$

$$J_{i+1/2} = \frac{KT}{\Delta x} \left(\frac{\mu_i + \mu_{i+1}}{2} \right) \left(n_{i+1} \cdot \text{Ber}(\phi_{i+1} - \phi_i) - n_i \cdot \text{Ber}(\phi_i - \phi_{i+1}) \right)$$

$$R[i] = \frac{n_i \cdot p_i - (\text{intrinsic})^2}{T_p(n_i + n_T) + T_n(p + p_T)}$$

$$T_p, T_n, \text{intrinsic} \Rightarrow \text{const} \quad P_T = n_T = \text{intrinsic}$$

assumption why?
most defects/impurities are generally at midgap,
(for easy calculation)

Issues -

- $\Rightarrow n_i = ?$
- \Rightarrow why arach code didn't converge?
- \rightarrow
- for $J_{i+1/2} - J_{i-1/2} = (n_{i-1}B_1 + n_iB_2 + n_{i+1}B_3)$
- $\frac{\partial J}{\partial x} = \frac{J(i)}{\Delta x}$
- $\frac{\partial n}{\partial x} = \nabla J + 0 \pm R$

$\frac{n_s(E+0.5) - n_s(E)}{\Delta x V_b} = N \cdot \frac{V_s V_b}{\pi^2 V_b F_z} \left[\frac{V_s V_b}{V_b} \right] [V_b(t+0) - V_b(t)] \quad t(t+0) \rightarrow \delta(t) \text{ (Gummel)}$

$$V_{in}(t+0.5) = V_{in} + \frac{V_s}{V_b} \sin(\omega_0 t) \quad \Rightarrow (V_{in} \in \dots)$$

$V_{in} - V_{in}$ symmetry for transient

$\Delta x \sim 0.5 \text{ nm} \sim w^{0.2} \quad a(0)$

$$\Delta x^{(0)} = \frac{w}{2} \quad \Delta x^{(0.5)} = \frac{w}{2}$$

$$\Delta x^{(1)} = \frac{w}{2} \quad \Delta x^{(1.5)} = \frac{w}{2}$$

$$\frac{d^2 V}{dx^2} = \rho / \epsilon_s, \quad \frac{d^2 V}{dx^2} = 0 \text{ in oxide}$$

$$\frac{\partial V}{\partial x} = 0$$

THANK YOU