Drift-Diffusion Model:
Time-Dependent Simulations
Sharfetter-Gummel Discretization

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Time-dependent simulations

The time-dependent form of the drift-diffusion equations can be used both for steady-state and transient calculations. Steady-state analysis is accomplished by starting from an initial guess, and letting the numerical system evolve until a stationary solution is reached, within set tolerance limits. This approach is seldom used in practice, since now robust steady-state simulators are widely available. It is nonetheless an appealing technique for beginners since a relatively small effort is necessary for simple applications and elementary discretization approaches. If an explicit scheme is selected, no matrix solutions are necessary, but it is normally the case that stability is possible only for extremely small time-steps.

The simulation of transients requires the knowledge of a physically meaningful initial condition, which can be obtained from a steady-state calculation. The same time-dependent numerical approaches used for steady-state simulation are suitable, but there must be more care for the boundary conditions, because of the presence of displacement current during transients. In a transient simulation to determine the steady-state, the displacement current can be neglected because it goes to zero when a stationary condition is reached. Therefore, it is sufficient to impose on the contacts the appropriate potential values provided by the bias network. In a true transient regime, however, the presence of displacement currents manifests itself as a potential variation at the contacts, superimposed to the bias, which depends on the external circuit in communication with the contacts. Neglect of the displacement current in a transient is equivalent to the application of bias voltages using ideal voltage generators, with zero internal impedance. In such a situation, the potential variations due to displacement current drop across a short circuit, and are therefore cancelled. In this arrangement, one will observe the shortest possible switching time attainable with the structure considered, but in practice an external load and parasitics will be present, and the switching times will be normally longer. A simulation neglecting displacement current effects may be useful to assess the ultimate speed limits of a device structure.

When a realistic situation is considered, it is necessary to include a displacement term in the current equations. It is particularly simple to deal with a 1-D situation. Consider a 1-D device with length W and a cross-sectional area A. The total current flowing in the device is

$$I_D(t) = I_n(x,t) + cA\frac{\partial E(x,t)}{\partial t} \tag{1}$$

The displacement term makes the total current constant at each position *x*. This property can be exploited to perform an integration along the device

$$I_D(t) = \frac{1}{W}\int_0^W I_n(x,t)dx + \frac{cA}{W}\frac{\partial V^*}{\partial t} \tag{2}$$

where $V^*(t)$ is the total voltage drop across the structure, with the ground reference voltage applied at $x=W$. The term $\frac{\varepsilon A}{W}$ is called cold capacitance. The 1-D device, therefore, can be studied as the parallel of a current generator and of the cold capacitance which is in parallel with the (linear) load circuit. At every time step, V^* has to be updated, since it depends on the charge stored by the capacitors.

To illustrate the procedure, consider a simple Gunn diode in parallel with an *RLC* resonant load containing the bias source. Calling C_o the parallel of cold and load capacitance, it is

$$I(t) = C_o\frac{\partial V^*(t)}{\partial t} + I_o(t) \tag{3}$$

where $I_o(t)$ is the particle current given by the first term on the right hand side of Eq. (1), calculated at the given time step with drift-diffusion (or any other suitable scheme). It is also

$$I(t) = -\frac{V^*(t)}{R} - \int\frac{V^*(t) - V_b}{L}dt \tag{4}$$

Upon time differencing this last equation, with the use of finite differences we obtain

$$V^*(t+\Delta t) = V^*(t) + \left[I(t) - I_o(t)\right]\frac{\Delta t}{C_o} \tag{5}$$

$$I(t+\Delta t) = I(t) - \frac{V^*(t+\Delta t) - V^*(t)}{R} - \left[V^*(t) - V_b)\right]\frac{\Delta t}{L} \tag{6}$$

This set of difference equations allows one to update the boundary conditions for Poisson's equation at every time step to fully include displacement current.

A robust approach for transient simulation should be based on the same numerical apparatus established for purely steady-state models. It is usually preferred to use fully implicit schemes, which require a matrix solution at each iteration, because the choice of the time-step is more likely to be limited by the physical time constants of the problem rather than by stability of the numerical scheme. In order to estimate the time-step limits, let's assume a typical electron velocity $v = 10^7 cm/s$ and a spatial mesh $\Delta x = 0.01 \mu m$. The C.F.L. condition necessary to resolve correctly a purely drift process on this mesh requires $\Delta t \le \Delta x / v = 10^{-15} s$. As calculated earlier, this value is not too far from typical values of the dielectric relaxation time in practical semiconductor structures.

When dealing with unipolar devices, as often used in many microwave applications, it is possible to formulate very simple time-dependent drift-diffusion models, which can be solved with straightforward finite difference techniques and are suitable for small student projects. If we can neglect the generation-recombination effects, the 1-D unipolar drift-diffusion model is reduced to the following system of equations

$$\frac{\delta n}{\delta t} = -\frac{d}{dx}\left[n v_d(E)\right] + \frac{d}{dx}\left[D(E)\frac{d}{dx}n\right] \tag{7}$$

$$\frac{d^2V}{dx^2} = \frac{q(n - N_D)}{\varepsilon} \tag{8}$$

where $v_d(E) = -\mu_n(E)E$ is the drift velocity. There are two physical processes involved: drift (advection) expressed by the first term on the right hand side of Eq. (7), and diffusion described by the second term. The continuity equation (7) is an admixture of competing hyperbolic and parabolic behavior whose relative importance depends on the local electric field strength. The

system (7) and (8) can be used for both transient or steady state conditions if the simulation is run $\frac{\delta n}{\delta t}=0$. A basic simple algorithm could consists of the following steps

1. Guess the carrier distribution $n(x)$.
2. Solve Poisson's equation to obtain the field distribution.
3. Compute one iteration of the discretized continuity equation with time step Δt. $v(E)$ and $D(E)$ are updated according to the local field value.
4. Check for convergence. If convergence is obtained, stop. Otherwise, go back to step (2) updating the charge distribution.

This is an uncoupled procedure, since Eqs. (7) and (8) are not solved simultaneously. Usually, explicit methods are used for computational speed. The time step must respect the limitations due to the C.F.L. condition (related to the advective component) and to the dielectric relaxation time. A simple discretization scheme could employ an explicit finite difference approach

$$n(i;k+1)=n(i;k)+\frac{\Delta t}{\Delta x}\left\{\left[v_d(i-1;k)n(i-1;k)-v_d(i;k)n(i;k)\right]+\frac{1}{\Delta x}D(i;k)\left[n(i-1;k)-2n(i;k)+n(i+1;k)\right]\right\};$$
$$v_d<0$$

$$n(i;k+1)=n(i;k)+\frac{\Delta t}{\Delta x}\left\{\left[v_d(i;k)n(i;k)-v_d(i+1;k)n(i+1;k)\right]+\frac{1}{\Delta x}D(i;k)\left[n(i-1;k)-2n(i;k)+n(i+1;k)\right]\right\};$$
$$v_d>0 \qquad (9)$$

where we have introduced upwinding for the drift term and we have assumed that the diffusion coefficient is slowly varying in space. There are of course many other possible explicit and implicit discretizations. Such simple finite difference approaches are in general a compromise which cannot provide at one time an optimal treatment of both advective and diffusive components. Because of spatially varying drift velocity, spurious diffusion and dispersion are present. This could be mitigated by using a nonuniform grid discretization, where the mesh size is locally adapted to achieve $v_d=\Delta x/\Delta t$ everywhere, which would involve interpolation to the new grid-points. The discretization for a diffusive process is better behaved with a fully implicit scheme (if the Crank-Nicholson approach is used, one needs to make sure that spurious

oscillations in the solution do not develop). On the other hand, the fully implicit algorithm for advection is not conservative. From these conflicting requirements, it emerges that it would be beneficial to split the drift and diffusion processes, and apply an optimal solution procedure to each. There are 1-D situations where this is known to be nearly exact. In well known experiments, a small concentration of excess carriers is generated in a semiconductor sample with a uniform electric field, and the motion of the centroid of the carrier envelope can be studied independently of the diffusive spread of the spatial distribution around the centroid itself. For an initial Gaussian distribution in space, a simple analytical solution shows that drift and diffusion can be treated as a sequential process, each using the total duration of the observation as simulation time. In analogy with this, the 1-D continuity equation can be solved in two steps, for instance

$$
\begin{aligned}
& n^*(j,i+1) = n(j,i) + v_d(j)\left[n(j-1,i) - n(j,i)\right]\frac{\Delta t}{\Delta x}; \\
& v_d < 0 \\
& n(j,i+1) = n^*(j,i+1) + D(j)\left[n(j-1,i+1) - 2n(j,i-1) + n(j+1,i+1)\right]\frac{\Delta t}{\Delta^2 x}
\end{aligned}
\qquad (10)
$$

where again a simple explicit upwinding scheme is used for the drift, while a fully implicit scheme is used for the diffusion.

Scharfetter-Gummel approximation

The discretization of the continuity equations in conservation form requires the determination of the currents on the mid-points of mesh lines connecting neighboring grid nodes. Since the solutions are accessible only on the grid nodes, interpolation schemes are needed to determine the currents. For consistency with Poisson's equation, it is common to assume that the potential varies linearly between two neighboring nodes. This is equivalent to assume a constant field along the mesh lines, and the field at the mid-point is obtained by centered finite differences of the potential values. In order to evaluate the current, it is also necessary to estimate the carrier density at the mid-points. The simplest approximation which comes to mind is to also assume a linear variation of the carrier density, by taking the arithmetic average between two neighboring nodes. This simple approach is only acceptable for very small potential variation between the

nodes, and indeed is exact only if the field between two nodes is zero, which implies the same exact carrier density on the two points.

In order to illustrate this, let's consider a 1-D mesh where we want to discretize the electron current

$$J_n = q\mu_n n\left(-\frac{d\psi}{dx}\right) + qD_n \frac{dn}{dx} \tag{11}$$

Here, the field is explicitly expressed by the derivative of the potential. The discretization on the mid-point of the mesh line between nodes x_i and x_{i+1} is given by

$$J_{i+\frac{1}{2}} = -q\mu_n n_{i+1/2} \frac{\psi_{i+1} - \psi_i}{\Delta x} + qD_n \frac{n_{i+1} - n_i}{\Delta x} \tag{12}$$

In the simple approach indicated above, the carrier density is expressed as

$$n_{i+1/2} \approx \frac{n_{i+1} + n_i}{2} \tag{13}$$

In Eq. (12), the assumed linearity of the potential between meshes, is implied by the use of the centered finite differences to express the field on the mid-point. We can now rewrite Eq. (12) including the approximation in Eq. (13) as

$$J_{i+\frac{1}{2}} = n_{i+1}\left[-q\frac{\mu_n}{2}\frac{\psi_{i+1} - \psi_i}{\Delta x} + q\frac{D_n}{\Delta x}\right] - n_i\left[\underbrace{q\frac{\mu_n}{2}\frac{\psi_{i+1} - \psi_i}{\Delta x}}_{a} + \underbrace{q\frac{D_n}{\Delta x}}_{b}\right] \tag{14}$$

If we assume a condition where $J_n = 0$ (equilibrium) and a >> b (negligible diffusion), it is easy to see that positivity of the carrier density is not guaranteed, since the solution oscillates as $n_{i+1} \approx -n_i$. Also, it can be shown that for stability we need to have $\psi_{i+1} - \psi_i > 2k_B T / q$, which requires very small mesh spacing to be verified.

The approach by Scharfetter and Gummel [1] has provided an optimal solution to this problem, although the mathematical properties of the proposed scheme have been fully recognized much later. We consider again a linear potential variation between neighboring mesh points, which is consistent with the use of finite differences to express the field. We express the current in the interval $[x_i; x_{i+1}]$ as a truncated expansion about the value at the mid-point

$$J_n(x) = J_n(x_{i+\frac{1}{2}}) + \left(x - x_{i+\frac{1}{2}}\right)\frac{\delta}{\delta x} J_n(x) \tag{15}$$

From Eq. (15) we obtain a first order differential equation for J_n which can be solved to provide $n(x)$ in the mesh interval, using as boundary conditions the values of carrier density n_i and n_{i+1}. We obtain

$$n(x) = [1 - g(x,\psi)]n_i + g(x,\psi)n_{i+1}; \quad x \in [x_i; x_{i+1}] \tag{16}$$

where $g(x,\psi)$ is the growth function

$$g(x,\psi) = \left[1 - \exp\left(\frac{\psi_{i+1} - \psi_i}{k_B T/q}\frac{x_i - x_i}{\Delta x}\right)\right] / \left[1 - \exp\left(\frac{\psi_{i+1} - \psi_i}{k_B T/q}\right)\right] \tag{17}$$

The result in Eq. (16) can be used to evaluate $n\left(x_{i+1/2}\right)$ for the discretization of the current in Eq. (15). It is easy to see that only when $\psi(i+1) - \psi(i) = 0$ we have

$$n_{i+1/2} = \left(1 - \frac{1}{2}\right)n_i + \frac{1}{2}n_{i+1} = \frac{n_i + n_{i+1}}{2} \tag{18}$$

The continuity equation can be easily discretized on rectangular uniform and nonuniform meshes using the above results for the currents, because the mesh lines are aligned exactly.

Extension of the Validity of the Drift-Diffusion Model

Due to the relative simplicity of the drift-diffusion equations, it would be very appealing to extend the validity of drift-diffusion-like models well into the hot electron regime. We have seen that the simplest attempt to include high-field effects is to make the mobility and the diffusion coefficient field dependent. The electron current in 1-D is

$$J(x,t) = qn(x,t)\mu(E)E + qD(E)\frac{\delta n(x,t)}{\delta x} \tag{19}$$

Here $\mu(E)E = v(E)$ is the (steady state) drift velocity for the case of homogeneous field E. The field is also space and time dependent, i.e. $E = E(x,t)$. Mobility and diffusion coefficients are steady state quantities, but the carrier velocity may differ considerably from the steady state value $v(E)$, due to abrupt space or time changes of the electric field. The steady state $v(E)$ can be considered accurate only if space or time variations of the field are very smooth (adiabatic). Velocity overshoot occurs when the average electron velocity exceeds the steady state (bulk) velocity. A modified version of the drift diffusion equation to include velocity overshoot was proposed by Thornber [2]:

$$J(x,t) = qn(x,t)\left[v(E) + W(E)\frac{\delta E}{\delta x} + B(E)\frac{\delta E}{\delta t}\right] + qD(E)\frac{\delta n(x,t)}{\delta x} + qA(E)\frac{\delta n(x,t)}{\delta t} \tag{20}$$

where three new terms have been added. The term with $W(E)$ contains the field gradient and corrects the local drift velocity for spatial velocity overshoot effects. The term with $B(E)$ contains the time derivative of the field and corrects for time-dependent velocity overshoot. The last term with $A(E)$ preserves the invariances of the total current (note that this term does not represent generation, recombination, trapping, etc., effects which may be incorporated with an additional term). The quantities $W(E)$, $B(E)$, and $A(E)$ must be tabulated from detailed transport calculations. In steady state the current equation simply becomes

$$J(x) = qn(x)\left[v(E) + W(E)\frac{\delta E}{\delta x}\right] + qD(E)\frac{\delta n}{\delta x} \tag{21}$$

and the resulting continuity equation is

$$\frac{\delta n(x)}{\delta x} = \frac{\delta}{\delta x}\left[n(x)v(E) + n(x)W(E)\frac{\delta E}{\delta x} + D(E)\frac{\delta n}{\delta x}\right] \tag{22}$$

Eq. (22) does not describe a real transient, since the time derivatives in the current equation have been neglected. Therefore Eq. (22) is valid in the steady state limit $\frac{\delta n}{\delta t} = 0$, i.e. $t \to \infty$. The equation may be used, however, to solve the pseudo-time-dependent problem until steady state is achieved. Since the Poisson equation is solved at each time step, the fields and the related variable are continuously updated in space. Alternatively, one may solve the steady-state equation obtained with $\frac{\delta n}{\delta t} = 0$, using Newton's method, for instance. Developing the space derivatives, Eq. (22) becomes [3]

$$\begin{aligned}\frac{\delta n}{\delta t} &= \frac{\delta n}{\delta x}v(E) + \frac{\delta v(E)}{\delta x}n(x) + \frac{\delta n}{\delta x}W(E)E_x + n(x)\frac{\delta}{\delta x}\left[W(E)\frac{\delta E}{\delta x}\right] + D(E)\frac{\partial^2 n}{\partial x^2} + \frac{\delta D(E)}{\delta x}\frac{\delta n}{\delta x} \\ &= \left(\frac{\delta v(E)}{\delta x} + \frac{\delta}{\delta x}\left[W(E)\frac{\delta E}{\delta x}\right]\right)n(x) + \left[v(E) + W(E)\frac{\delta E}{\delta x} + \frac{\delta D(E)}{\delta x}\right]\frac{\delta n}{\delta x} + D(E)\frac{\partial^2 n}{\partial x^2}\end{aligned} \tag{23}$$

Finally, the pseudo-time-dependent equation has form

$$\frac{\delta n}{\delta t} = a(x,t)\frac{\partial^2 n}{\partial x^2} + b(x,t)\frac{\partial n}{\partial x} + c(x,t)n \tag{24}$$

Since from Gauss law $\frac{\delta E}{\delta x} = \rho/\varepsilon$ and ρ depends on the carrier density $n(x)$, the coefficients $b(x,t)$ and $c(x,t)$ are also functions of $n(x)$ and Eq. (24) is nonlinear. Often the overshoot parameter $W(E)$ is rewritten in terms of mobility, as $W(E) = \mu(E)L(E)$, where $L(E)$ is called length coefficient. Monte Carlo calculations as well as analytical models for the length coefficient have been presented in the literature. Extension to 2-D is not trivial when confining fields (barriers) besides accelerating fields are present. An approximate approach allows the extension to 2-D by using the gradient of the quasi-Fermi levels (very flat inside barrier regions

but following the potential profile in accelerating regions) as the functional parameter for the length coefficient [4].

References

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