Chapter 1

Introduction

The construction of semiconductor devices is a complex process. While the mass production of semiconductors is inexpensive, the creation of a few prototypes can be prohibitively costly and time consuming. By using a mathematical model of the devices developers can investigate the properties of hypothetical devices before actually constructing one. The use of simulations reduces the number of prototypes constructed, with a corresponding reduction of costs and time commitments. This thesis examines the application of the multigrid method to the numerical simulation of semiconductor devices.

The equations which govern the behaviour of semiconductors were first developed by van Roosbroeck in the early 1950’s [38]. The basic semiconductor device equations are a system of nonlinear partial differential equations which describe the electrostatic potential, current flow, and carrier concentrations. These equations are singularly perturbed, and are subject to both Dirichlet and Neumann boundary conditions. Internal boundary layers, where the solution varies rapidly, arise in the interior of the domain.

Early studies of the equations employed simplifying, and sometimes drastic, assumptions to make the model more accessible to analytic techniques [34]. More recently, asymptotic analysis has been used to provide qualitative information about the solution structure [26]. These analytic approaches often involve assumptions which limit their applicability in technologically interesting cases.
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The need for solutions to realistic problems has led to the use of numerical simulations based directly on the fundamental equations. The first numerical model of a one dimensional bipolar transistor was developed by Gummel in 1964 [17], and a modified approach was later applied to a \textit{pn}-junction by De Mari [12]. Slotboom [35] first used a full two dimensional model of a bipolar transistor in 1969, and two dimensional simulations of the static equations are now almost standard in the development of prototypes [31]. Three dimensional simulations have been performed in recent years [11], but their usefulness is often limited due to the intensive computations required. Solutions of the time dependent problem have been reported by Mock [26] and Yamaguchi [39]. Several surveys of numerical simulations have been published, including [31], [30] and [6].

The numerical solution of the semiconductor equations is an interesting and challenging problem. A nonstandard discretization of the equations must be used, and the equations are poorly scaled. The sharp internal layers (internal boundary layers) require that a highly nonuniform mesh be used to provide a uniformly accurate resolution of the solution efficiently. The iterative procedure which is needed to deal with the nonlinearities must be both robust and efficient, since simulations are usually performed for a wide range of operating conditions.

The multigrid method [9] is an efficient numerical algorithm for solving the algebraic equations which arise from the discretization of differential equations. Relaxation sweeps are combined with coarse grid correction steps to produce a scheme which is, theoretically, optimally efficient. The method has been successfully used for many problems, but it is not always obvious how it should be implemented to attain the maximum efficiency for a new problem. Previous attempts to apply the multigrid method to the semiconductor equations ([7], [15] and [19]) have met with limited success, and do not always appear to be as efficient as possible. This thesis evaluates several modifications
to the basic multigrid algorithm, and demonstrates that the multigrid method can be successfully used for semiconductor device modelling in one space dimension.

An overview of semiconductor device modelling is presented in Chapter 2. §2.1 contains a simple introduction to semiconductor devices, and a derivation of the governing equations is presented in §2.2. Some analytic aspects of the problem, including the boundary conditions, an appropriate scaling, and a reformulation of the problem in terms of new dependent variables, are discussed in §2.3. The form of the physical parameters occurring in the equations is detailed in §2.4. §2.5 outlines certain aspects of the numerical solution of the problem, presenting a stable discretization of the equations and describing the two methods which are commonly used to solve the nonlinear equations.

Chapter 3 contains a brief introduction to the multigrid method. §3.1 discusses the multigrid idea and presents the fundamental algorithms. The components of the algorithm are discussed in more detail in §3.2, while the extension of the basic method to systems of nonlinear equations is outlined in §3.3. §3.4 discusses the application of the multigrid method to the semiconductor equations. The problems which are expected to arise are outlined, and the behaviour of a straightforward implementation is described.

Improvements to the basic algorithm are described in Chapter 4. Symmetric relaxation iterations, prolongations based on the discretized equations, and local relaxation sweeps all significantly improve the convergence of the method. These modifications, and their effects, are described in §4.1. The most successful variants are collected into one program (SC-1). §4.3 demonstrates that SC-1 is successful for a variety of problems, including the modelling of a thyristor. §4.4 compares SC-1 to an adaptation of a multigrid implementation described by Hemker [19]. For the problems considered, our program is more efficient and more robust than Hemker's version.
Chapter 5 summarizes the findings of this thesis, and contains some suggestions for future work in this area.