Current continuity discretization is much more difficult and central differencing is out. The reason is very large variation of concentrations. Recall the current continuity eq.:

$$\vec{\nabla} \cdot (D_n \nabla n - \mu_n n \nabla \psi) - R(\psi, n, p) = \frac{\partial n}{\partial t} \tag{1}$$

or in 2-D

$$\frac{\partial}{\partial x}\left(D_n \frac{\partial n}{\partial x} - \mu_n n \frac{\partial \psi}{\partial x}\right) +$$
$$\frac{\partial}{\partial y}\left(D_n \frac{\partial n}{\partial y} - \mu_n n \frac{\partial \psi}{\partial y}\right) - R = 0$$

The terms inside parenthesis are current densities flowing in x and y directions.

Approximate $\partial/\partial x, y$ at mid pts by using central differencing

$$\frac{-J_{nx}|_{i+1/2,j} - (-J_{nx})|_{i-1/2,j}}{1/2(h_i + h_{i-1})} + O(h)\frac{\partial^2 J_{nx}}{\partial x^2}\bigg|_{i,j} \ldots = 0. \qquad (2)$$

This gives us approx. for divergence term at the point (i,j). Completely analogous for holes.

We can't just plug in some more central differences in order to obtain mid-point values for currents in terms of independent variables (n, p, ψ). Instead, expand J around mid-point

$$J_{nx} = J_{nx}|_{i+1/2,j} + \left(x - x_i - \frac{h_i}{2}\right)\frac{\partial}{\partial x}\, J_{nx}|_{i+1/2,j}$$
$$+O(h^2)\frac{\partial^2}{\partial x^2}\, J_{nx}|_{i+1/2,j} \cdots$$

By neglecting 2nd order terms and assuming constant gradient of potential on the interval and known ratio of mobility and diffusivity, the resulting diff. eq. can be solved in n. As it turns out, the term containing $\partial J_{i,j}/\partial x$ can be neglected resulting in

$$n(x \in [x_i, x_{i+1}], y_j) = (1 - g^x_{i,j})n_{i,j} + g^x_{i,j}n_{i+1,j} \tag{3}$$

where g^x is the "growth" function

$$g^x_{i,j} = \frac{1 - \exp\left(\frac{\psi_{i+1,j} - \psi_{i,j}}{Ut}\ \frac{x - x_i}{h_i}\right)}{1 - \exp left(\frac{\psi_{i+1,j} - \psi_{i,j}}{Ut}} \tag{4}$$

By defining Bernoulli function $B(x) = x/(e^x - 1)$ final expressions for current densities can be simplified to

$$J_{nx}\big|_{i+1/2,j} = \frac{D_n\big|_{i+1/2,j}}{h_i}$$
$$\left[B\left(\frac{\psi_{i,j} - \psi_{i+1,j}}{Ut}\right) n_{i,j} - B\left(\frac{\psi_{i+1,j} - \psi_{i,j}}{Ut}\right) n_{i+1,j}\right] \ldots$$

All that is left is to plug these equations in the first approximation for the divergence of current density at node (i,j).

Local truncation error linearly proportional to the mesh spacing and the sum of the first and second partial derivatives of current density components.

An alternative approach (simpler) to deriving expressions for current densities is from original Scharfetter Gummel paper.

Or, look at it from box integration point of view. Here, once the current density at mid-point is known, it is integrated along that side of the box — assumption is that current is constant along the path of integration. To derive the current at mid-pint, the expression for $n(x) \in [x_i, x_{i+1}]$ is emplyed. Also, diffusivities (mobilities) are assumed constant.

For recombination we keep the volume integral and assume that it is constant over the box.

Discretized BCs for current continuity eqs.:

- ideal voltage controlled contact (ohmic)
- ideal current controlled contact

$$\int_{\partial D_0}(\vec{J}_n + \vec{J}_p)d\vec{A} - I_D = 0 \tag{5}$$

  and also $(\psi - \psi_b)|_{\partial D_0}$. Example

- reflection boundaries: $\vec{J} \cdot \vec{n} = 0$
- interface to oxide: $\vec{J} \cdot \vec{n} = 0$

Finally, care needed when coding Bernoulli functions — problems with underflow, overflow and round-off errors.

Different variables can be picked up as independent. Two standard choices are ψ, n, p and ψ, ϕ_n, ϕ_p. Each has its strengths and weaknesses.

How to solve nonlinear sets of equations?

Fixed point is a solution of equation : $g(x) = x$; basis for fixed point iteration

Newton-Raphson is concerned with $f(x) = 0$; many ways to derive, e.g. from Taylor expansion

$$f(x) = f(\bar{x}) + (x - \bar{x})f'(\bar{x}) + \frac{(x - \bar{x})^2}{2} f''(\xi(x)) \tag{6}$$

and the final expression is

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})} \tag{7}$$

for initial guess close to the solution the method converges

What about systems of nonlinear equations?

using vector notation the system is $\mathbf{F}(\mathbf{x}) = \mathbf{0}$.

def: fixed point of system of equations $\mathbf{M}(\mathbf{w}) = \mathbf{w}$. Fixed points important for generating sequences that converge to the true solution.

In fact, Newton's method stems from the requirement that (vectors and matrices are implied from now on)

$$M(x) = x - A(x)^{-1}F(x) \tag{8}$$

gives quadratic convergence. If matrix A is chosen to be the Jacobian matrix, where $J_{ij} = F'_{ij} = \partial F_i / \partial x_j$, this requirement is satisfied producing the iteration procedure

$$x^{(k)} = M(x^{(k-1)}) = x^{(k-1)} - F'(x^{(k-1)})^{-1}F(x^{(k-1)}) \tag{9}$$

Provided F'^{-1} exists and sufficiently accurate initial guess is given, a quadratic convergence is expected. Never done in this form! Instead, use a two step procedure: 1) solve $F'(x)\Delta x = -F(x)$, and 2) update x $x^{(k)} = x^{(k-1)} + \Delta x$.

Advantage: self correcting!

Disadvantage: Jacobian must be recomputed every time. Tricks: use old Jacobian for a few more calculations; numerically calcuate the derivatives instead of evaluating given functions etc.

Finally, stopping criterion most often used is

$$\|x^{k+1} - x^k\| < \epsilon \|x^{k+1}\| \tag{10}$$

Care needed if large damping is used. Additional measure can be $\|F(x^{k+1})\| < \delta$ but $F(x)$ must be properly scaled.