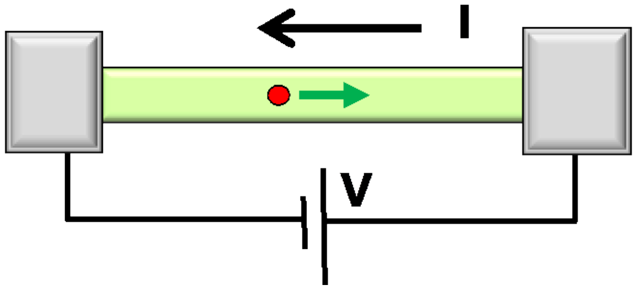
Section 18
Semiconductor Equations

18.3 Numerical Solutions

Gerhard Klimeck
gekco@purdue.edu

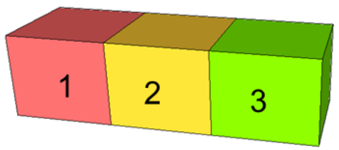
PURDUE UNIVERSITY

School of Electrical and Computer Engineering



$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area

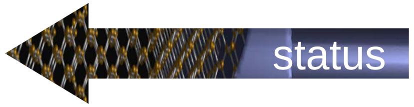


Vid

Vid

Vid

- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - » Basic Transport Equations
  - » Gridding and finite differences
  - » Discretizing equations and boundary conditions
  - » Iterative Solution Approach



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

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

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

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

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

Preface

- The 5 equations we derived the past few lectures have been used for the longest time in the industry and in academia to understand carrier transport in devices.

- It is useful to know the essentials of how these equations are *implemented* on a modern computer so that one understands some of the finer details involved in creating tools that simulate thee phenomena.

- Understanding some of these details helps one become a ‘power user’ of the simulation tools that implement the physics. One also understands the limitations re. numerical issues and applicability ranges of results.

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

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

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

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

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

Equations to be solved

Band-diagram →

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

Diffusion approximation,
Minority carrier transport,
Ambipolar transport →

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

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

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

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

1) The Semiconductor Equations

Conservation Laws: not specific to a particular problem - Universal

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

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

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

(steady-state)

Constitutive relations: specific to problem at hand – reflect physics of the problem

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

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

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

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

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

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

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

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

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

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

The "Semiconductor Equations"

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

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

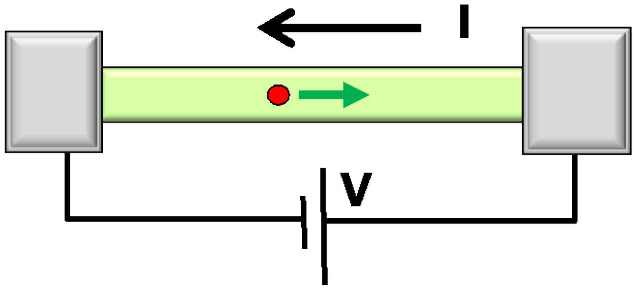
$$\nabla \bullet \left(\vec{J}_p / q \right) = \left(g_N - r_N \right)$$

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

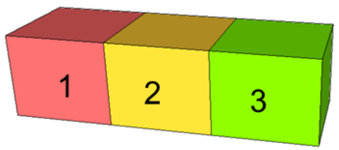
$V(\vec{r})$ $n(\vec{r})$ $p(\vec{r})$

Why are these equations coupled?
Potential→Field→current→changes potential→changes field and so on…

Conservations laws: **exact**
Transport eqs. (drift-diffusion): **approximate**



$$I = G \times V$$
$$= q \times n \times v \times A$$



Vid
Vid
Vid

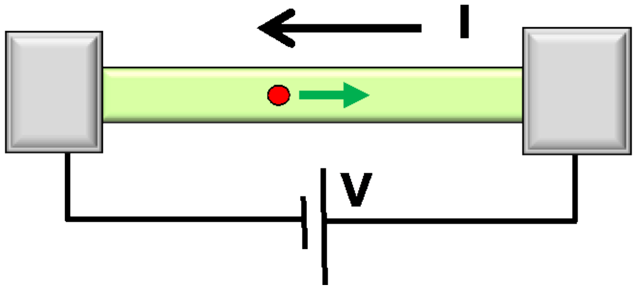
- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations

status

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

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \bullet \mathbf{J}_N - r_N + g_N$$
$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$
$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \bullet J_P + g_P - r_P$$
$$\mathbf{J}_P = qp\mu_P E - qD_P \nabla p$$
$$\nabla \bullet D = q\left(p - n + N_D^+ - N_A^-\right)$$

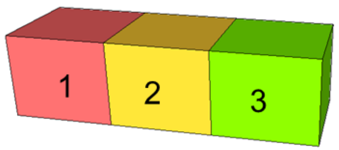
Semiconductor Equations



$I = G \times V$

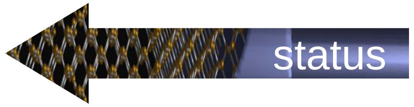
$= q \times n \times v \times A$

charge density velocity area



Vid
Vid
Vid

- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations
  - »Gridding and finite differences



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

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

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

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

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

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

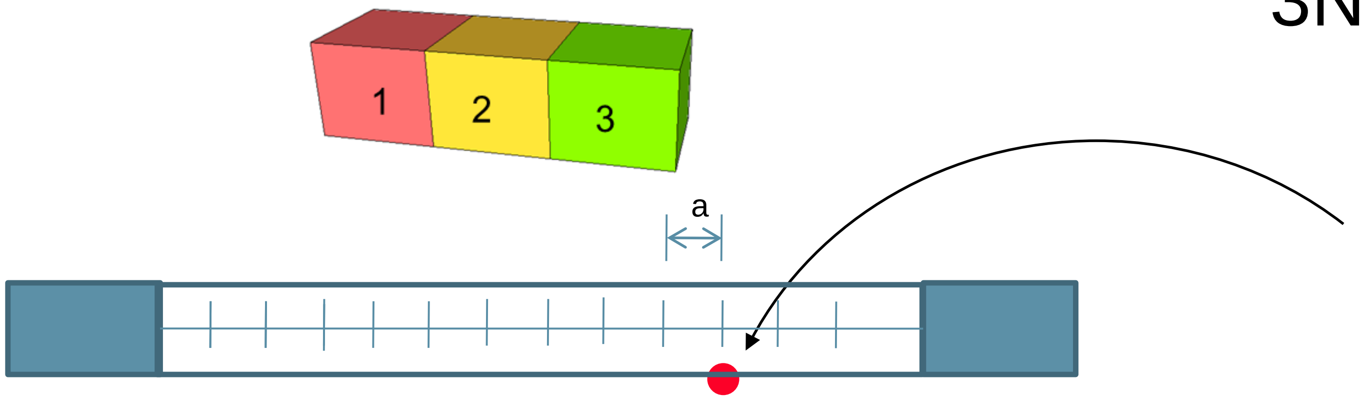
$$\nabla \bullet \left(\vec{J}_n / -q\right) = \left(g_N - r_N\right)$$

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

2) The Grid

(ii) "exact" numerical solutions

N nodes
3N unknowns



$$V_i \quad n_i \quad p_i$$

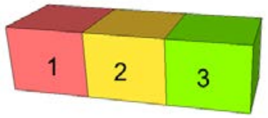
'Gridding'– total length divided into 'N' parts
- equal (uniform gridding) , or
- unequal (adaptive and non-uniform gridding)

Variables described at each point '*i*'.

V_o and V_{n+1} is known because these are voltages at source and drain.

$$\frac{df}{dx} = ?$$

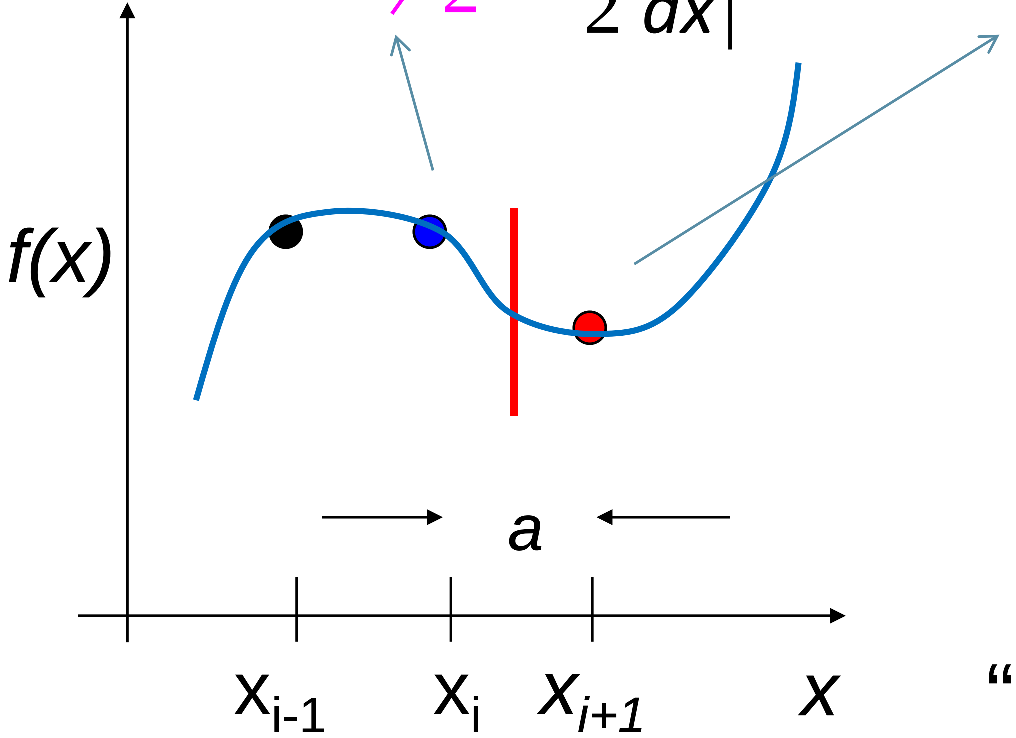
Finite Difference Expression for Derivative



$$\frac{df}{dx}$$

$$f(x_o) = f\left(x_o + \tfrac{a}{2}\right) - \frac{a}{2}\frac{df}{dx}\bigg|$$

$$f(x_o + a) = f\left(x_0 + \tfrac{a}{2}\right) + \frac{a}{2}\frac{df}{dx}\bigg|$$



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

“centered difference”

$$\frac{d^2 f}{dx^2} = ?$$

The Second Derivative …

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

$$\frac{d^2 f}{dx^2} = ?$$

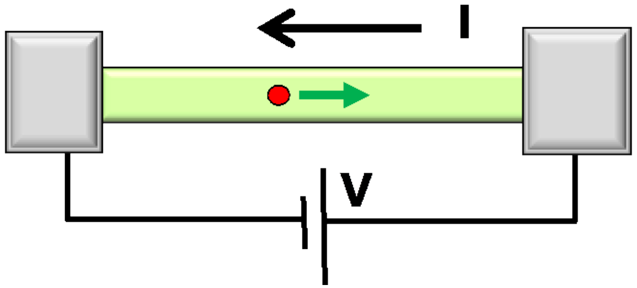
$$f\left(x_0 + a\right) = f\left(x_0\right) + a\left.\frac{df}{dx}\right|_{x_0 = a} + \frac{a^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x_0 = a} + \ldots$$

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

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

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

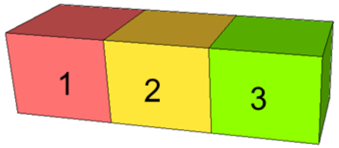
→ 3 point formula, could be extended to N points depending on the number of derivatives we carry in our expansion



I = G x V

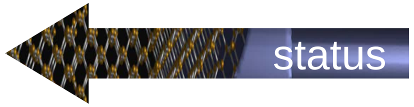
= q x n x v x A

charge density velocity area



Vid
Vid
Vid

- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations
  - »Gridding and finite differences



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

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

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

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

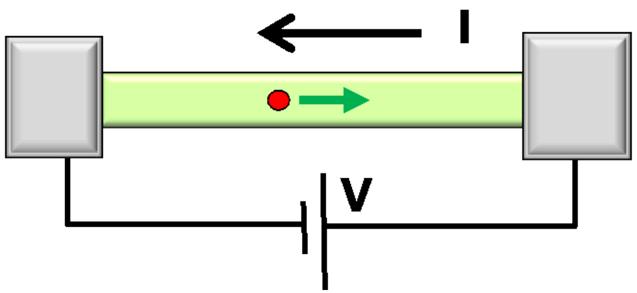
$$\nabla \bullet D = q(p - n + N_D^+ - N_A^-)$$

$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a} \qquad \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

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

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

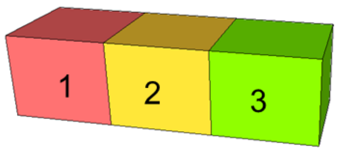
$$\nabla \bullet \left(\vec{J}_p / \; q\right) = \left(g_N - r_N\right)$$



I = G x V

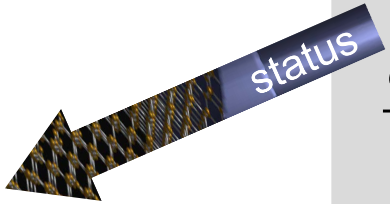
= q x n x v x A

charge density velocity area



Vid
Vid
Vid

- 18.1 Continuity Equation
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations
  - »Gridding and finite differences
  - »Discretizing equations and boundary conditions



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

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

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

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

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

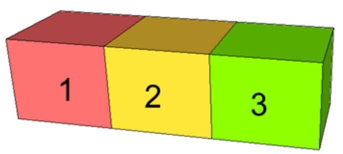
$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a} \qquad \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

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

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

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

2) Control Volume



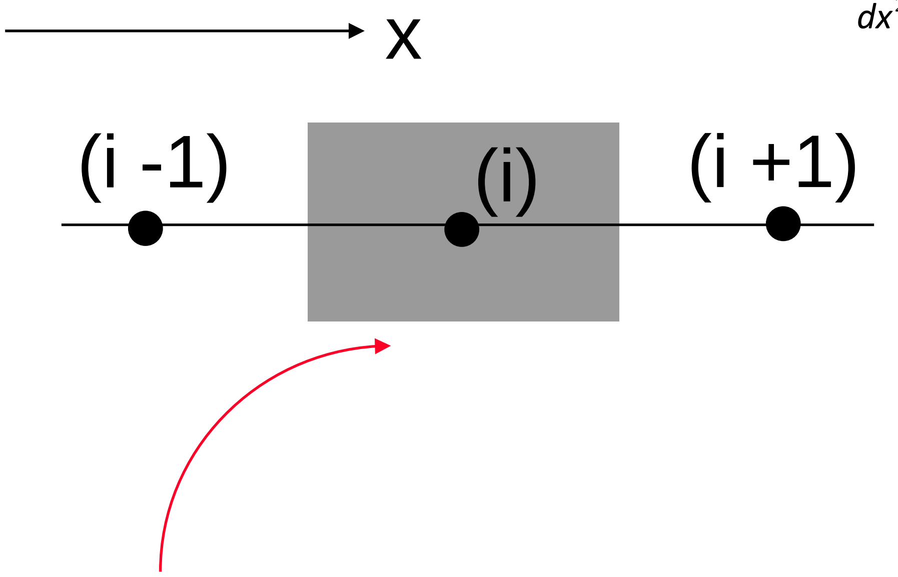
$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a}$$

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

3 unknowns at each node:

$$V_i, n_i, p_i$$

Need 3 equations at each node

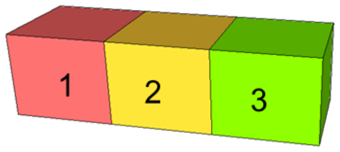


“control volume”

Discretizing Poisson's Equation

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

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

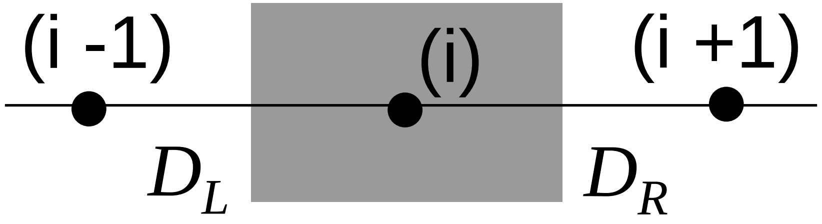


$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a}$$

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

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

Since V_o and V_{-1} are known, as are carrier concentration on doping (or lack thereof) in contacts, we find V_1 and iterate from this point to solve for potential.

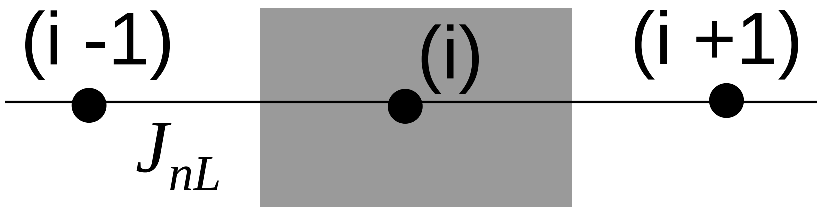


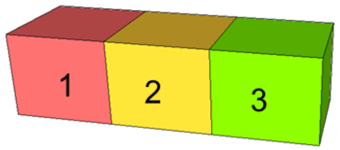
$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

→ Once this potential is found, solve continuity equation to obtain new carrier concentrations

Discretizing Continuity Equations

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





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

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

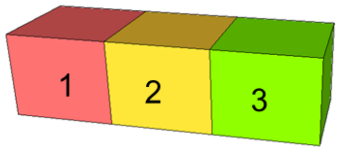
$$J_{nL} = -nq\mu_n \frac{dV}{dx} + kT\mu_n \frac{dn}{dx}$$

The simplest approach…..

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

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

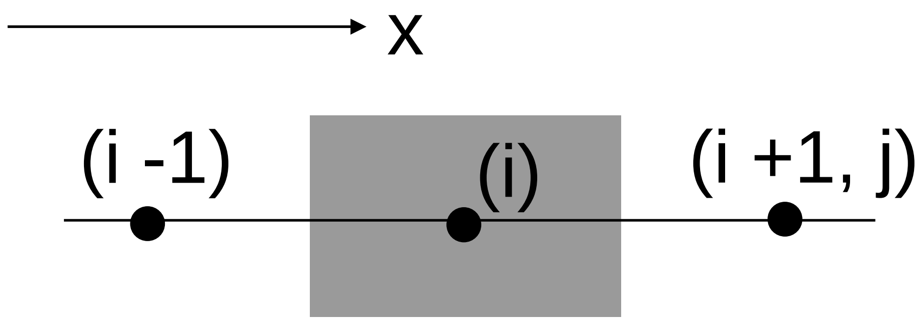
Three Discretized Equations



$$F_V^i = 0$$

$$F_n^i = 0$$

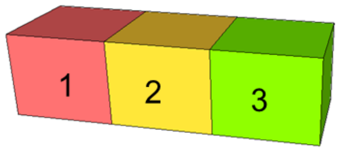
$$F_p^i = 0$$



3 unknowns at each node
N nodes
3N unknowns and 3N equations (coupled to each other)

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

Numerical Solution – Poisson Equation Only

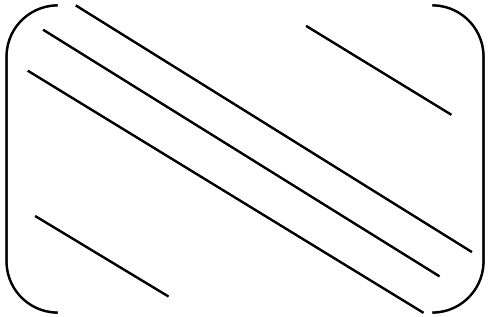


3 unknowns at each node
N nodes
3N unknowns and 3N equations (coupled to each other)

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

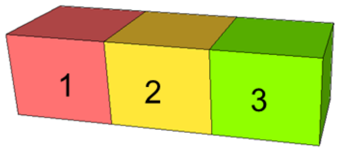
$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

linear if n_i and p_i are known $[A]\vec{V} = \vec{b}$

[A]: 

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

Boundary conditions

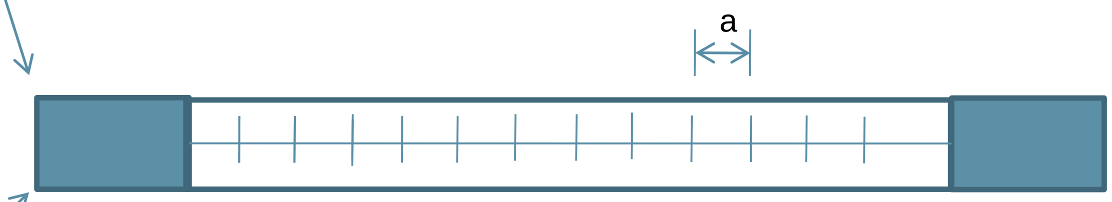


Contacts are assumed large and in equilibrium
→ detailed balance and law of mass-action apply!!

$$n_0 p_0 = n_i^2$$

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

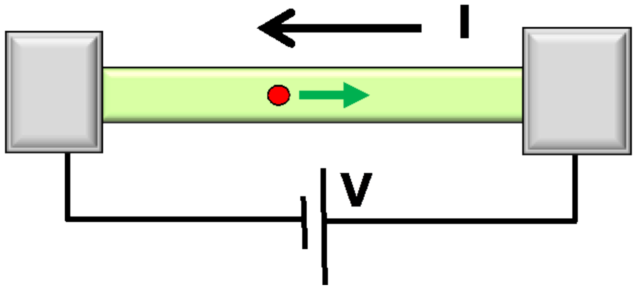
Dopant density



$$V = V_A$$

One could have unequal materials on the two contact sides, one must be careful to use the right intrinsic concentration <-> material.

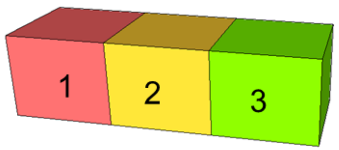
$$V = 0$$



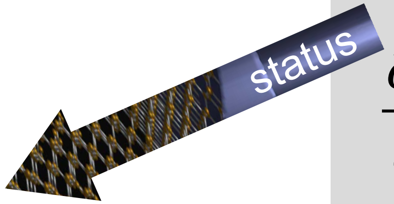
$I = G \times V$

$= q \times n \times v \times A$

charge density velocity area



- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - » Basic Transport Equations
  - » Gridding and finite differences
  - » Discretizing equations and boundary conditions



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

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

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

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

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

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

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

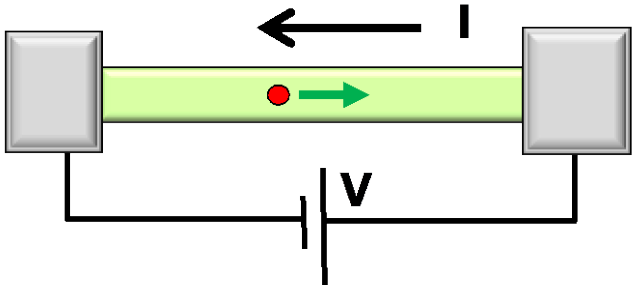
$$\nabla \bullet \left(\vec{J}_p / \ q\right) = \left(g_N - r_N\right)$$

$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a} \qquad \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

Vid

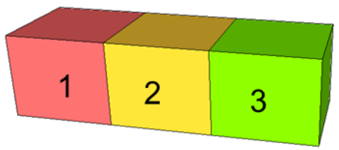
Vid

Vid



$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area



Vid
Vid
Vid

- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations
  - »Gridding and finite differences
  - »Discretizing equations and boundary conditions
  - »Iterative Solution Approach

status

$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a} \qquad \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

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

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

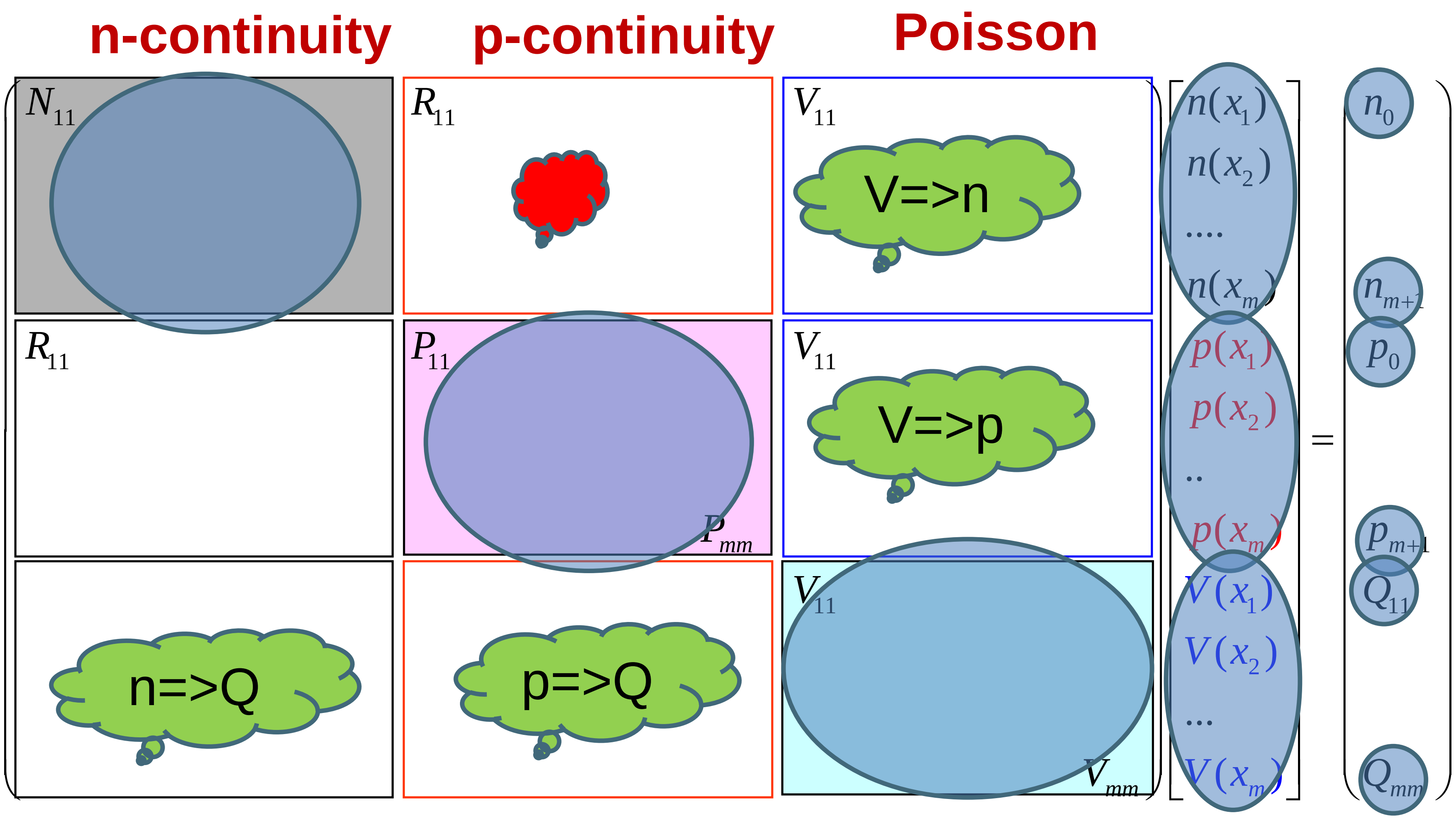
$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$

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

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

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

Numerical Solution...

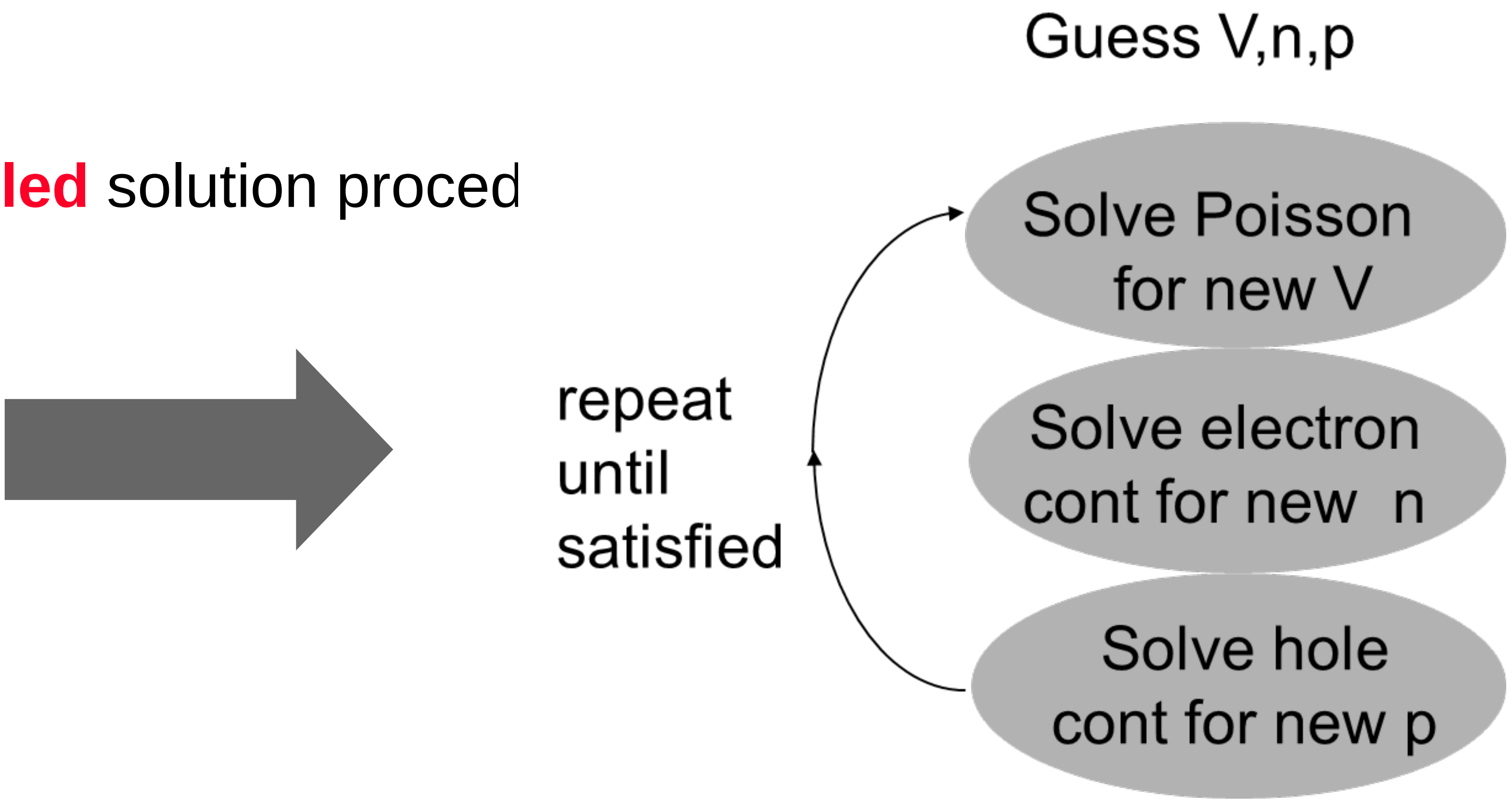


Off-diagonal terms are Poisson-Continuity equations talking to each other.
Recombination-generation terms also feed into continuity equations.

3) Uncoupled Numerical Solution

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

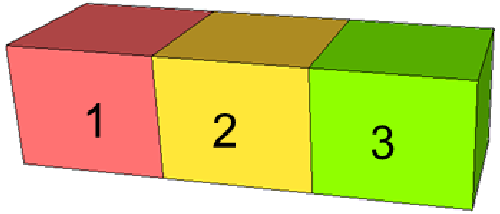
Uncoupled solution proced



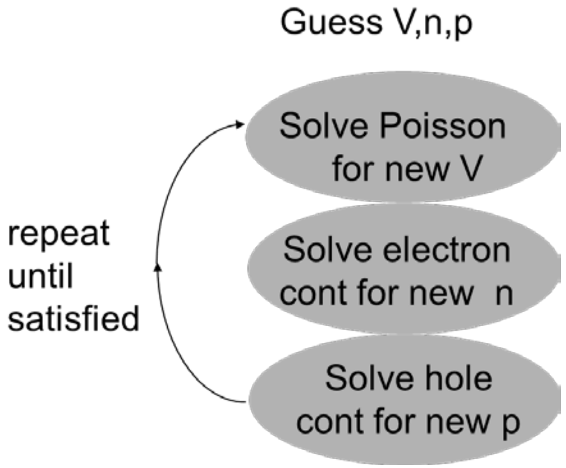
Summary

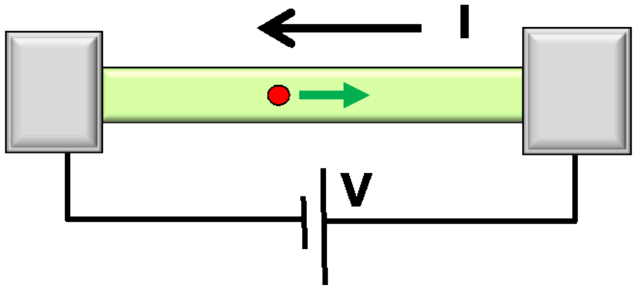
1) Two methods to solve drift-diffusion equation consistently – analytical and numerical.

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



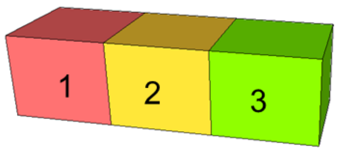
3) Numerical solution is more versatile.
   1) One begins with a set of equations and boundary conditions,
   2) discretize the equations on a grid with N nodes to obtain 3N nonlinear equations in 3N unknowns, and
   3) solve the system of nonlinear equations by iteration.





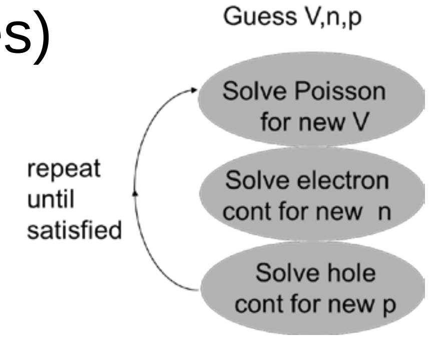
$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area



Vid
Vid
Vid

- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - »Basic Transport Equations
  - »Gridding and finite differences
  - »Discretizing equations and boundary conditions
  - »Iterative Solution Approach



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

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

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

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

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

$$\left.\frac{df}{dx}\right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a} \qquad \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2}$$

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