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ECE606: Solid State Devices
Lecture 19: Numerical Solution of Transport Equations

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Outline

1) **Basic Transport Equations**
2) Gridding and finite differences
3) Discretizing equations and boundary conditions
4) Conclusion

REF. A primer on semiconductor device simulation
… M. Lundstrom (nanohub.org)

Equations to solve … analytical/numerical approach

$$\nabla \bullet D = q\left(p - n + N_D^+ - N_A^-\right)$$

← Band-diagram

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \bullet \mathbf{J}_N - r_N + g_N$$

$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$

$$\frac{\partial p}{\partial t} = \frac{-1}{q}\nabla \bullet \mathbf{J}_P - r_P + g_P$$

$$\mathbf{J}_P = qp\mu_P E - qD_P \nabla p$$

← Diffusion approximation, Minority carrier transport, Ambipolar transport

1) The Semiconductor Equations

Conservation Laws:

$$\nabla \bullet \vec{D} = \rho$$

$$\nabla \bullet \left(\vec{J}_n / -q \right) = \left(g_N - r_N \right)$$

$$\nabla \bullet \left(\vec{J}_p / \ q \right) = \left(g_P - r_P \right)$$

(steady-state)

Constitutive Relations:

$$\vec{D} = \kappa \varepsilon_0 \vec{E} = -\kappa \varepsilon_0 \vec{\nabla} V$$

$$\rho = q\left(p - n + N_D^+ - N_A^- \right)$$

$$\vec{J}_n = nq\mu_n \vec{E} + qD_n \vec{\nabla} n$$

$$\vec{J}_p = pq\mu_p \vec{E} - qD_p \vec{\nabla} p$$

$$g_{N,P} = f\,(n, p) \text{ etc.}$$

1) The Mathematical Problem

The "Semiconductor Equations"

$$\nabla \bullet \vec{D} = \rho$$

$$\nabla \bullet \left(\vec{J}_n / -q \right) = \left(g_N - r_N \right)$$

$$\nabla \bullet \left(\vec{J}_p / \ q \right) = \left(g_N - r_N \right)$$

3 coupled, nonlinear, second order PDE's for the 3 unknowns:

$$V(\vec{r}) \quad n(\vec{r}) \quad p(\vec{r})$$

Conservations laws: **exact**

Transport eqs. (drift-diffusion): **approximate**

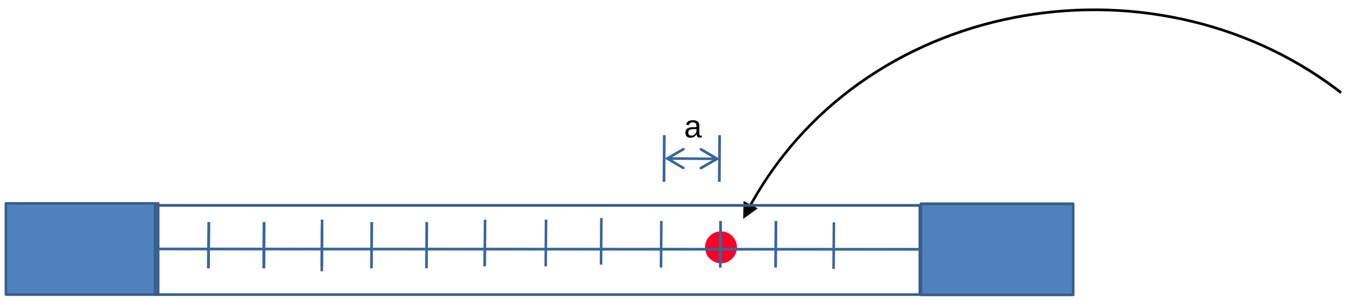
Outline

1) Basic Transport Equations
2) **Gridding and finite differences**
3) Making up the matrix and boundary conditions
4) Conclusion

2) The Grid

(ii) "exact" numerical solutions

N nodes
3N unknowns



V_i

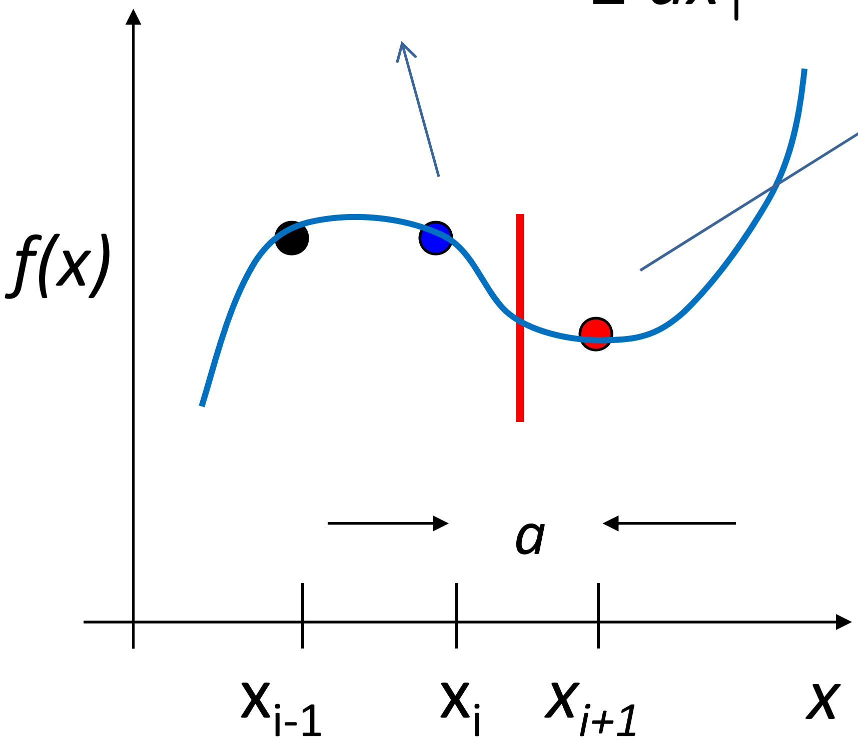
n_i

p_i

Finite Difference Expression for Derivative

$$f(x_o) = f(x_o + a/2) - \frac{a}{2}\frac{df}{dx}\Big|$$

$$f(x_o + a) = f(x_0 + a/2) + \frac{a}{2}\frac{df}{dx}\Big|$$



$$\frac{df}{dx}\Big|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a}$$

"centered difference"

The Second Derivative ...

$$f(x_0+a) = f(x_0) + a\left.\frac{df}{dx}\right|_{x_0=a} + \frac{a^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x_0=a} + \ldots$$

$$f(x_0-a) = f(x_0) - a\left.\frac{df}{dx}\right|_{x_0=a} + \frac{a^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x_0=a} - \ldots$$

$$f(x_0+a) + f(x_0-a) - 2f(x_0) = a^2\left.\frac{d^2 f}{dx^2}\right|_{x_0=a}$$

$$\left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

Outline

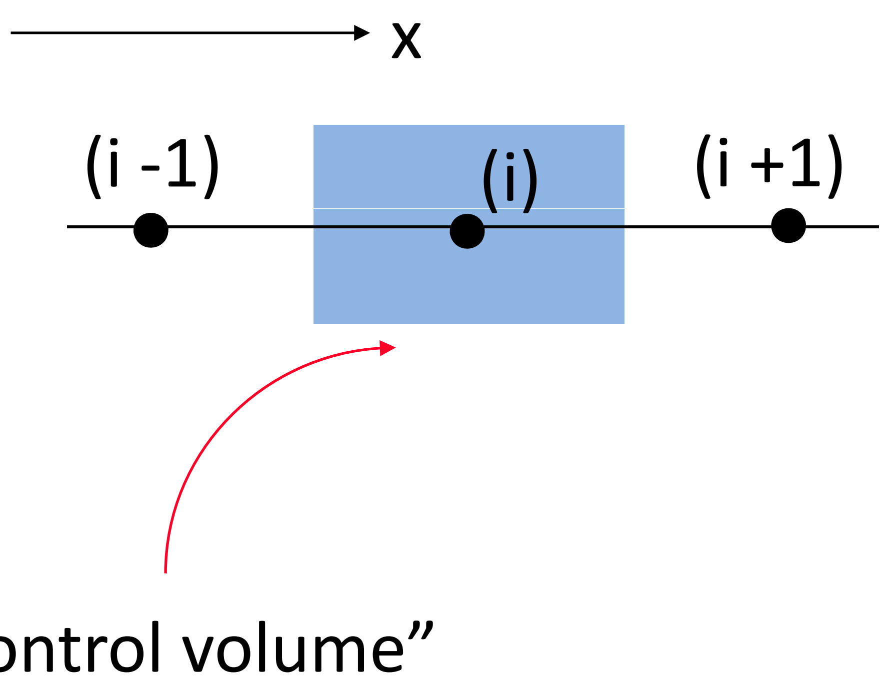
1) Basic Transport Equations
2) Gridding and finite differences
3) **Discretizing equations and boundary conditions**
4) Conclusion

2) Control Volume

3 unknowns at each node:

$$V_i, n_i, p_i$$

Need 3 equations
at each node

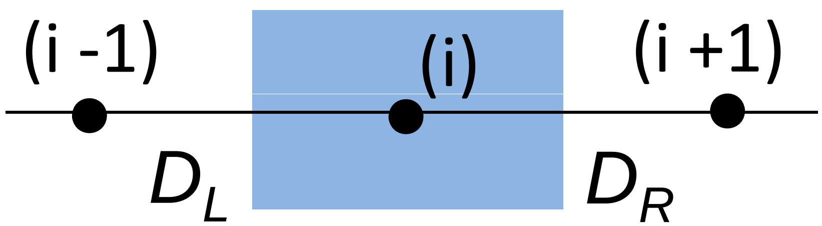


Discretizing Poisson's Equation

$$\nabla^2 V = -\rho / K_s \varepsilon_o$$

$$\nabla \bullet D = \rho \qquad D = K_s \varepsilon_0 \mathcal{E} = -K_s \varepsilon_0 \nabla V$$

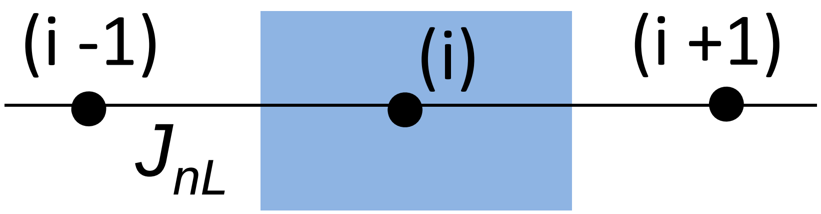
$$\frac{V(i-1) - V(i) + V(i+1)}{a^2} = -\frac{q}{K_s \varepsilon_0}\left(p_i - n_i + N_{D,i}^{+} - N_{A,i}^{-}\right)$$



$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

Discretizing Continuity Equations

$$\nabla \bullet \vec{J}_n = -q\left(g_N - r_N\right)$$



$$J_{nL} = -nq\mu_n \frac{dV}{dx} + kT\mu_n \frac{dn}{dx}$$

The simplest approach.....

$$\frac{J_{nL}}{kT\mu_n} = -\left(\frac{n_{i-1}+n_i}{2}\right)\left(\frac{V_i - V_{i-1}}{a\left(kT/q\right)}\right) + \left(\frac{n_i - n_{i-1}}{a}\right)$$

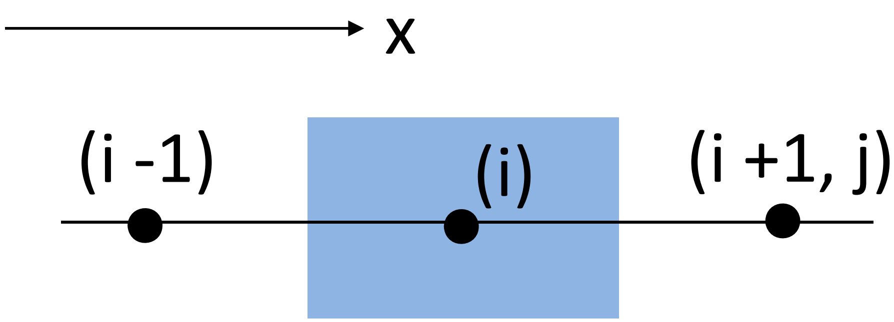
$$F_n^i\left(V_{i-1}, V_i, n_i, n_{i-1}, p_i, p_{i-1}\right) = 0$$

Three Discretized Equations

$$F_V^i = 0$$

$$F_n^i = 0$$

$$F_p^i = 0$$



3 unknowns at each node

N nodes

3N unknowns and 3N equations (nonlinear!)

Numerical Solution – Poisson Equation Only

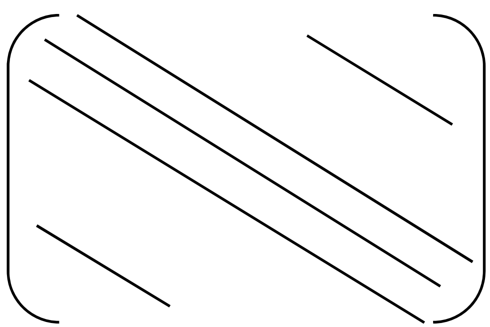
- Have a system of 3N nonlinear equations to solve

- Recall Poisson's equation at node (i):

$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

<u>linear</u> if n_i and p_i are known $\quad [A]\vec{V} = \vec{b}$

[A]:

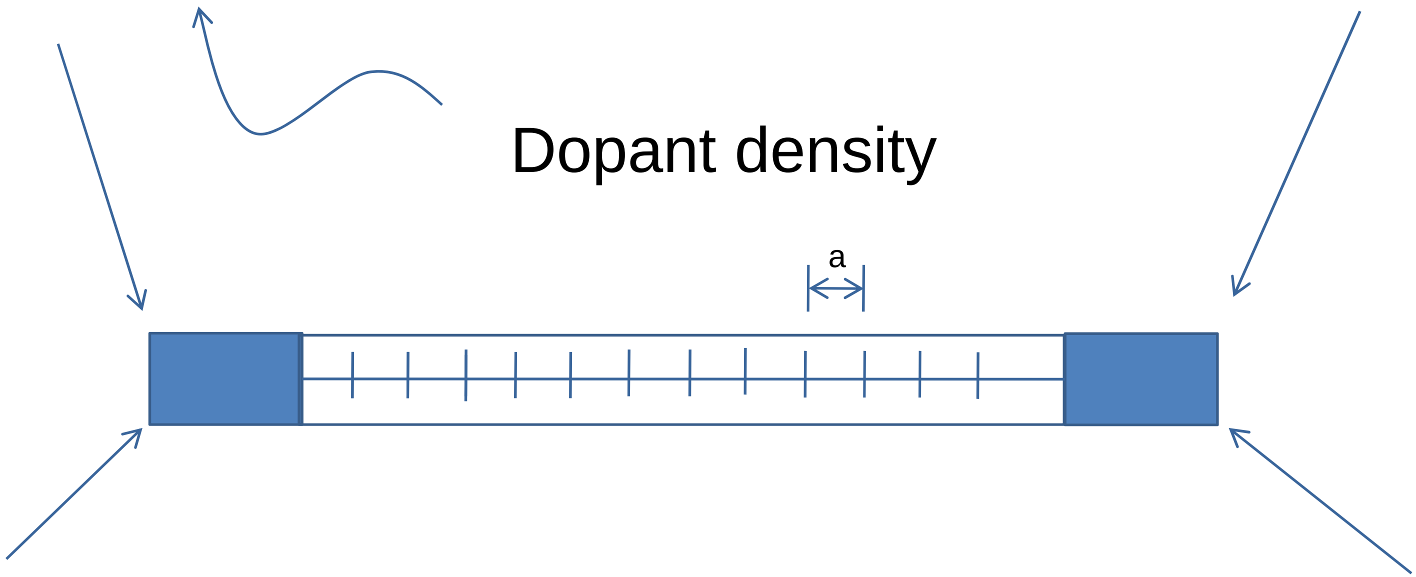


$$\vec{V} = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_N \end{bmatrix}$$

Boundary conditions

$$n_0 p_0 = n_i^2$$

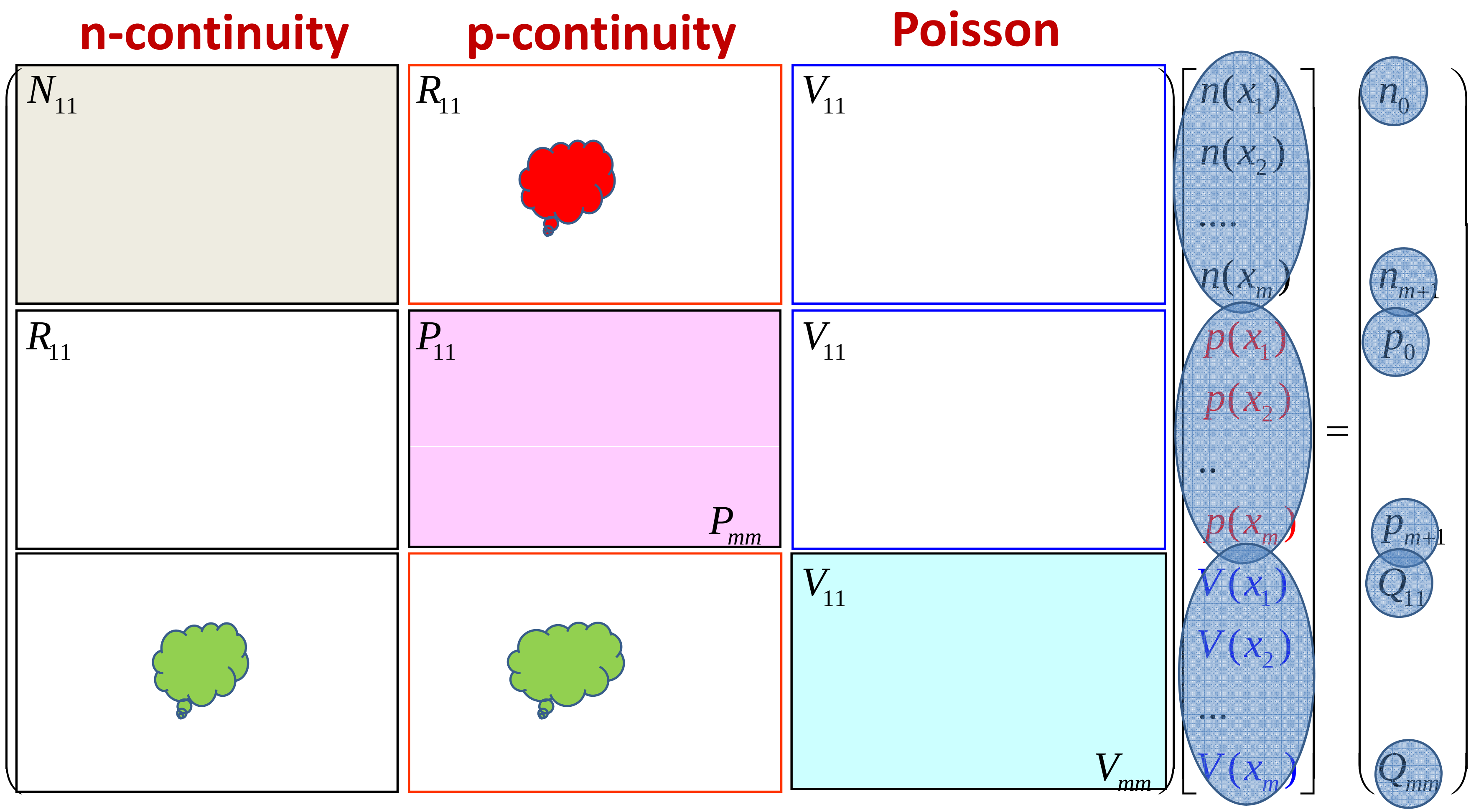
$$n_{N+1} p_{N+1} = n_i^2$$



$$V = V_A$$

$$V = 0$$

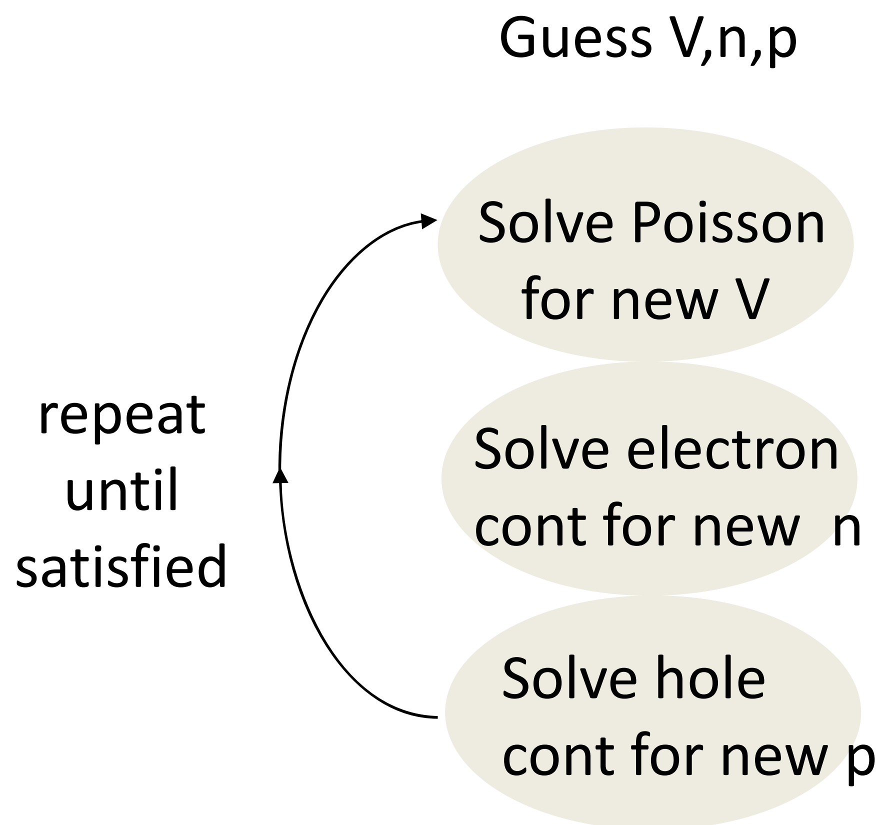
Numerical Solution…



3) Uncoupled Numerical Solution

The semiconductor equations are nonlinear!
(but they are linear individually)

Uncoupled solution procedure



Summary

1) Two methods to solve drift-diffusion equation consistently – analytical and numerical.

2) Analytical solution provides great insight and the solution methodology is similar to that of Schrodinger equations.

3) Numerical solution is more versatile. One begins with a set of equations and boundary conditions, discretize the equations on a grid with N nodes to obtain 3N nonlinear equations in 3N unknowns, and solve the system of nonlinear equations by iteration.