"FINITE BOXES" - A GENERALIZATION OF THE FINITE DIFFERENCE METHOD UTMOST SUITABLE FOR SEMICONDUCTOR DEVICE SIMULATION.

A.F.FRANZ[1], G.A.FRANZ[1], S.SELBERHERR[1]

C.RINGHOFER[2], P.MARKOWICH[2]

1) Institut für Allgemeine Elektrotechnik
TU Wien, Gußhausstraße 27, A-1040 Vienna, AUSTRIA
2) Institut für Angewandte Mathematik
TU Wien, Gußhausstraße 27, A-1040 Vienna, AUSTRIA

Two dimensional numerical simulation of complex semiconductor structures requires an approach that improves the classical methods. Regions where a broad grid spacing is sufficient may alternate with domains where a fine mesh is necessary. In our approach the discretization of the carrier transport equations is performed by replacing the partial derivatives with finite differences. To be able to treat non rectangular geometries, we developed the concept of "finite boxes", which is a generalisation of the "terminating lines" approach introduced by Adler /1/. The grid is generated automatically according to the specified device geometry and adapted during the solution process to equidistribute the local discretisation error. /2/. The representation of the mesh by a directed graph permits efficient utilisation of computer resources. A modified Newton method is used for solving the discretized nonlinear system. The coefficients of the Jacobian are calculated analytically for Poisson's equation and numerically for the continuity equations using the algorithm published by Curtis & Reid. /3/. This allows for correct calculation of the derivatives of the physical parameters (mobility and generation - recombination). The commonly known overshooting of Newton's method is prohibited by a modification of the Jacobian as suggested by /4/. This allows the use of a very efficient iterative algorithm as long as the error is relatively large. After some accepted iterations we switch to a more accurate sparse Gauß solver. Since the calculation of the Jacobian is rather time consuming, a rank one update as well as a bypass of some equations of the system increase the speed of calculation without loosing accuracy or convergence. An efficient ordering algorithm of the equations ("minimum degree" /5/ modified for directed graphs) minimizes fill in during Gaußian elimination. Our current investigations concentrate on power devices (thyristor) and GaAs MESFET.

/1/ Adler M.S., **"A Method for Achieving and Choosing Variable Density Grids in Finite Difference Formulations and the Importance of Degeneracy and Band Gap Narrowing in Device Modelling"**, Proc. NASECODE I Conf., pp.3-30, 1979

/2/ Ringhofer C., **"A Singular Perturbation Approach for the Analysis of the Fundamental Semiconductor Equations"**, submitted to Conf. on Numerical Simulation of VLSI Devices, Boston 1982

/3/ Curtis A.R., Reid J.K., **"The Choice of Step Lengths When Using Differences to Approximate Jacobian Matrices"**, J. Inst. Maths. Applics., Vol. 13, pp.121-126, 1974

/4/ Bank R.E., Rose D.J., **"Parameter Selection for Newton-Like Methods Applicable to Nonlinear Partial Differential Equations"**, SIAM J.Numer.Anal., Vol.17, pp.806-822, 1980

/5/ George A., Liu J.W.H., **"A Minimal Storage Implementation of the Minimum Degree Algorithm"**, SIAM J.Numer.Anal., Vol.17, pp.282-299, 1980