Currently, AdaptUSim is implemented using devsim[1], [2] and the following formalism following the conventional Scharfetter-Gummel stable differences approximation[3] with some relationships and non-idealities obtained from other publications[4]–[9].

# Continuity Equations

The electron and hole continuity equations are

Where and refer to electron and hole densities respectively, is the current density, is the fundamental charge, G is the net generation-recombination rate, is the spatially and field dependent mobility, is the quasi-Fermi level potential. Limiting to non-degenerate doping cases we use the Boltzmann relation

Such that is the electrostatic potential, is the electron affinity, is the thermal potential with the Boltzmann constant, and the absolute temperature in Kelvin. By starting with these relations after some algebraic manipulation we arrive at a finite differences relationship which is suitable for numeric simulation. We consider two adjacent nodes at position on a given mesh, location and and the current between them defined at . Namely,

Yet for small changes in potential across nodes, , care must be taken to evaluate, thus we refactor the expression as

Defining for convenience and evaluating it piecewise based on the magnitude of for numerical stability:

In this piecewise definition for expanding out , precision is maintained for 16 digits of z and obviates risks of numerical overflow. Similarly we define the current density for holes as

# Poisson’s Equation

The third equation that we must simultaneously solve is Poisson’s equation at each gridpoint node. That is

Where is the effective density of ionized donors and is the effective density of ionized acceptors, as the density of trap states with charge , and with being the dielectric constant of the material. Using the above definitions of current we introduce the displacement field and electric field as approximated by

Requiring that

With as the density of conduction band states, the density of valence band states, being the bandgap between the conduction and valence band edge, as the intrinsic carrier concentration, and as the intrinsic fermi level potential derived from the conduction and valance band potentials.

This formalism then requires we specify the net generation-recombination rate . For this term, defects may be specified with particular energy levels, densities, effective charges, and capture cross sections. In this way a host of behavior can be simulated by using known realistic defect energies.

Now introducing the thermal voltage from the effective mass .

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# Functionality

With the above formalism in place and implemented, [] lists the number of supported features and the roadmap of future feature additions planned.

Table 1. List of Adaptusim features both implemented and planned.

|  |  |  |
| --- | --- | --- |
| **Name** | **Implemented** | **Comments** |
| 3D mesh support | Yes | Devsim feature |
| Spatially dependent recombination with deep and shallow charge states | Yes | [5] |
| Spatially, thermally and doping dependent bandgap | Yes | Pseudo-bulk |
| Thermionic emission and Anderson model heterojunctions | Yes | [4] |
| Field-dependent mobility including scattering processes | Yes | Analytic expression |
| Simulated electrical cross-talk | Yes | Devsim feature |
| Optical generation rates | Yes | Beer’s law absorption |
| Classes and scripting interface | Yes |  |
| Graphical Interface | Planned | [10], [11] |
| Band-to-Band tunneling | Planned |  |
| Trap-assisted tunneling | Planned | [12], [13] |
| Barrier tunneling | Planned | [14] |
| Surface recombination | Planned |  |
| Interfacial trap states and charge | Planned | Devsim feature |
| Time-dependent signal analysis (CV, noise) | Planned | Devsim feature |