Recall the Poisson's equation (written a bit differently)

$$\lambda^2 \nabla^2 \psi = -(p - n + N_D^+ - N_A^-) \tag{1}$$

Three steps to solving this problem:

- Define the domain (or geometry) and partition it into finite number of subdomains. Reason: on smaller subdomains an approximation can be made on solution
- Approximate partial differential equation(s) (PDEs) on subdomains by algebraic equations involving only values of variables at discrete points. This results in large system of nonlinear equations.

- Solve this system of equations

This is an approximate solution of the original equation!

Several methods available for tasks 1. and 2.:

- Finite differences,
- Finite boxes, and
- Finite elements.

We start with Finite differences.

FYI, the PDEs are classified as

1. elliptic, such as

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y) \tag{2}$$

2. parabolic, such as

$$\frac{\partial u}{\partial t}(x,t) - \alpha^2 \frac{\partial^2 u}{\partial x^2}(x,t) = 0 \tag{3}$$

3. hyperbolic, such as

$$\alpha^2 \frac{\partial^2 u}{\partial x^2}(x,t) = \frac{\partial^2 u}{\partial t^2}(x,t) \tag{4}$$

Examples are Poisson's eq., heat eq., and wave eq., respectively.

After the first step is done (see graphs), we need approximations for derivatives and function values on a discrete grid. Taylor expansion is at root of most of the approximations.

In 1-D Taylor expansion of function $y(x)$ around point x_i gives

$$y(x) = y(x_i) + (x - x_i)y'(x_i) + \frac{(x - x_i)^2}{2}y''(\xi_i) \tag{5}$$

By evaluating this at $x = x_{i+1}$ and setting $h_i = x_{i+1} - x_i$, we obtain

$$y'(x_i) = \frac{y(x_{i+1}) - y(x_i)}{h_i} - \frac{h_i}{2}y''(\xi_i) \tag{6}$$

This is forward-difference approximation. By going in the opposite direction, a backward-difference approximation is obtained.

By assuming constant spacing and doing some algebra, a central-difference formula is obtained

$$y'(x_i) = \frac{y(x_{i+1} - y(x_{i-1})}{2h} - \frac{h^2}{6} y^{(3)}(\xi_1) \tag{7}$$

By expansion to fourth order and evaluating at x_{i+1}, x_{i-1} we get

$$y''(x_i) = \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} - \frac{h^2}{12} y^{(4)}(\xi_i) \tag{8}$$

We will assume two-dimensional domain (2-D). There are two approaches to Poisson's eq. (PE) discretization: one applies finite differences directly, the other utilizes Gauss' theorem.

Notation: $h_i = x_{i+1} - x_i$, $k_j = y_{j+1} - y_j$. Also, for various functions $u_{i,j} = u(x_i, y_j)$, $u_{i+1/2,j} = u(1/2(x_i + x_{i+1}), y_j)$, and $u_{i,j+1/2} = u(x_i, 1/2(y_j + y_{j+1}))$

For the first order partial derivatives, central difference approximation is used

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{1/2(h_i + h_{i-1})} + \frac{h_{i-1} - h_i}{4}\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} + \ldots \tag{9}$$

Local truncation error: residual which occurs when inserting the solution of the continuous problem into the discrete scheme.

$O(h), O(h^2)$ etc. signify terms in the truncation error that are controlled by linear, quadratic etc expressions in the local mesh spacing. h and k are the maximum spacings on the domain.

By plugging in $\partial\psi/\partial x, y$ into the central difference formula and applying that to PE we get:

$$\lambda^2 \left(\frac{\left.\frac{\partial\psi}{\partial x}\right|_{i+1/2,j} - \left.\frac{\partial\psi}{\partial x}\right|_{i-1/2,j}}{1/2(h_i + h_{i-1})} + O(h) \left.\frac{\partial^3\psi}{\partial x^3}\right|_{i,j} + \right.$$

$$\left. \frac{\left.\frac{\partial\psi}{\partial y}\right|_{i,j+1/2} - \left.\frac{\partial\psi}{\partial y}\right|_{i,j-1/2}}{1/2(k_i + k_{i-1})} + O(k) \left.\frac{\partial^3\psi}{\partial y^3}\right|_{i,j} \right) -$$

$$n_{i,j} + p_{i,j} + C_{i,j} = 0$$

Express $\partial\psi/\partial x, y$ at mid-pints with central differences, e.g.:

$$\left.\frac{\partial\psi}{\partial x}\right|_{i+1/2,j} = \frac{\psi_{i+1,j} - \psi_{i,j}}{h_i} + O(h^2)\left.\frac{\partial^3\psi}{\partial x^3}\right|_{i+1/2,j} \tag{10}$$

These approximations do not increase the order of the local truncation error. After substitution and neglecting truncation error terms the final expression for discretized Poisson's equation is:

$$\lambda^2\left(\frac{\frac{\psi_{i+1,j}-\psi_{i,j}}{h_i} - \frac{\psi_{i,j}-\psi_{i-1,j}}{h_{i-1}}}{1/2(h_i + h_{i-1})} + \frac{\frac{\psi_{i,j+1}-\psi_{i,j}}{k_j} - \frac{\psi_{i,j}-\psi_{i,j-1}}{k_{j-1}}}{1/2(k_j + k_{j-1})}\right) - n_{i,j} + p_{i,j} - C_{i,j} = 0$$

A different approach: box integration method. Based on utilizing Gauss' (Green's) theorem:

$$\int\int_{D_{ij}} \vec{\nabla} \cdot (P \nabla u) dx dy = \int_{\partial D_{i,j}} \left(P \frac{\partial u}{\partial x} dy - P \frac{\partial u}{\partial y} dx \right) \tag{11}$$

The idea is to utilize the properties of function u which may be better known on the surface $\partial D_{i,j}$ than inside the volume $D_{i,j}$. The domain is a "box" around each point and they don't overlap.

For Poisson's eq. we have

$$\int_{x_i-1/2h_{i-1}}^{x_i+1/2h_i} \int_{y_j-1/2k_{j-1}}^{y_j+1/2k_j} \lambda^2 \nabla^2 \psi dy dx -$$
$$\int_{x_i-1/2h_{i-1}}^{x_i+1/2h_i} \int_{y_j-1/2k_{j-1}}^{y_j+1/2k_j} (n - p - C) dy dx = 0$$

The first part is transformed into surface integral, while the second stays as it is.

One approximation is to use central-differences for partial derivatives and assume that those stay the same along the given line of integration, resulting in

$$\text{right hand side of Gauss' theorem} \approx$$
$$P_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_i}\,\frac{k_{j-1}+k_j}{2}+P_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{k_j}\,\frac{h_{i-1}+h_i}{2}+$$
$$P_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_{i-1}}\,\frac{k_{j-1}+k_j}{2}-P_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{k_{j-1}}\,\frac{h_{i-1}+h_i}{2}$$

For PE P-s are =1. What to do with the volume integral of the carrier and doping concentrations? No really good answer, but what works is to assume they are constant over the box and equal to the value at node i, j.

The final PE becomes

$$\lambda^2 \left(\frac{\psi_{i+1,j} - \psi_{i,j}}{h_i} \frac{k_{j-1} + k_j}{2} \frac{\psi_{i,j+1} - \psi_{i,j}}{k_j} \frac{h_{i-1} + h_i}{2} + \frac{\psi_{i-1,j} - \psi_{i,j}}{h_{i-1}} \frac{k_{j-1} + k_j}{2} + \frac{\psi_{i,j-1} - \psi_{i,j}}{k_{j-1}} \frac{h_{i-1} + h_i}{2} \right) - (n_{i,j} - p_{i,j} - C_{i,j}) \frac{k_{j-1} + k_j}{2} \frac{h_{i-1} + h_i}{2} = 0.$$

which is the same as the eq. derived in a different way.

To complete the discretization we need boundary conditions.

Types of BCs: Dirichlet, reflection, interface

Both mathematical and physical in nature.

Dirichlet: specifies value of the variable (n,p,ψ) at the boundary, Example: ohmic contacts

Ohmic contact assume infinite surface recombination velocity and charge neutrality: $np - n_i^2 = 0$ and $n - p - C = 0$ giving

$$n = \frac{\sqrt{C^2 + 4n_i^2} + C}{2} \text{ and } p = \frac{\sqrt{C^2 + 4n_i^2} - C}{2} \tag{12}$$

For PE alone, we only need potential BC and by assuming voltage drive we have: $\psi(t) - \psi_b - \psi_{appl}(t) = 0$. Many other BCs can be applied depending on the physical situation (e.g. Schottky contacts)

Interfaces, such as silicon-silicon dioxide? At those point we need Gauss' law

$$\epsilon_{semi} \frac{\partial \psi}{\partial \vec{n}}\bigg|_{semi} - \epsilon_{ins} \frac{\partial \psi}{\partial \vec{n}}\bigg|_{ins} = Q_{ins} \tag{13}$$

Further simplifications: 1. for thick oxide el. field in oxide ≈ 0 2. interface charge neglected; results in $\frac{\partial \psi}{\partial \vec{n}} = 0$

Artificial BCs: reflection (or symmetry) BC also state $\frac{\partial \psi}{\partial \vec{n}} = 0$ but the reasoning is different

How about discretization of BCs? It's pretty straightforward. For Dirichlet BCs the values are already specified so that's no problem. For BCs that involve normal derivatives (=0) mirror imaging (reflection) can be used. It is based on introducing imaginary equi-distant point across the interface giving

$$\left.\frac{\partial \psi}{\partial y}\right|_{i,j+1/2} = -\left.\frac{\partial \psi}{\partial y}\right|_{i,j-1/2} + O(k^2)\left.\frac{\partial^3 \psi}{\partial y^3}\right|_{i,j} \tag{14}$$

Alternative explanation based on box-integration method.

The first part of PE looks like

$$\lambda^2 \left(\frac{\left.\frac{\partial \psi}{\partial x}\right|_{i+1/2,j} - \left.\frac{\partial \psi}{\partial x}\right|_{i-1/2,j}}{1/2(h_i + h_{i+1})} + \frac{-2\left.\frac{\partial \psi}{\partial y}\right|_{i,j-1/2}}{k_{j-1}} \right) \ldots \qquad (15)$$

Things are a little bit more complicated if interface charge is present: the second fraction has additional $2\, Q_{int}|_{i,j}$

For Gauss' law application we need to be more careful (see additional notes).

We need models for various "constants" we left unspecified. Also, we may need to modify the semiconductor eqs. according to the physical situation.

Carrier concentrations can become dependent on background doping: bandgap narrowing effect. At very large concentrations, impurities start forming a band of their own that can merge with the conduction or valence band, or it provides additional states ("tail" states) inside the forbiden bandgap.

Quick fix: introduce "effective intrinsic concentration" n_{ie} which hides all the details of physics into simple increase of intrinsic concetration due to rigid band-edge shifts so that

$$n = n_{ie} exp\left(\frac{q(\psi - \phi_n)}{kT}\right) \tag{16}$$

The most often used model for BGN is Slotboom's, although more physically based models keeps appearing. Caution: evaluate the extraction of model parameters — does it include degeneracy or not. Also, in its most common application, it does not matter which dopand is used, which is not eniterely consistent, but it works. In other words, the bandgap change is equally divided between conduction and valance bands. This restriction can be avoided but the problem needs to be re-formulated.

Two way to approach mobility: heuristic and physics based. It can be viewed as proportionality "constant" between electric field and velocity (i.e. $v = \mu E$), or it is defined through average momentum relaxation times. The latter point of view is better suited to physical interpretation. Think of these relaxation times as average time the electrons are free to move around with thermal velocity before they are scattered.

Scattering mechanisms: thermal lattice vibrations (phonons), ionized impurities, neutral impurites, vacancies, interstitials, dislocations, surfaces and carrier-carrier scattering. The most fundamental is phonon scattering but there are several types. "Acoustic deformation potential" lattice scattering represents scattering off the acoustic waves traveling around the crystal. Two types: longitudinal and transverse. Acoustic phonons displace neighbouring atoms in the same direction; optical phonons displace them in opposite directions. The distinguishing feature: temperature dependence is $\sim T^{-3/2}$. Model:

$$\mu_n^L = \mu_n^0 \left(\frac{T}{300}\right)^{-\alpha_n} \tag{17}$$

Mathiessen's rule may be applied to sum up the individual contributions to mobility (extreme caution).

Impurity scattering: features $\sim T^{3/2}$ dependence. Complications at high doping because of "screening": Conwell and Weiskopf, Brooks-Herring, Ridley models.

How to combine phonon (L) and impurtity (i) models into one mobility? Mathiessen's rule is a poor choice. Best to resort to heuristics — Caughey-Tomas model

$$\mu_{n,p}^{LI} = \mu_{n,p}^{\min} + \frac{\mu_{n,p}^{L} - \mu_{n,p}^{I}}{1 + \left(\frac{CI}{C_{n,p}^{ref}}\right)^{\alpha_{n,p}}} \tag{18}$$

or, even simpler, Scharfetter-Gummel model

$$\mu_{n,p}^{LI} = \frac{\mu_{n,p}^{L}}{\left(1 + \frac{CI}{C_{n,p}^{ref} + \frac{CI}{S_{n,p}}}\right)^{1/2}} \tag{19}$$

Arora's model for temperature dependence of various constants in Caughey-Thomas' model.

Large scatter of experimental results!

Carrier-carrier scattering difficult to model and introduces numerical problems. Likely use: high injection cases.

Experimentally we know that velocity saturates vs. electric field. This saturation needs to be modeled. Not much in terms of theory, but this one works:

$$\mu_{n,p}^{LICNE} = \frac{\mu_{n,p}^{LICN}}{\left(1 + \left(\frac{\mu_{n,p}^{LICN} E_{n,p}}{v_{n,p}^{sat}}\right)^{\beta_{n,p}}\right)^{1/\beta_{n,p}}} \tag{20}$$

Another popular choice is Scharfetter-Gummel model.

For GaAs devices there is a "hump" in v vs. E curve. In Si, velocity monotonically reaches the saturation value, but not so in GaAs. One way to include this effect is

$$\mu_{LIE} = \frac{\mu_n^{LI} + v_n^{sat} \frac{E_n^3}{\left(E_n^{crit}\right)^4}}{1 + \left(\frac{E_n}{E_n^{crit}}\right)^4} \tag{21}$$

For MOS devices surface scattering needs to be treated.

Auger recombination: three particle interaction; either two electrons and one hole, or two holes and one electron.

Four basic processes:

a) electron capture; highly energetic electron transmits its energy to another electron in conduction band and moves to the valence band where it recombines with a hole

b) hole capture: instead of transmitting energy to an electron in conduction band as in a), the energy is transmitted to a hole in the valence band. Electron again recombines with a hole.

c) electron emission: highly energetic electron in the conduction band excites an electron in the valence band into the conduction band which leaves a hole behind in the valence band

d) hole emission: inestead of an electron from conduction band as in c), a highly energetic hole in the valence band provides energy to excite an electron from valence band into the conduction band leaving a hole behind.

Note: these are direct band-to-band transitions. The question remains how realistic this is in indirect bandgap materials such as Si and Ge.