Computational Microelectronics
Lecture 7 Newton-Raphson Method

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Nonlinearity

Discretized diffusion equation

- It is much more difficult.
  - Although it can be generally written as

$$\frac{C(x_i, t_k) - C(x_i, t_{k-1})}{\Delta t}\Delta x = -F_{C,i+0.5} + F_{C,i-0.5}$$

  - Now, the flux terms are nonlinear, because of

$$F_C = -DC\left[\frac{\partial}{\partial x}\log C \pm \frac{\partial}{\partial x}\left(\log\frac{n}{n_{int}}\right)\right]$$

  - Note that the electron density is a nonlinear function of C.

Is it $\boldsymbol{Ax = b}$?

- Try to construct a matrix, A, for the flux term.
  - What is the entry for $C(x_i, t_k)$?

- Recall the previous case.
  - In our previous simple problem, the discretized form was

$$\frac{C(x_i, t_k) - C(x_i, t_{k-1})}{\Delta t} \Delta x$$
$$= D \frac{1}{\Delta x} [C(x_{i+1}, t_k) - C(x_i, t_k)] - D \frac{1}{\Delta x} [C(x_i, t_k) - C(x_{i-1}, t_k)]$$

Nonlinearity is the key.

- At present, we cannot solve the problem, because it is nonlinear.
  - Let us learn how to solve a nonlinear problem!
- An example, calcation of n under the charge neutrality.

$$N_D^+ + p = N_A^- + n$$
$$np = n_{int}^2$$

  - By eliminating p, we find an equation of

$$n^2 - (N_D^+ - N_A^-)n - n_{int}^2 = 0$$

  - Of course, we know the solution. However, instead of using the known formula, just calculate n with a numerical method.

Newton method

- First, we assume an initial solution, n_0.
  - Of course, there is no guarantee that n_0 is the solution. Therefore,
  $$n_0^2 - (N_D^+ - N_A^-)n_0 - n_{int}^2 = r_0 \neq 0$$
  - However, we assert that an improved solution, n_1, is the real solution. Our assertion can be written as
  $$n_1^2 - (N_D^+ - N_A^-)n_1 - n_{int}^2 = 0$$
  - We can take the difference between two equations:
  $$(n_1 + n_0)(n_1 - n_0) - (N_D^+ - N_A^-)(n_1 - n_0) = -r_0$$
  - We CANNOT solve, because it is still a nonlinear equation of n_1.
  - Instead, we can solve the following (approximate) equation:
  $$2n_0(n_1 - n_0) - (N_D^+ - N_A^-)(n_1 - n_0) = -r_0$$

Iteration

- Unfortunately, the solution, $n_1 - n_0$, is not exact.
  - Anyway, from n_0 and $n_1 - n_0$, we can calcultate (inaccurate) n_1.
  - Then, from n_1, we again assert that n_2 is the real solution.
  - Again, n_2 will not be perfect.
  - Even though it is not perfect, it may approach to the solution.
  - Repeat this procedure until the error is sufficiently reduced.

HW#7

- Due: AM08:00, September 20
- Problem#1
  - Calculate the electron density, n, under the charge neutrality. Adopt the Newton method. Verify your results at two temperatures (300 K and 1200 K) and three dopants densities, $N_D^+ - N_A^-$ (10^{20} cm^{-3}, 10^{18} cm^{-3}, and 10^{16} cm^{-3}). Of course, your solution should be very close to the analytic solution.

Generalization

- We want to solve $f(\phi) = 0$.
  - A temporal solution, ϕ_0, is ***NOT*** a solution.
$$f(\phi_0) \neq 0$$
  - However, we assert that an improved solution, ϕ_1 , is the real solution.
$$f(\phi_1) = f(\phi_0 + \delta\phi) = 0$$
  - A linearized form of $f(\phi_0 + \delta\phi)$ is used:
$$f(\phi_0 + \delta\phi) \approx f(\phi_0) + \left.\frac{df}{d\phi}\right|_{\phi_0} \delta\phi = 0$$
  - The update, $\delta\phi$, can be calculated by solving
$$\delta\phi = -\left(\left.\frac{df}{d\phi}\right|_{\phi_0}\right)^{-1} f(\phi_0)$$

Newton-Raphson method

Extension to multi-variable cases

- We want to solve $f(x,y) = 0$ and $g(x,y) = 0$ simultaneously.
  - Again, x_0 and y_0 do ***NOT*** satisfy the equations

$$f(x_0, y_0) \neq 0 \text{ and } g(x_0, y_0) \neq 0$$

  - Following the same procedure, we assert that

$$f(x_1, y_1) = 0 \text{ and } g(x_1, y_1) = 0$$

  - In thee linearized form,

$$f(x_0, y_0) + \left.\frac{df}{dx}\right|_{x_0,y_0} \delta x + \left.\frac{df}{dy}\right|_{x_0,y_0} \delta y = 0$$

$$g(x_0, y_0) + \left.\frac{dg}{dx}\right|_{x_0,y_0} \delta x + \left.\frac{dg}{dy}\right|_{x_0,y_0} \delta y = 0$$

$\boldsymbol{Ax = b}$, once again

- Express the previous equations in the $Ax = b$ form.
  - What is the x vector (update vector) ? $[\delta x \quad \delta y]^T$ 🡐 It is not $[x \quad y]^T$.
  - What is the matrix, A (Jacobian matrix)?

$$A = \begin{bmatrix} \left.\frac{df}{dx}\right|_{x_0,y_0} & \left.\frac{df}{dy}\right|_{x_0,y_0} \\ \left.\frac{dg}{dx}\right|_{x_0,y_0} & \left.\frac{dg}{dy}\right|_{x_0,y_0} \end{bmatrix}$$

  - What is the b vector (residue vector)? $-[f(x_0, y_0) \quad g(x_0, y_0)]^T$
- We can repeat the above calculation, again and again.

An example

- Three variables
  - Calculate the solution, ϕ_1, ϕ_2, ϕ_3.

$$f_1(\phi_1, \phi_2, \phi_3) = \phi_2 - 2\phi_1 - e^{\phi_1} = 0$$
$$f_2(\phi_1, \phi_2, \phi_3) = \phi_3 - 2\phi_2 + \phi_1 - e^{\phi_2} = 0$$
$$f_3(\phi_1, \phi_2, \phi_3) = -2\phi_3 + \phi_2 - e^{\phi_3} + 4 = 0$$

  - The Jacobian matrix reads

$$\begin{bmatrix} -2 - \exp\phi_1 & 1 & 0 \\ 1 & -2 - \exp\phi_2 & 1 \\ 0 & 1 & -2 - \exp\phi_3 \end{bmatrix}$$

Solution procedure

- Initial guess is important.
  - Starting from $[0 \quad 0 \quad 0]^T$ or $[10 \quad 10 \quad 10]^T$.

```
0 [[0.]
 [0.]
 [0.]]
1 [[-0.39130435]
 [-0.17391304]
 [ 0.86956522]]
2 [[-0.43431205]
 [-0.22153048]
 [ 0.79160481]]
3 [[-0.43519241]
 [-0.22324493]
 [ 0.78862027]]
4 [[-0.43522526]
 [-0.22333163]
 [ 0.78841154]]
```

```
0 [[10.]
 [10.]
 [10.]]
1 [[8.99959144]
 [8.99999997]
 [8.999773  ]]
2 [[7.9986041 ]
 [7.99999971]
 [7.99927931]]
3 [[6.9962551 ]
 [6.99999788]
 [6.99827256]]
4 [[5.99078014]
 [5.99998625]
 [5.99644714]]
```

HW#7

- Problem#2
  - Solve the previous example. Select various initial guesses and measure the number of Newton iterations. The convergence criterion is the maximum absolute update smaller than 10^{-10}.

Thank you!