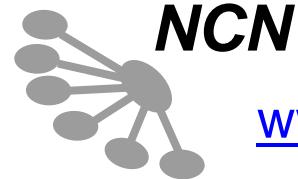


EE-612:

Lecture 2: Introduction to

Device Simulation

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www.nanohub.org

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Introduction

This is a short version of a presentation, “A Primer on Semiconductor Device Simulation,” by Mark Lundstrom.

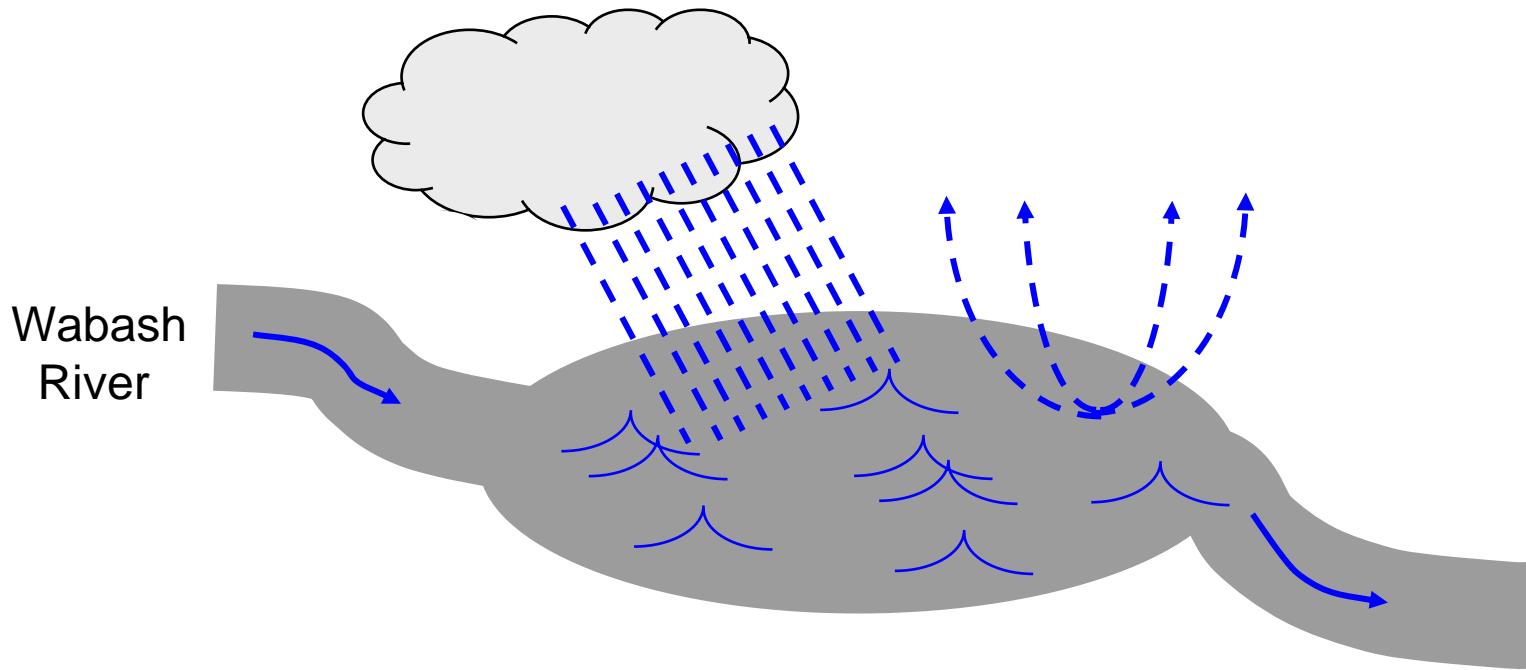
That presentation can be found at www.nanohub.org.

To find the longer presentation, search “Lundstrom” using the nanoHUB search box.

Outline

- 1) The Semiconductor Equations
- 2) Numerical vs. analytical solutions
- 3) Discretization
- 4) Numerical Solution
- 5) Physical Models
- 6) Examples
- 7) Concluding Thoughts

1) A Continuity Equation



Rate of increase of
water level in lake = (in flow - outflow) + rain - evaporation

$$\frac{\partial p}{\partial t} = -\nabla \cdot (\vec{J}_p/q) + G - R$$

1) The Semiconductor Equations

Conservation Laws:

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

$$\nabla \bullet (\vec{J}_n / -q) = (G - R)$$

$$\nabla \bullet (\vec{J}_p / q) = (G - R)$$

(steady-state)

Constitutive Relations:

$$\vec{D} = \kappa \epsilon_0 \vec{E} = -\kappa \epsilon_0 \vec{\nabla} V$$

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

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

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

$$R = f(n, p)$$

etc.

1) The Mathematical Problem

The “Semiconductor Equations”

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

$$\nabla \bullet (\vec{J}_n / -q) = (G - R)$$

$$\nabla \bullet (\vec{J}_p / q) = (G - R)$$

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

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

Conservation laws:

Transport eqs. (drift-diffusion):

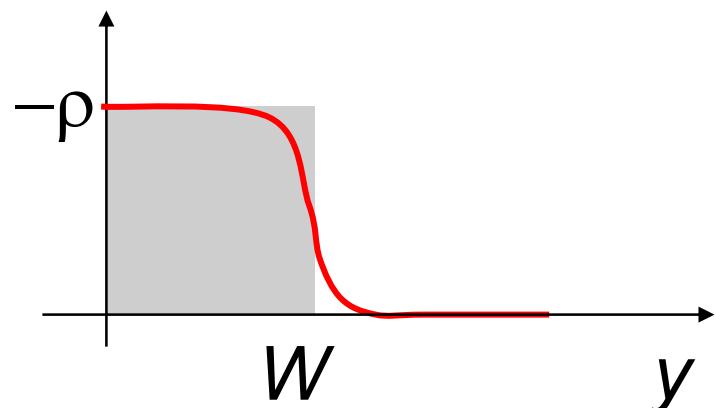
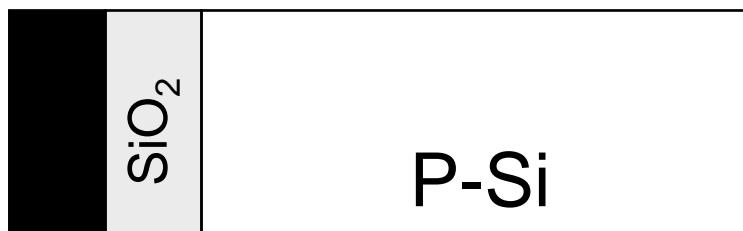
“exact”

approximate

2) Numerical vs. Analytical: The Depletion Approximation

(i) analytical solutions (e.g. depletion approximation)

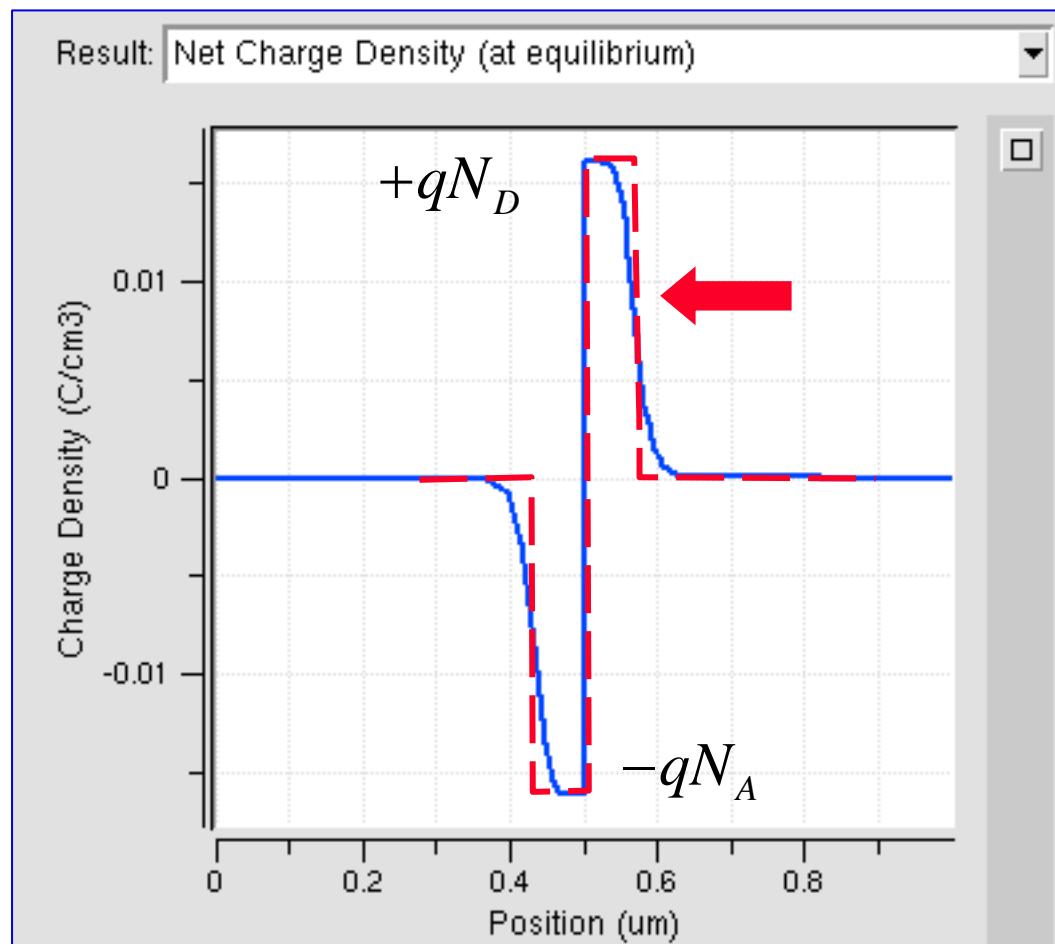
$$0 < V_G < V_T$$



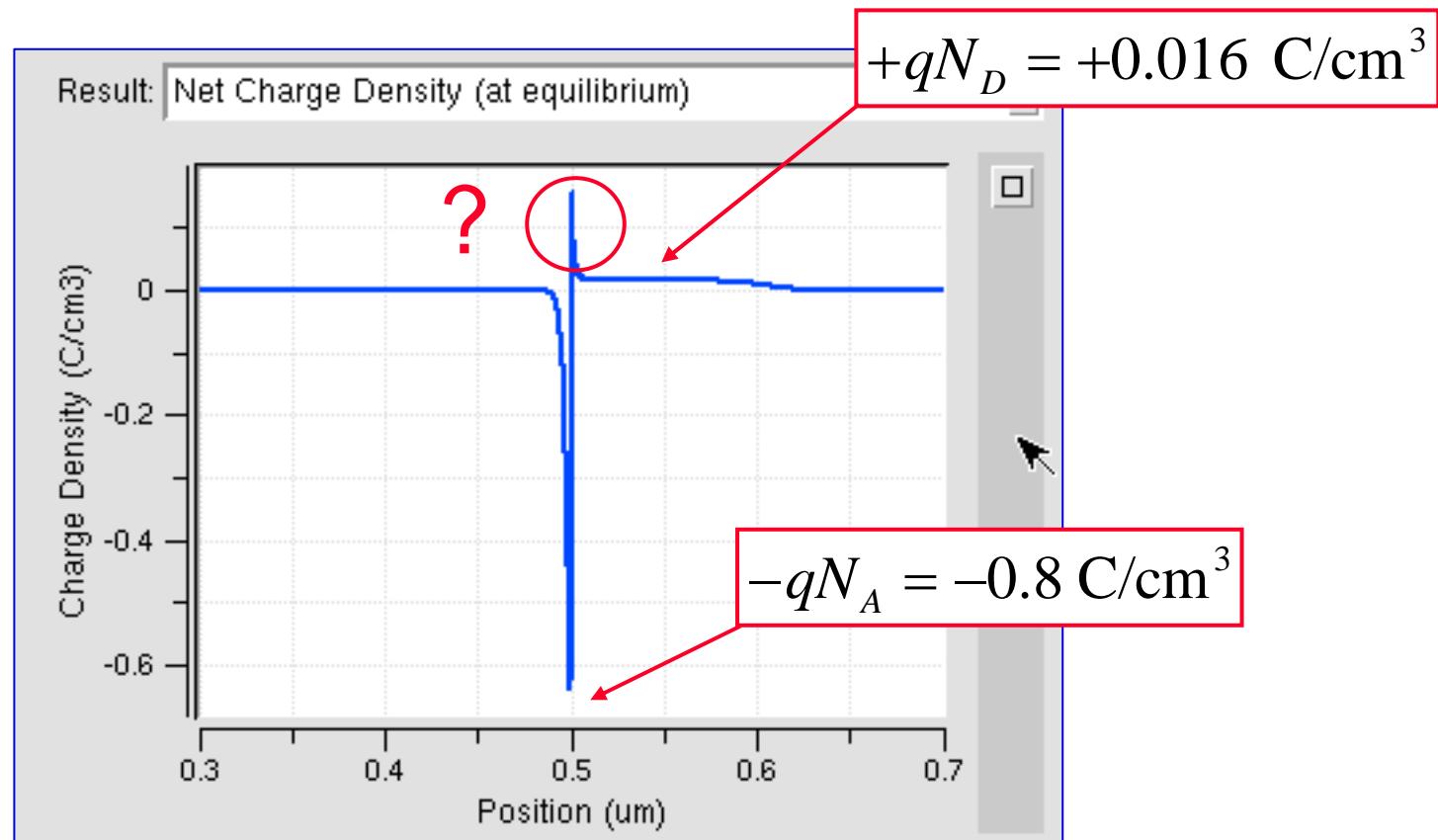
$$\frac{dD}{dx} = q(p - n - N_A)$$

$$\frac{d^2V}{dx^2} = \frac{qN_A}{\kappa_S \epsilon_0} \quad (x < W)$$

2) The Depletion Approximation vs. Numerical Solution

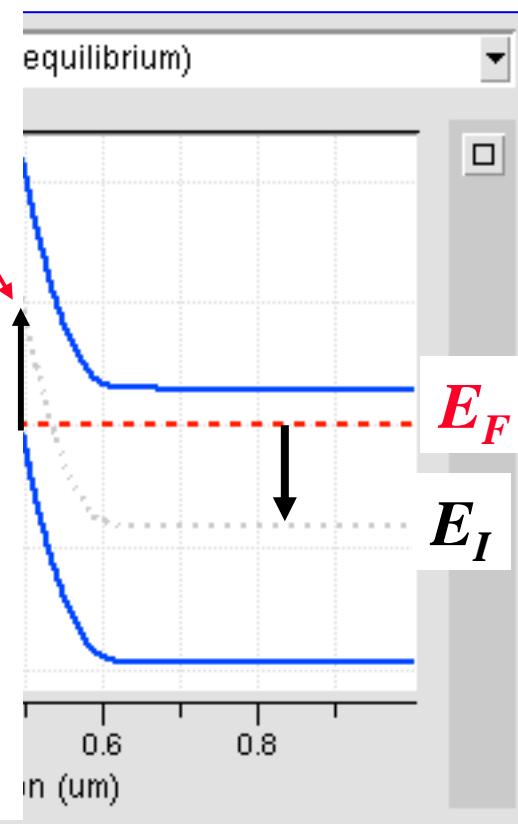


2) Asymmetric Junction



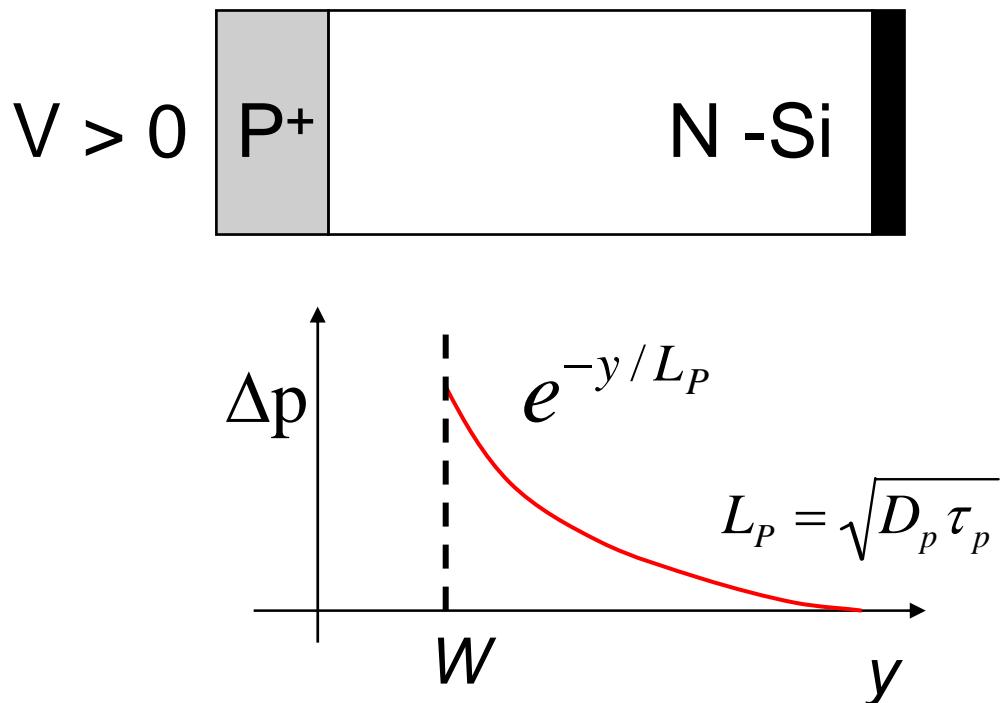
2) Asymmetric Junction

inversion layer
in a PN junction!



2) The Minority Carrier Diffusion Equation

(i) analytical solutions (e.g. minority carrier diffusion eq)



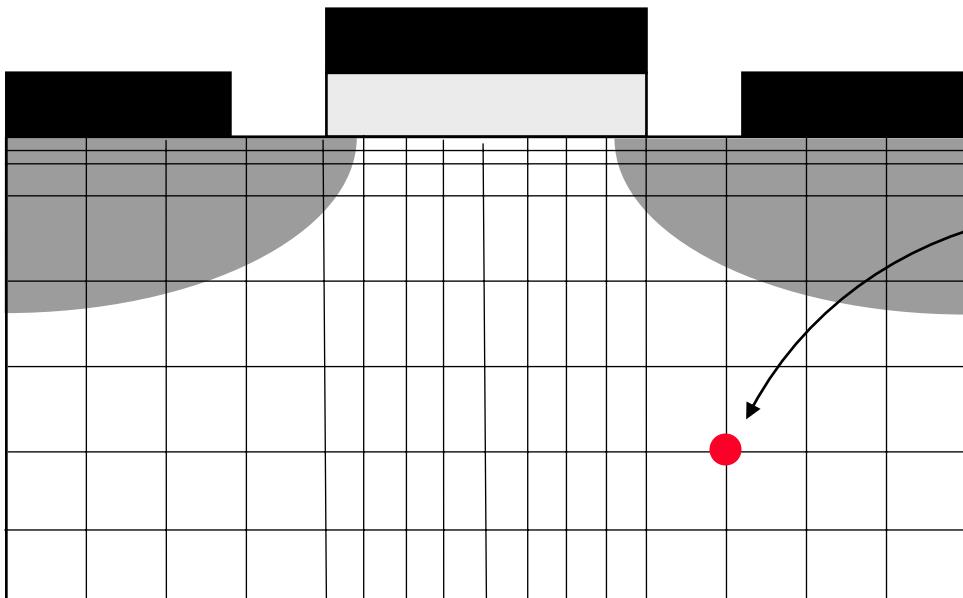
$$J_p = pq \cancel{\tau_p} E - qD_p \frac{dp}{dy}$$

$$\frac{d(J_p/q)}{dy} = -R \approx -\frac{\Delta p}{\tau_p}$$

$$D_p \frac{d^2 \Delta p}{dy^2} - \frac{\Delta p}{\tau_p} = 0$$

3) Discretization: The Grid

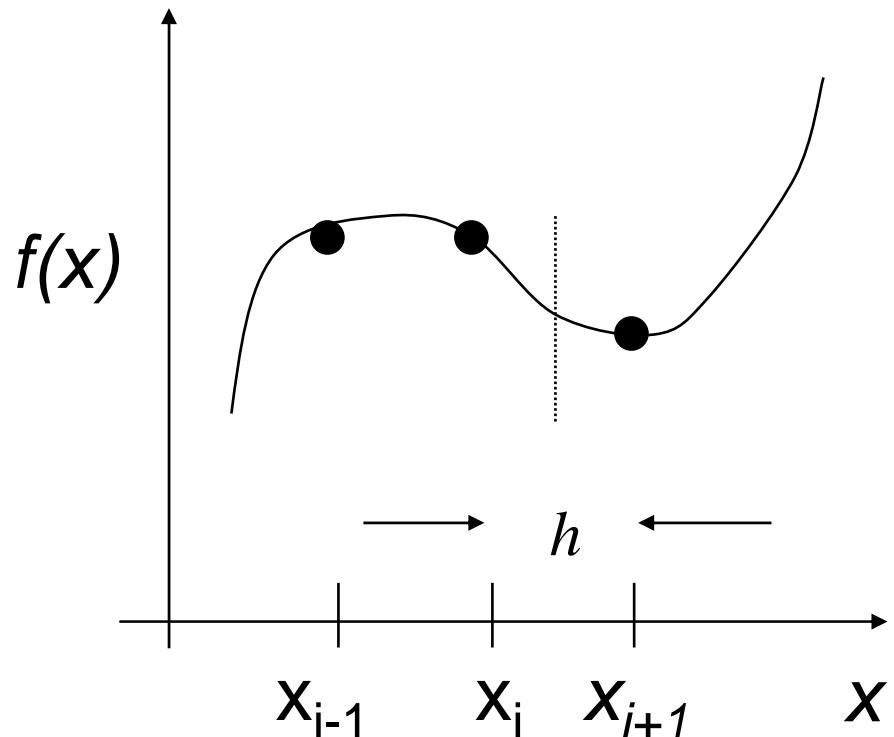
(ii) “exact” numerical solutions



N nodes
3N unknowns

$$\begin{matrix} V_{i,j} \\ n_{i,j} \\ p_{i,j} \end{matrix}$$

3) Discretization

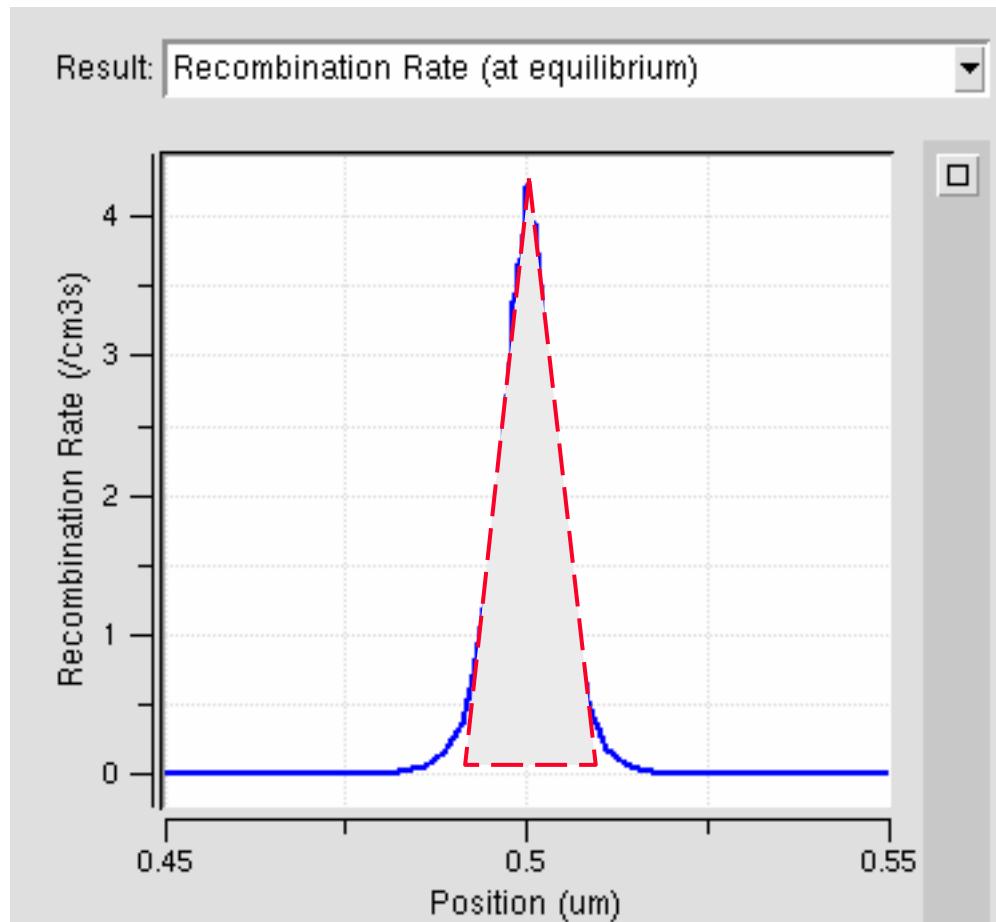


$$\left. \frac{df}{dx} \right|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{h} + O(h^2)$$

“centered
difference”

Local truncation error
(LTE)

3) Numerical Error: Example



$$J = q \int_0^L R(x) dx \text{ A/cm}^2$$

$$J \approx 1.3 \times 10^{-24} \text{ A/cm}^2$$

let $A = 10\mu\text{m} \times 10\mu\text{m}$

$$I \approx 1.3 \times 10^{-30} \text{ A}$$

1 electron every 15M years!

3) Discretization: Tips

Gridding tips

- place nodes where V , p , and n are expected to vary
- avoid abrupt changes in h
- ***verify the accuracy*** of the grid by re-solving with a finer grid

3) Discretizing a PDE

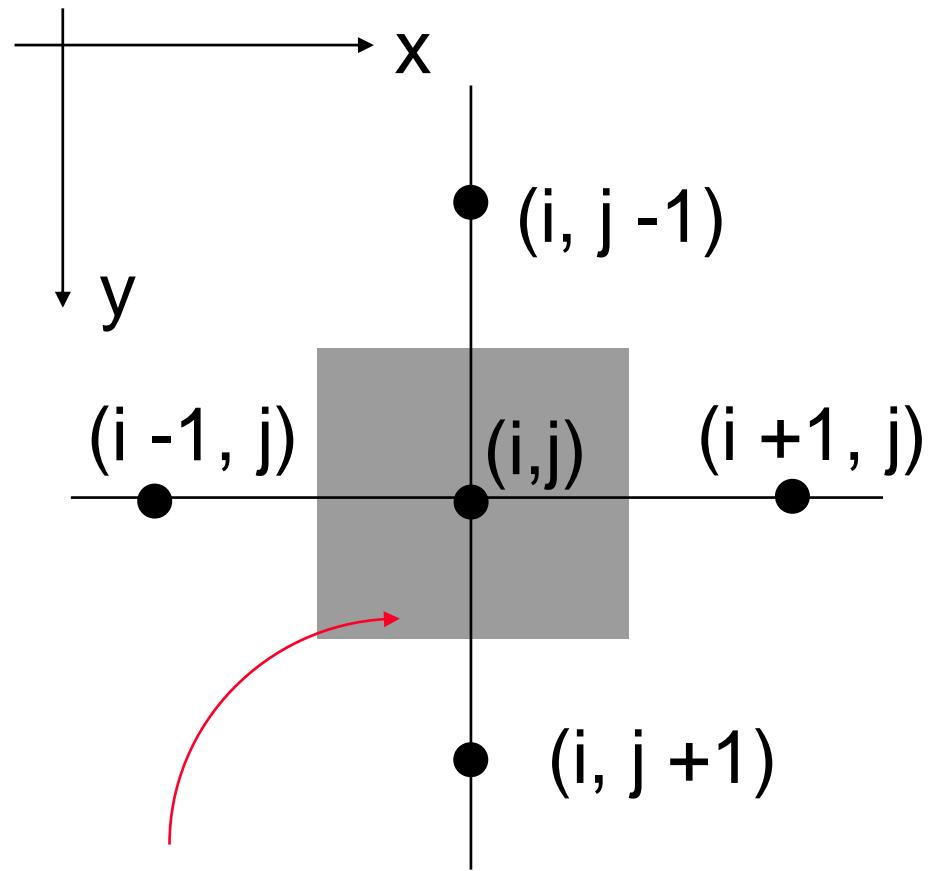
Poisson

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

$$\int_{\Omega} \nabla \bullet \vec{D} d\Omega = \int_{\Omega} \rho d\Omega$$

$$\oint_S \vec{D} \bullet d\vec{S} = \int_{\Omega} \rho d\Omega$$

“control volume”

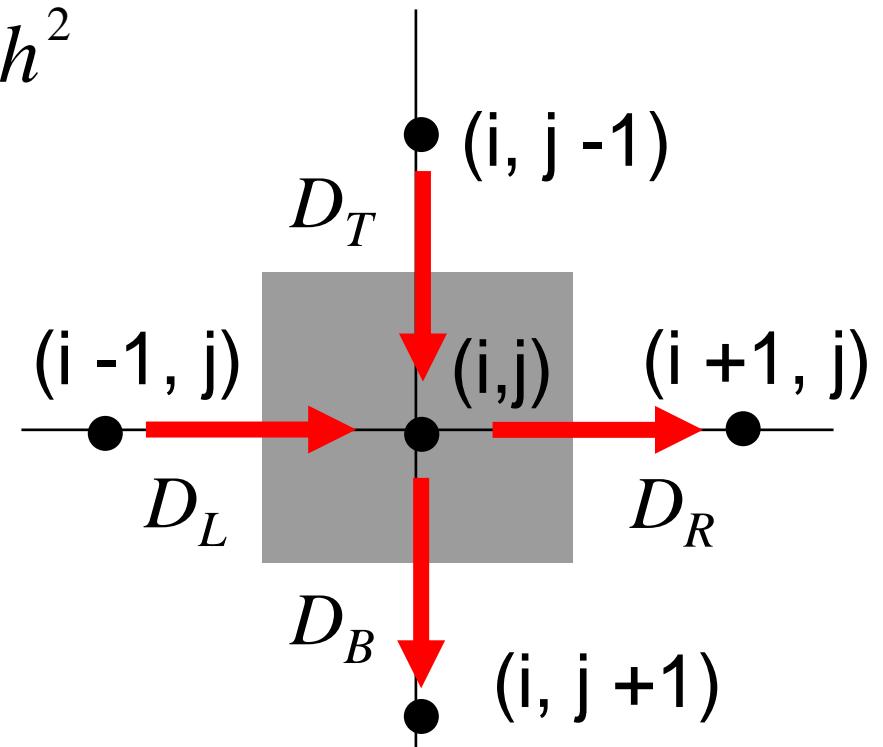


3) Discretizing Poisson's Equation

$$(D_R + D_B - D_L - D_T)h = \rho_{i,j} h^2$$

$$D_L = \kappa_S \epsilon_0 E_L$$

$$D_L \approx \frac{\kappa_S \epsilon_0}{h} (V_{i-1,j} - V_{i,j})$$



$$F_V^{i,j}(V_{i,j-1}, V_{i-1,j}, V_{i,j}, V_{i+1,j}, V_{i,j+1}, n_{i,j}, p_{i,j}) = 0$$

3) Discretizing the semiconductor equations

Current Continuity

$$\nabla \bullet \vec{J}_n = -q(G - R)$$

$$\int_{\Omega} \nabla \bullet \vec{J}_n d\Omega = \int_{\Omega} -q(G - R) d\Omega$$

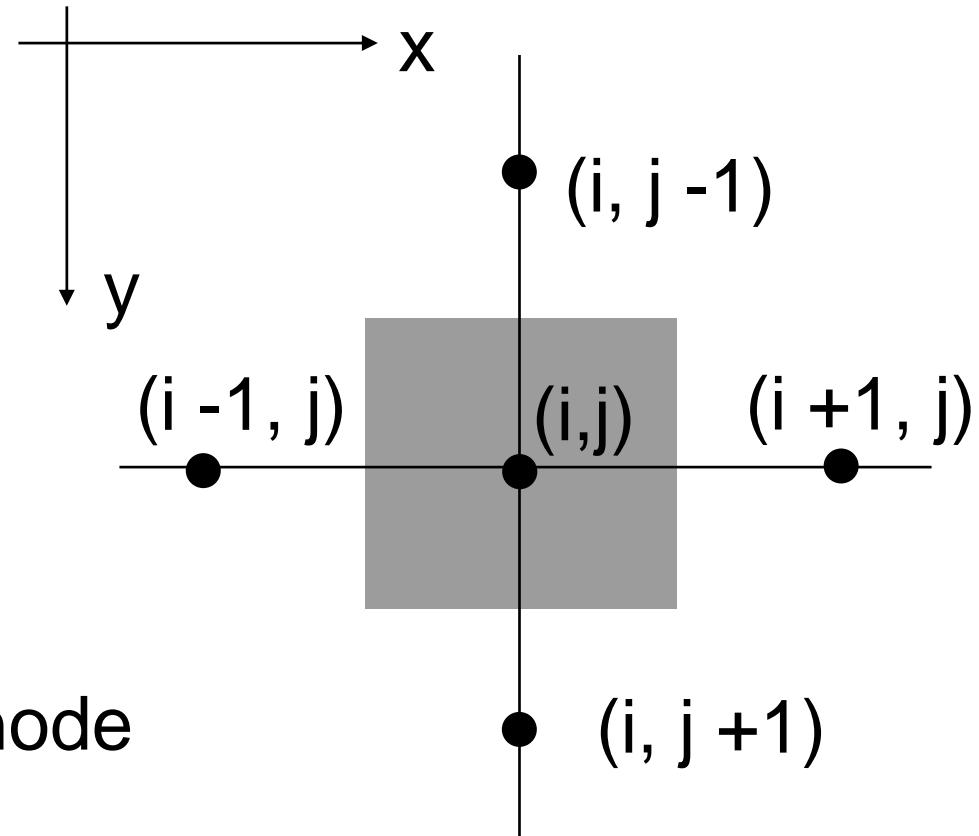
$$\oint_S \frac{\vec{J}_n}{-q} \bullet d\vec{S} = \int_{\Omega} (G - R) d\Omega \quad (\text{steady-state})$$

3) The 3 Discretized Equations

$$F_V^{i,j} = 0$$

$$F_n^{i,j} = 0$$

$$F_p^{i,j} = 0$$



3 unknowns at each node

N nodes

$3N$ unknowns and $3N$ equations
(nonlinear!)

need boundary and initial conditions too...

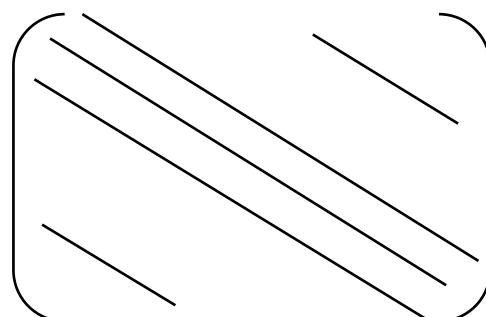
4) Numerical Solution

- have a system of $3N$ nonlinear equations to solve
- recall Poisson's equation at node (i,j) :

$$F_V^{i,j}(V_{i,j-1}, V_{i-1,j}, V_{i,j}, V_{i+1,j}, V_{i,j+1}, n_{i,j}, p_{i,j}) = 0$$

linear if n_{ij} and p_{ij} are known $[A]\vec{V} = \vec{b}$

$[A]:$



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

4) Curse of Dimensionality

Linear systems:

1D $N \sim 100$ nodes $[A]: 100 \times 100$

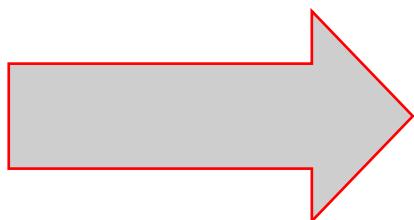
2D $N \sim 10,000$ $[A]: 10,000 \times 10,000$

3D $N \sim 100,000$ $[A]: \text{huge!}$

4) Numerical Solution of 3 coupled, nonlinear PDE's

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

sequential solution procedure



repeat
until
satisfied
“iteration”

Guess V,n,p

Solve Poisson
for new V

Solve electron
cont for new n

Solve hole
cont for new p

4) Numerical Solution: Stopping

How do we know when we're done?

1)

$$\begin{pmatrix} \vec{F}_V \\ \vec{F}_n \\ \vec{F}_p \end{pmatrix} = \vec{0} \quad \begin{pmatrix} \vec{F}_V(\vec{V}^k, \vec{n}^k, \vec{p}^k) \\ \vec{F}_n(\vec{V}^k, \vec{n}^k, \vec{p}^k) \\ \vec{F}_p(\vec{V}^k, \vec{n}^k, \vec{p}^k) \end{pmatrix} = \vec{r}$$

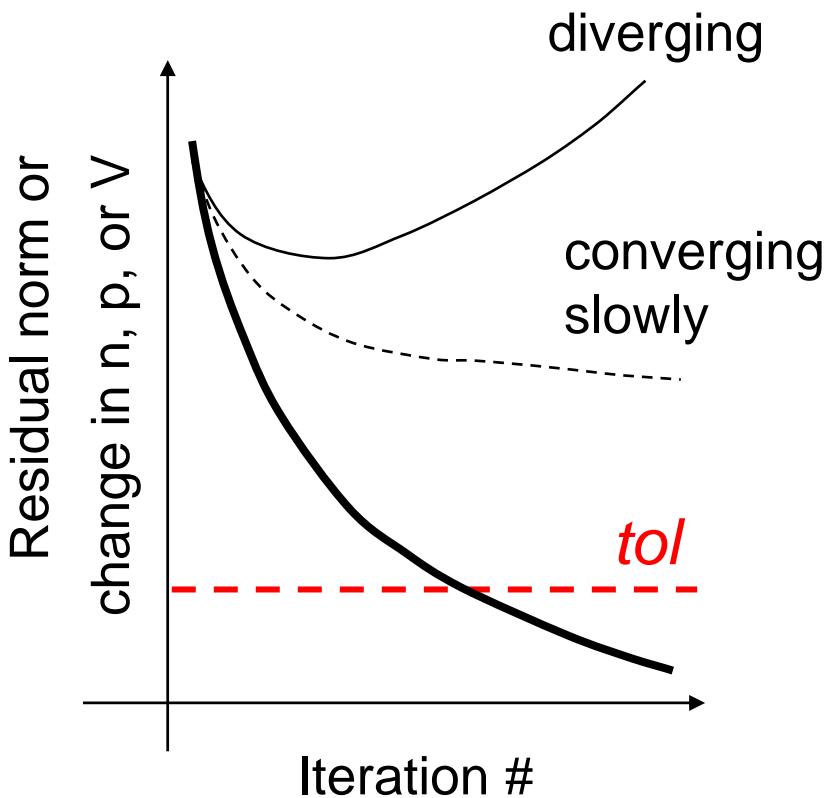
$\| r \|$

Is a measure of the numerical error

2)

$$\Delta V^k = V^{k+1} - V^k \quad \Delta V^k \rightarrow 0 \text{ as } k \rightarrow \text{infinity}$$

4) Convergence



Convergence tips:

- check problem definition
- take small steps in voltage
- increase k_{max} if converging
- change convergence criterion
- try another method

4) Numerical Solution

Summary: Solving Partial Differential Equations

- 1) Begin with a set of equations, boundary conditions, and initial conditions
- 2) Discretize the equations on a grid with N nodes to obtain $3N$ nonlinear equations in $3N$ unknowns
- 3) Solve the system of nonlinear equations by iteration

5) Physical Models

The physical parameters in the semiconductor equations need to be modeled.

e.g.

- 1) doping dependent mobility $\mu = \frac{\mu_i}{1 + N_D/N^\alpha}$
- 2) field dependent mobility $\mu = \frac{\mu_o}{\sqrt{1 + E/E_{cr}}}$
- 3) recombination $R = \frac{np - n_i^2}{(n + n_1)\tau_{po} + (p + p_1)\tau_{no}}$
- 4) etc.

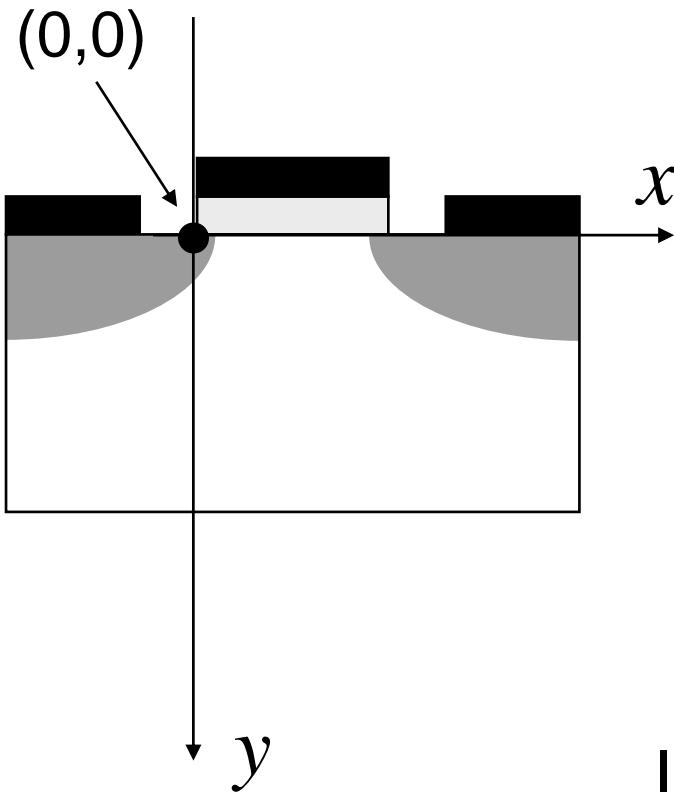
5) Physical Models

Tips for dealing with physical models

- **understand** the models available in the tool
- **understand** the parameters in the model you select
- **know** the default models and their parameters
- **check** for conflicts between various models
(i.e. if model A is selected, then model B can't be used)

Proper selection and specification of physical models is critical!

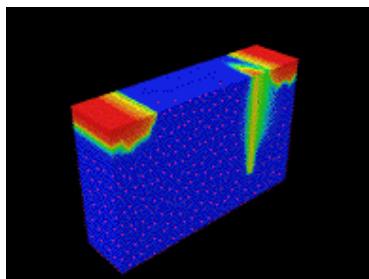
6) Example: The MINIMOS program



```
* EXAMPLE MINIMOS 6.0 SIMULATION
DEVICE CHANNEL=N GATE=NPOLY
+
TOX=150.E-8 W=1.E-4 L=0.85E-4
BIAS UD=4. UG=1.5
PROFILE NB=5.2E16 ELEM=AS DOSE=2.E15
+
TOX=500.E-8 AKEV=160.
+
TEMP=1050. TIME=2700
IMPLANT ELEM=B DOSE=1.E12 AKEV=12
+
TEMP=940 TIME=1000
OPTION MODEL=2-D
OUTPUT ALL=YES
END
```

Input directives are described in Ch. 3
of the MINIMOS 6.0 User's Guide

6) Example: The PADRE program



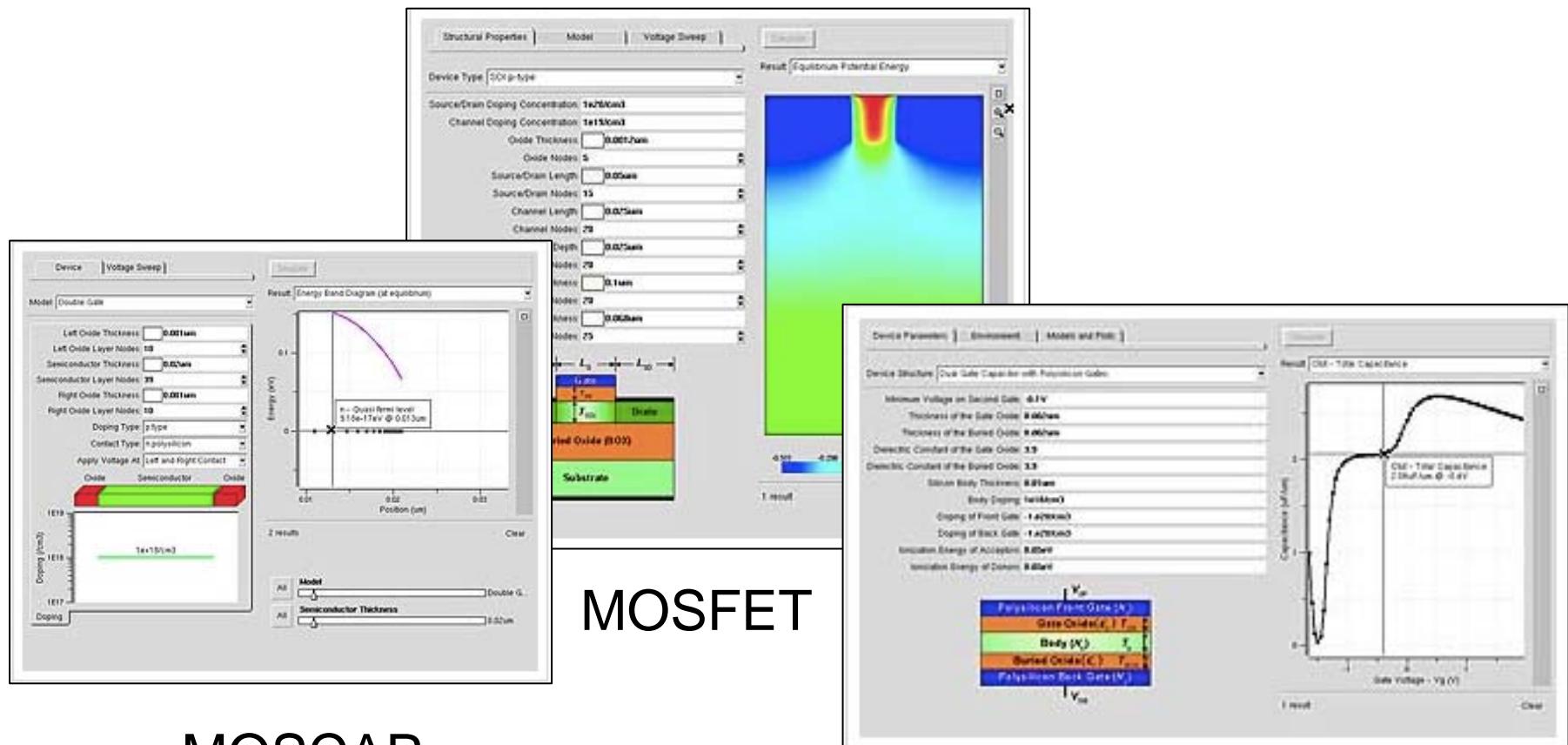
M. Pinto, R.K. Smith, M.A. Alam, Bell
Labs

```
title      MOSFET - NMOS
MESH RECT NX=51NY=51
X. M N=1 LOC=0
X. M N=15 LOC=0.05 RATIO=0.8
X. M N=26 LOC=0.0625 RATIO=1.25
X. M N=36 LOC=0.075 RATIO=0.8
X. M N=51 LOC=0.125 RATIO=1.25

Y.M N=1 LOC=0
Y.M N=25 LOC=0.068 RATIO=0.8
Y.M N=36 LOC=0.0805 RATIO=1.25
Y.M N=46 LOC=0.093 RATIO=0.8
Y.M N=51 LOC=0.0942 RATIO=1.25

# Substrate
REGION NUM=1 ix.l=1 ix.h=51 iy.l=1 iy.h=25 silicon
# Source
REGION NUM=2 ix.l=1 ix.h=15 iy.l=25 iy.h=46 silicon
# Drain
REGION NUM=3 ix.l=36 ix.h=51 iy.l=25 iy.h=46 silicon
# Channel
REGION NUM=4 ix.l=15 ix.h=36 iy.l=25 iy.h=46 silicon
# Gate
REGION NUM=5 ix.l=15 ix.h=36 iy.l=46 iy.h=51
...
```

6) More examples (EE-612 / nanoHUB)



MOSCAP

MOSFET

Schred

6) Tips on using a new simulation tool

- Understand what the tool does
 - what equations are being solved?
 - what numerical methods are used?
 - what physical models are implemented?
- Try a simple problem first to be sure you get the correct answer
- Look for example files - close to the problem you're interested in.
- Know what the default settings are
- Ask an experienced user for help

7) Concluding Thoughts

- 1) Don't be a 'Spice monkey' - think about the simulation before you do it and understand the results before you do another.
- 2) All software has limitations, and these are not always clearly understood. Check your results, and don't be afraid to 'stand up to a computer'.
- 3) Simulation gives us an ability to look inside a device in a way that is hard to do experimentally. Use that capability to develop your understanding of the problem. Remember Hamming:
“The purpose of computing is insight - not numbers.”
- 4) Simulation can be a tool that makes a good engineer better or a crutch that makes an engineer lazy. Learn to use simulation effectively, and it will pay off.

Where to get more information

- 1) *Analysis and Simulation of Semiconductor Devices*, S. Selberherr, Springer-Verlag, New York, 1984. (discusses numerical methods)
- 2) "MINIMOS - A Two-Dimensional MOS Transistor Analyzer," by S. Selberherr, A. Schutz, and H.W. Potzl, *IEEE Transactions on Electron Devices*, **27**, pp. 1540-1550, 1980
- 3) MINIMOS 6.0 User's Guide, October, 1994
(available from the MINIMOS page of the nanoHUB)
- 4) Padre User's Guide
(available from the Padre page of the nanoHUB)
- 5) Additional simulation tools and instructional material is available on the nanoHUB: www.nanoHUB.org