The grant helped to support the IMA summer program Semiconductors, held July 15 -- August 9, 1991. This was an intensive, interdisciplinary program which involved many of the leaders in the field. The proceedings will be published in the series IMA Volumes in Mathematics and its Applications (Springer-Verlag).
VIII. SCIENTIFIC DESCRIPTION OF SUMMER SEMICONDUCTORS PROGRAM.

Coordinators: Farouk Odeh (Chairman), IBM, Yorktown Heights, New York
Julian Cole, Rensselaer Polytechnic Institute, Troy, New York
William M. Coughran, Jr., AT&T Bell Labs, Murray Hill, New Jersey
Peter Lloyd, AT&T Bell Labs, Allentown, Pennsylvania
Jacob White, Massachusetts Institute of Technology, Cambridge

General Description

Semiconductors have become the foundation of high technology. This is evidenced by the fact that every piece of sophisticated electronic equipment currently contains integrated circuits with thousands to nearly 1.5 million transistors. The improved production of such equipment is thus tied up with the efficient and reliable manufacture of very small semiconductor devices and with accelerating the design of mega-transistor circuits. These latter issues are increasingly tied up with improved modeling and better understanding of various models by means of mathematical and computational analysis. This is because the cost of experiments is very high and because many of the phenomena of interest are not susceptible to direct measurements. The subject offers a uniquely rich source of mathematical problems such as free boundary problems arising from modeling surface oxide growth during processing, uniqueness and bifurcation questions for systems of nonlinear elliptic equations in the case of the drift-diffusion model of a single device, existence of solutions for the Boltzmann equation in more realistic device models, analysis and numerical methods for large systems of differential-algebraic systems arising in circuitry, and so on. New challenges in modeling, computations and analysis have recently surfaced due to the rapidly decreasing dimensions of devices.

The goal of this program was to foster interaction in this interdisciplinary field which involves electrical engineers, computer scientists, semiconductor physicists and mathematicians, from both university and industry. The program particularly encouraged the participation of numerical and mathematical analysts with backgrounds in ordinary and partial differential equations and helped get them involved in the mathematical aspects of semiconductor models and circuits. Leading engineers in semiconductors were invited to present the significant industrial issues as well as to concentrate on those models which were most relevant to mathematicians. The main topics of the program were:

1. Processing modeling (1 week) July 15-19, 1991
2. Device modeling (1 1/2 weeks) July 22-31, 1991
3. Quantum effects (1 week) July 31-August 2, 1991
4. Circuit analysis (1 week) Aug. 5-9, 1991

The proceedings will be published as two volumes in the series IMA Volumes in Mathematics and its Applications (Springer-Verlag).

**Week 1 - Processing Modeling, July 15-19, 1991**

Process simulation is concerned with the solution of physical equations which model impurity distribution, oxide growth and other standard wafer-processing steps (i.e., those necessary to fabricate complete device structures) such as thermal annealing, oxidation and etching. The multitude of processing steps involves a corresponding array of mathematical problems. For example, stiff nonlinear system of parabolic reaction-diffusion equations are used to model point defect assisted diffusion; oxidation leads to singular perturbation problems and to the study of nonlinear viscoelastic time-dependent equations and hyperbolic problems, replete with shocks, appear in the study of reactive ion etchings. Moreover, in addition to the traditional numerical analysis questions associated with the above, delicate computational geometry questions arise in the attempt to create appropriate moving grids for obtaining the impurity distributions within domains with free boundaries.

**Week 2 - Device Modeling (1\frac{1}{2} weeks), July 22-31, 1991**

Device modeling, primarily concerned with electrical characterization of a single device, is described by coupling electromagnetics - Maxwell equations or some of their approximations - to charge carrier transport equations. In current and near future technologies, carriers may be regarded as pseudo particles and a generalized Boltzmann equation, with a momentum-dependent mass and a complicated collision term incorporating a fair amount of physics, govern the transport of carriers. Numerical methods which are based on the Monte Carlo approach or some of its versions, are appropriate for understanding the basic transport phenomena. Simpler models, involving the first few moments of the Boltzmann equation, provide the tool for the modeling of actual devices, with all of their complicated geometries and impurity concentration profiles. The traditional model, referred to as the drift-diffusion model, comprises, in the stationary case, a system of three nonlinear equations of elliptic type, and has received most of the attention so far in the mathematical literature. Although existence theorems and numerical and asymptotic methods for this model have been an active research area, some basic questions such as uniqueness and the shape of the I-V curve remain unsolved (from the viewpoint of rigorous mathematics). Also, numerical approaches to three dimensional devices have not yet been satisfactorily developed. More sophisticated models, which fit in between drift-diffusion and Boltzmann, are necessary for the near future submicron devices. For example, one such (hydrodynamic) model in 2D comprises five nonlinear equations of a mixed hyperbolic-elliptic type even
in the stationary case. Most of the mathematical as well as the computational aspects of such models are quite open.

Week 3 - Quantum Effects (½ week), July 31 – Aug. 2, 1991

As the dimensions of modern devices decrease to ultrasmall levels, quantum effects begin to play a major role. Examples are the quantization of states in confined regions - thin channels, quantum-wires etc. - and tunneling phenomena in resonant diodes. This involves a coupling of electromagnetics directly to quantum mechanics, i.e. to eigenfunctions of the Schroedinger equation. New transport models, such as the Wigner psuedo-differential equation and/or what may be loosely called quantum-Boltzmann have to be applied for an adequate description of "quantum devices". Path integrals, psuedo-differential operators and numerical techniques for eigenvalues and eigenfunctions are expected to provide the mathematical tools for this area.

Week 4 - Circuit Analysis, August 5–9, 1991

The high cost of integrated circuit fabrication, both in time and materials, forces designers to simulate their complete designs in as much detail as possible. Typically, the approach of choice is to construct a differential algebraic (DAE) system that describes the circuit, and solve that system numerically for a given set of inputs. More specifically, the circuit is assumed to be an interconnection of lumped elements (e.g. resistors, capacitor, inductors and transistors), characterized by a relation between the terminal voltages and terminal currents. The equation system that describes such a network is then constructed using the Kirchoff voltage and current laws, and this leads to an index 1 system of differential-algebraic equations where the state variables are not always readily identified. In general, the system of equations generated from most circuits is very stiff, even if the algebraic equations are not present. Also, the system is quite nonlinear, and this makes finding an initial solution which satisfies the initial conditions and the algebraic constraints rather difficult.

The circuit simulation problem can be broken into two classes: solving large initial value problems, with as many as 10,000 unknowns, efficiently; and computing periodic or quasi-periodic solutions for smaller problems, with 10 to 100 unknowns. For solving the large initial value differential-algebraic systems, the topics of interest are techniques for stiff systems; techniques for solving large nonlinear systems where the Jacobian can be much more than one rank deficient; multirate integration methods; and iterative techniques for very nonsymmetric problems. For computing periodic or quasi-periodic solutions to these DAE systems, topics of current interest are existence and uniqueness of solutions, high order methods for very stiff problems, spectral methods, mixed time-frequency methods and other types of collocation methods.
INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS
FINAL REPORT TO AFOSR

(1) CONTRACT OR GRANT NUMBER: AFOSR-89-0165
(2) PERIOD COVERED BY REPORT: November 15, 1989 - November 15, 1991
(3) TITLE OF PROPOSAL: NONLINEAR WAVES, DYNAMICAL SYSTEMS AND OTHER APPLIED MATH PROGRAMS
(4) NAME OF INSTITUTION: University of Minnesota, Minneapolis
(5) AUTHOR OF REPORT: Willard Miller, Jr.
(6) LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER AFOSR SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

STEVEN ALTSCHULER


DAVID DOBSON


MICHAEL JOLLY

[1] WITH H.S. BROWN AND I.G. KEVREKIDIS, A minimal model for spatio-temporal patterns in thin film flow, IMA Preprint Series # 790 and A minimal model for

P. Smereka


(7) Scientific Personnel supported by this project and degrees awarded during this reporting period:

1990–1991 Postdocs:
Steven Altschuler
David Dobson
Peter Smereka

1989–1990 Postdocs:
M. Jolly
S. Laederich
SCHEDULE FOR JULY 15 - AUGUST 9

Week 1 - Processing Modeling, July 15-19, 1991
(Julian Cole will be in residence and in charge of week 1)

Process simulation is concerned with the solution of physical equations which model impurity distribution, oxide growth and other standard wafer-processing steps (i.e., those necessary to fabricate complete device structures) such as thermal annealing, oxidation and etching. The multitude of processing steps involves a corresponding array of mathematical problems. For example, stiff nonlinear system of parabolic reaction-diffusion equations are used to model point defect assisted diffusion; oxidation leads to singular perturbation problems and to the study of nonlinear viscoelastic time-dependent equations and hyperbolic problems, replete with shocks, appear in the study of reactive ion etchings. Moreover, in addition to the traditional numerical analysis questions associated with the above, delicate computational geometry questions arise in the attempt to create appropriate moving grids for obtaining the impurity distributions within domains with free boundaries.
Monday, July 15

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:00 am  Registration and coffee  Reception Room EE/CS 3-176

9:30 am  Welcome and Orientation  Conference Hall EE/CS 3-180

9:40 am  Leonard Borucki  
          Motorola Corporation  Modeling the growth and annealing of dislocation loops

Abstract: Accounting for the nucleation, growth and annealing kinetics of dislocation loops is becoming increasingly important for understanding the diffusion behavior of the dopants that are commonly used in the silicon semiconductor industry. It has been hypothesized, for example, that the absorption and emission of silicon interstitials by end of range dislocation loops has a significant transient effect on the diffusion of ion-implanted boron during rapid thermal processing and during low temperature processing. A better understanding of this transient diffusion effect is desirable because it would in turn permit better prediction and control of processes used to create some of the boron-doped structures that are used in current technologies. Although a detailed simulation of the relevant phenomena is not currently practical, something can be learned from an analysis of simpler cases. This paper examines some of the solutions and approximations that are in the literature for the pressure field around a pure prismatic dislocation loop. A boundary value problem is formulated for the growth or shrinkage of a loop due to the interaction of interstitials and vacancies with the pressure field. An issue of primary concern is the boundary condition at the core of the loop. Numerical solutions of the boundary value problem are presented that explore the characteristics of the model and their relationship to the observed diffusion phenomena.

10:40 am  Coffee Break  Reception Room EE/CS 3-176

11:00 am  P. Lloyd  
          AT&T Bell Labs  IC technology CAD overview

Abstract: This paper will provide an overview of IC Technology CAD in terms of process modeling, device modeling and circuit analysis. These are the major topics of the 1991 IMA Summer Program on Semiconductors. The talk will discuss the integration of the various simulation tools and discuss industrial applications in process development and product design.

2:00 pm  Martin Giles  
          University of Michigan  Point defect diffusion modeling and transient diffusion effects

Abstract: Dopant diffusion in silicon has been studied for several decades, but is still the subject of active research and unexpected experimental results continue to be obtained. Current models consider dopant diffusion to occur through interaction with point defects - silicon vacancies and self-interstitials. A background concentration of point defects exists in silicon at thermal equilibrium, and they can also be generated by processes such as oxidation and ion implantation, and can be removed at the surface or at dislocation or precipitation sites within the wafer. Point defects also exist in various charge states controlled by the local fermi level. Macroscopic diffusivity is the net result of dopant-defect pair formation and diffusion for each charge state. Part of the difficulty in modeling this system is the wide range of timescales involved, from electronic equilibrium in nanoseconds through dopant-defect pair formation and defect diffusion in milliseconds and seconds to macroscopic dopant diffusion in minutes and hours.

For ion implanted dopant, the process of ion implantation generates point defects with concentration several orders of magnitude above the background level. During subsequent annealing, these may recombine, rapidly diffuse away, or may coalesce to form extended defects. While excess defects remain, dopant diffusion will be greatly enhanced. Experimentally, diffusion is seen to be enhanced by factors of more than 1000 for times on the order of 20 minutes at 800 C and 5 seconds at 1000 C. For higher implantation doses, extended defects are formed in a narrow band in the tail of the implantation distribution. Since these are strong sinks for interstitials, defect concentrations and dopant diffusivity have a strong variation in space as well as time.
During this talk we will review the development of the models currently used for diffusion and ion implantation, and the experimental results which provide the physical justification for the models. Examples will illustrate the capabilities offered and difficulties encountered which might be overcome with improved mathematical methods.

4:00 pm Vincent Hall 502 IMA Tea (and more!)
(The IMA Lounge)

Tuesday, July 16

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am J.R. King University of Nottingham
Asymptotic analysis for models for impurity-defect pair diffusion

Abstract: The coupled diffusion of impurities and point defects in silicon may be modelled by systems of reaction-diffusion equations. These systems usually contain several widely different time and space scales, and asymptotic methods provide a systematic means of reducing their complexity. We discuss some of these physically significant asymptotic limits, identifying the appropriate parameter ranges in each case. Problems in both one and higher dimensions are considered. Some of the mathematically unusual features of the resulting simplified problems are highlighted.

10:30 am Coffee Break Reception Room EE/CS 3-176

11:00 am Ken Suto Tohoku University
Atomic diffusion in GaAs with controlled deviation from stoichiometry

Abstract: Although several models for atomic diffusion in GaAs have been presented, they have not given strong attention on the effect of the arsenic vapor pressure, i.e., the deviation from stoichiometry, or some of them are thought to be unrealistic.

On the other hand, we have shown that the crystal growth from solution or melt under applied vapor pressure i.e., temperature difference method under controlled vapor pressure, can be explained by the equality of the arsenic chemical potentials, and the dominating point defects are arsenic interstitial atoms and arsenic vacancies, but not gallium vacancies and gallium interstitials.

On the basis of this theory, we will present the models for atomic diffusion of impurities and point defects, particularly with attention on the interstitial atoms. They can well explain the arsenic vapor pressure dependence, and the comparison with known experiments gives reasonable values for formation energies and migration energies.

Joint work with Jun-ichi Nishisawa.

2:00 pm Walter Richardson University of Texas at San Antonio
Reaction-diffusion systems arising from phosphorous diffusion

Abstract: A five-species reaction-diffusion system is derived to model the nonequilibrium diffusion of phosphorous in silicon during a high-concentration predisposition. Mathematically interesting because it is partly dissipative, i.e., substitutional phosphorous is considered immobile, the system is challenging numerically because it is stiff and ultimately needs to be solved in 3 dimensions. The numerical method for this has been used to implement the model in 3-D using LSODP and various matrix-free iterative methods from the NSPCG package. Results indicate that a large Krylov subspace dimension is required on difficult problems and that for realistic goals preconditioning is more important than the choice of an iterative method.

Wednesday, July 17

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am Michael J. Johnson IBM, Lexington
An interface method for semiconductor process simulation
Abstract: The diffusion of multiple species of dopants in silicon at high temperatures is modeled by a nonlinear parabolic system of PDEs on a two-dimensional region with a moving boundary. A numerical solution using the L-stable TRBDF2 time integration method and a "box method" spatial discretization is described. Details are given of the methods used to specify curves, to manipulate curves, and to define arbitrary simply-connected regions by their boundary curves. Numerical experiments comparing alternative choices of matrix representation, timestep size selection, and operator linearization are described and analyzed.

10:30 am Coffee Break Reception Room EE/CS 3-176

11:00 am P. Dean Gerber IBM The extended proximity effect equation in electron beam lithography

Abstract: In electron beam lithography the applied electrons scatter away from their targeted points to nearby (proximate) points. This is known as the proximity effect, and correction of this effect is necessary for practical lithographic applications. The scattering is commonly modeled by a multiple diffusion equation, so the correction problem is formulated as an inverse diffusion problem. The computational complexity of this problem is a function of the number of shapes in the lithographic pattern, which can run in the hundreds of millions. We discuss this problem, which is both ill-posed and ill-conditioned, and obtain a practical solution by means of a "geometric regularization" technique.

2:00 pm B. Lojek Motorola Corporation Rapid thermal annealing: Diffusion and stress

Abstract: Rapid thermal annealing (RTA) of implanted layers is a new technology which has been widely studied to replace conventional thermal processing. However, experimental results reveal that the physical phenomena accompanying RTA lead to many anomalies in diffusion behavior which in the literature are usually called transient diffusion. Previously, various models mostly based on the time dependent diffusivity or epitaxial realignment of damaged layers had been proposed to explain these phenomena without either solid theoretical support or unique experimental evidence. There is no theory which can interpret electrical and chemical profile redistribution during RTA.

It has been found that the prediction of the lattice position and the electronic configuration of the implanted atoms is one of the most formidable problems in diffusion modeling. Based on evaluation of available data a new approach is presented. The impurity atom is forced by the local topological constraint of the silicon lattice into three electronic configurations: for group III impurities - acceptor configuration with tetrahedral bonding configuration $sp^3$; natural configuration with planar $sp^2$ configuration and finally the nonbonding (interstitial) configuration $s^2$. Similar configurations can be found for the group IV of impurities: donor, natural and precipitates configurations. In any case the natural electronic configuration is possible only if a vacancy defect is in the vicinity of the impurity. More important however is that the impurity is in this configuration electrically inactive. For example in this context only the VAs complex is energetically favorable and can lead to electrical deactivation. Another unwanted side effect of RTA processing is the potential to generate plastic deformation in the wafer. During plastic deformation a large number of dislocations is introduced into certain crystallographic planes. These dislocations have impact not only on impurity diffusion but also if the thermal stress is large enough, permanent crystallographic slip occurs.

The main purpose of this paper is twofold: first to review the RTA processing and provide evidence that the defect-impurity, in particular vacancy-impurity interaction is the governing process which determines the electrical activity of implant and subsequent relaxation from metastable state into equilibrium. Secondly, we will discuss the origin of thermoelastic stress originated by RTA which can give rise to the slip.

Thursday, July 18

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am Mark Law IBM Automatic grid generation for diffusion models University of Florida
Abstract: A description of the diffusion equations for advanced point-defect based models of dopant diffusion in silicon will be presented. These models require the solution of stiff, non-linear partial differential equations in multiple dimensions. The equations require accurate solutions over time ranges from milliseconds to hours, and space ranges from 100 angstroms to 500 microns. In addition, these problems are typically solved over domains which are changing in time. Consequently, space and time discretisation is critical for controlling both errors and limiting computer time.

Of current interest is manufacturing simulation, for which not only the nominal case but the variances are solved for. For this situation, control of the spatial and temporal discretisation is essential so that the numerical error can be controlled to be less than the process variances of interest. Techniques for solving these problems will be discussed.

10:30 am Coffee Break
11:00 am Andrzaj Strojwas
Carnegie Mellon University
New numerical techniques for efficient simulation of diffusion and lithography
2:00 pm S. Hamaguchi
IBM, Yorktown Heights
The Boltzmann-Poisson system in weakly collisional sheaths

Abstract: The energy distribution of an ion flux bombarding a cathode surface is important information in plasma-processing tools for etching and plasma-enhanced chemical vapor deposition (PECVD). In particular, theoretical understanding of such ion dynamics in recent high-density, low-pressure tools, in which plasma sheaths are almost collisionless, is of significant interest. In this paper, we discuss ion kinetics in weakly collisional sheaths described by boundary-value problems of the Boltzmann-Poisson system.

First, we discuss direct-current (DC) sheaths or steady-state solutions of the system. Assuming that elastic hard-sphere collision is the dominant collision mechanism and that the ion mean-free path is much larger than the sheath thickness, we obtain the ion distribution function at the cathode to the lowest order of the collisionality parameter (i.e. the ratio of the sheath thickness to the ion mean free path). Subsequently, angular and energy distributions of the ion flux are calculated based on the distribution function, which provide important information on etching/PECVD microscopic profiles.

Second, we discuss radio-frequency (RF) sheaths, where a boundary value of the system (the cathode potential) is a periodic function in time. Since the RF frequency $\omega$ is comparable to the ion plasma frequency $\omega_{pi}$ in most RF processing tools, the oscillating electric field exerts a nonlinear force (called ponderomotive force or Miller force) and push traveling ions inward (toward the bulk plasma) in an RF sheath. Using a multi-time expansion method, we calculate ponderomotive force in the limit of a high RF frequency $(\omega_{pi}/\omega)^2 << 1)$ and estimate decrease of the ion bombardment energy in an RF sheath from that in the corresponding DC sheath.

The theoretical predictions described above are also compared with Monte-Carlo simulations.

5:30 pm 502 & 570 Vincent Hall Semiconductors Pizza Party

Pizza, salad and desert.

Friday, July 9

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am Contributed Talks

Contact the organizers if you wish to give a contributed talk during this period.

9:30 am Sadasivan Shankar
University of Minnesota
Numerical solution of Boltzmann equation for electrons in glow discharges or non-equilibrium plasmas
Abstract: With the advent of very large scale integrated circuits, need for precise control of various micro-electronic devices have become important. The study of plasma is an analysis of the dynamics of a wide variety of particles like electrons, positive ions, photons, metastables, free radicals, and so on. The talk will be divided into four major sections: (i) Background of plasma processes (ii) Current work which includes particle approach to studying plasmas. (iii) Contributions and conclusions of the above study, and (iv) Future applications to realistic plasma processes. We have observed that in nonequilibrium plasmas or glow discharges, due to low degrees of ionization and large spatial variations in electric fields, determination of electron behavior is dependent on electron velocity distribution function (EVDF) and a particle approach is essential. We developed an approach to numerically evaluate the EVDF by solving the Boltzmann equation of electrons in a plasma. We have also used features like multitasking, vectorization, and optimization on supercomputers like Cray-XMP and Cray-2. From our detailed study of electron kinetics, we have been able to calculate transport properties like mean energy, radial and longitudinal fluxes, and densities. Drift velocities were also computed from these functions. The output of the algorithm also included macroscopic transport variables like diffusion coefficients and mobilities. These properties also serve to validate various models which need the energy dependence of transport variables. Evaluation of reaction rate constants like excitation and ionization rate constants are necessary to understand the role of various active species in plasma reactors. The algorithm supplies these as functions of electron energy and applied electrical fields. This study is important, since it is useful in studying the chemistry plasma processes and the link between plasma physics and plasma processing.

Joint work with Klavs F. Jensen.

10:30 am Coffee Break

Reception Room EE/CS 3-176

Industrial Postdocs Seminar

1 - 3:30 pm Eleventh Meeting

The format of the seminar is:
1) Presentation of projects and problems from industry (3M and Honeywell) on which the industrial postdocs are working.
2) Informal suggestions and discussion among the participants.

The seminar is directed by Avner Friedman and Walter Littman. The topic today is "Diffractive Optics". Those wishing to participate should contact A. Friedman.

The SEMINAR meets in Vincent Hall 570

Week 2 - Device Modeling (1 1/2 weeks), July 22-31, 1991

(Farouk Odeh and Bill Coughran will be in residence and in charge of weeks 2 and 3)

Device modeling, primarily concerned with electrical characterization of a single device, is described by coupling electromagnetics - Maxwell equations or some of their approximations - to charge carrier transport equations. In current and near future technologies, carriers may be regarded as pseudo particles and a generalized Boltzmann equation, with a momentum-dependent mass and a complicated collision term incorporating a fair amount of physics, govern the transport of carriers. Numerical methods which are based on the Monte Carlo approach or some of its versions, are appropriate for understanding the basic transport phenomena. Simpler models, involving the first few moments of the Boltzmann equation, provide the tool for the modeling of actual devices, with all of their complicated geometries and impurity concentration profiles. The traditional model, referred to as the drift-diffusion model, comprises, in the stationary case, a system of three nonlinear equations of elliptic type, and has received most of the attention so far in the mathematical literature. Although existence theorems and numerical and asymptotic methods for this model have been an active research area, some basic questions such as uniqueness and the shape of the I-V curve remain unsolved (from the viewpoint of rigorous mathematics). Also, numerical approaches to three dimensional devices have not yet been satisfactorily developed. More sophisticated models, which fit in between drift-diffusion and Boltzmann, are necessary for the near future submicron devices. For example, one such (hydrodynamic)
model in 2D comprises five nonlinear equations of a mixed hyperbolic-elliptic type even in the stationary case. Most of the mathematical as well as the computational aspects of such models are quite open.

Monday, July 22

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am  Giorgio Baccarani  Università di Bologna  A critical review of the fundamental semiconductor equations

Abstract: Physical models for numerical device simulation are reviewed in an engineering perspective, and their derivation from more general physical principles is examined. More specifically, the limitations of the basic semiconductor equations within both the drift-diffusion and the hydrodynamic models are discussed and their validity range is assessed with emphasis on silicon devices. Special attention is devoted to the issue of hot-carrier effects and related simulation problems. Techniques alternative to the Monte Carlo approach for the solution of the Boltzmann Transport Equation (BTE) are shortly addressed. Open problems both in the area of physical models and numerical techniques are identified, showing the need of further work to improve our ability of reliably predicting device performance in an engineering environment.

Joint work with Antonio Gnudi and Davide Ventura.

10:30 am  Coffee Break  Reception Room EE/CS 3-176

2:00 pm  Peter A. Blakey  Motorola Corporation  An applications-oriented view of semiconductor device simulation

Abstract: This presentation will focus on the issues faced by the developers and users of device simulation codes. An understanding of these issues can help specialised mathematically-oriented researchers to maximize the utility of their efforts. The general goals of the talk are: to supply a context for tasks that deal with specialized topics; to provide background information that can help in selection and prioritisation of research; and to give nonengineers an interesting glimpse into the world of applications.

Code developers bridge specialised research and applications. The tasks involved in implementing a device simulator will therefore be reviewed first. The tasks include: selecting physical models; selecting numerical techniques; selecting a software engineering strategy; defining capabilities for data collection, analysis and visualization; and coding. Trade-offs between factors such as generality, efficiency, stability, robustness, and ease of implementation are required. The choices in each area will be surveyed. A by-product of this exercise is a framework for classifying device simulators.

The second part of the presentation will focus on user issues. The generic modes of use include: obtaining physical insight; predicting trends; design; optimization; developing models for use by circuit simulators; and obtaining parameters required by circuit models. A discussion of why many device engineers are reluctant to use simulators leads to the identification of high priority research areas. Additional discussion will center on the cost-benefit concerns of management, market size constraints, and manpower limitations.

The last part of the talk will describe specific examples of the successful use of device simulation in the development of microelectronic products. These examples will include microwave diodes, power transistors, and bipolar and MOS technology development.

3:00 pm  Christian Schmeiser  TU-Wien-Austria  The derivation of analytic device models by asymptotic methods

Abstract: In circuit simulation, device models should be as simple as possible. On the other hand, physically sound models for the electrical behaviour of semiconductor devices involve nonlinear systems of partial differential equations posed on domains with complicated geometries. Therefore simplifications have to be introduced corresponding to certain idealizing assumptions. By the use of asymptotic methods the simplification procedure can be carried out in a mathematically justifiable way.

This talk gives an overview of recent results on steady-state voltage-current characteristics of multidimensional devices as well as a new approach to the modelling of the transient behaviour via integral equations.
Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180.

9:30 am  B. Meinershagen  On the consistent modeling of impact ionization and hot electron oxide emission in NMOS devices
           University of Aachen

Abstract: In the first part of this talk experimental results on hot electron oxide emission (gate current) and impact ionization (substrate current) are reviewed and different methods of modeling these effects are studied. This leads to the conclusion that neither the drift diffusion (DD) model nor local hot electron models (based on local electric field and/or electron temperature) can be used for a consistent modeling of both effects. Moreover it is shown that such a consistent modeling can be achieved by a combination of a hydrodynamic (HD) model and a nonlocal field line based lucky electron (LE) model.

In the second part of the talk an advanced Monte Carlo (MC) Model is used as a physical reference to confirm the conclusions drawn at first from experimental results. Finally a generalised HD model that is consistent to the MC model is introduced and it is demonstrated that the internal distributions of electrostatic potential, electron density, electron temperature and impact ionization rate resulting from the combination of the generalised HD model and the nonlocal LE model are in good agreement with the corresponding results from the MC model.

10:30 am  Coffee Break

11:00 am  Josef Bürgler  Combined device-circuit simulation of advanced semiconductor structures
           ETH, Zürich

Abstract: To develop and optimize semiconductor devices it is common practice to advocate numerical device modeling by using simulation programs. Typically the simulation of a unit is split into levels, starting with process simulation (to study the effect of wafer-processing steps) and device simulation (to study the electrical behavior), to circuit simulation (to study the electrical features of an ensemble of devices), leading possibly to the logic simulation of a whole unit. Unfortunately, this approach makes it very hard to model the interaction of the device and the circuit in the transient case: therefore, in order to optimize the transient behavior of a particular device it is necessary to include the effects of both the drive (i.e., control part), as well as the load circuit.

During the last year, we have developed a software environment for combined device-circuit simulation studies dedicated to semiconductor power devices, magnetic field sensors, and BiCMOS structures augmented with simple circuits. In our work we discuss some critical points in detail. These include the grid generation and adaptation, the scaling of the unknowns (i.e. how to deal with high voltages), the numerical procedures used to solve the transient problem (with special attention to supercomputer architectures), the assembly of the device (element assembly versus edge assembly) and circuit equations as well as the physical models used.

We show that it is essential to choose properly the numerical techniques to obtain accurate and reliable results. Studies of the turn-off of power devices, the switching of BiCMOS structures, and of magnetic field sensors indicate the success of the current approach.

2:00 pm  Carl L. Gardner  Electron shock waves in a submicron semiconductor device
           Duke University

Abstract: The hydrodynamic model treats electron flow in a semiconductor device through the Euler equations of gas dynamics (with heat conduction) coupled to Poisson's equation for the electric potential. The hydrodynamic model PDEs thus have hyperbolic, parabolic, and elliptic modes.

The nonlinear hyperbolic modes support shock waves. Numerical simulations of a steady-state electron shock wave in a submicron semiconductor device will be presented using a steady-state upwind method. The
electron shock wave has a finite width, due to heat conduction. The width of the shock profile as a function of heat conduction will be analyzed.

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**Wednesday, July 24**

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

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<th>Time</th>
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<td>9:30 am</td>
<td>Carlo Cercignani</td>
<td>Methods of the kinetic theory of gases relevant to the kinetic models for semiconductors</td>
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<tr>
<td>10:30 am</td>
<td>Coffee Break</td>
<td>Reception Room EE/CS 3-176</td>
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<tr>
<td>11:00 am</td>
<td>F. Poupaud</td>
<td>Boundary value problems in semiconductors for the stationary Vlasov-Maxwell-Boltzmann equations</td>
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**Abstract:** When the transport of charges in a semiconductor is considered on a sufficiently large time scale, then the motion of the carriers is decidedly influenced by the short range interactions with the crystal lattice, which can be described, in a classical picture, by particle collisions. The basic tool, in this situation, is the Boltzmann equation, which may be simplified by excluding the short range interactions between carriers, which only play a role when the particle density is very large. The basic unknown then becomes the distribution function, a function of position $x$, velocity $v$ and time $t$. Even if we exclude the interactions between carriers, we obtain a nonlinear equation because of the Pauli exclusion principle. The nonlinearity is, however, different from that occurring in the Boltzmann equation for gases; here the nonlinearity can make life easier because it ensures that $f$ is bounded. In many applications the nonlinear term can be neglected. Then many properties of linear transport equations can be applied. There is, of course, no difficulty in establishing existence theorems for both initial and boundary value problems. As an approximate computational tool it is important to recall the variational principle for the steady case in a given electric field, which can be useful to evaluate global quantities such as currents and jumps near contacts and interfaces in an accurate way. One can also study the Green's function and particular solutions that are extremely useful in order to gain insight into the qualitative behavior of solutions. The talk will be devoted to a survey of the abovementioned topics.

References

4) F. Poupaud, Boundary value problems for the stationary Vlasov-Maxwell system, Forum Math., to appear
2:00 pm  Luis G. Reyna  On the treatment of the collision operator for hydrodynamic models
IBM Watson Research Center

Abstract: The study of the charge transport in semiconductor devices has been traditionally based on the Drift-Diffusion model. Smaller devices need to take into account ballistic electrons effects. An almost complete description of these effects can be obtained form computationally expensive Monte Carlo simulations. An alternative approach is given by Hydrodynamic models.

In this work we propose an alternative treatment of the collision operator in the Boltzmann equation leading to Hydrodynamic models. We start with a trial displaced Maxwellian function for the distribution function and by explicit integration of the collision term, we obtain a set of differential equations that lies in between the Drift-Diffusion model and the Hydrodynamic model.

We present numerical results obtained from these equations for a simple one dimensional $N+ N N+$ structure. We include the interaction of electrons with acoustic and optical phonons and discuss the possibility of including non-parabolic bands and intervalley scattering. The present approach could be suitable for simulations based on a mixed Monte Carlo-Hydrodynamic description.

Joint work with Andres Saul.

Thursday, July 25

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am  Thomas Kerkhoven  Numerically stable three dimensional finite element discretizations of drift-diffusion equations
University of Illinois, Urbana

Abstract: The drift-diffusion current continuity semiconductor equations are usually brought in self-adjoint form in terms of Slotboom variables by an exponential upwinding technique. The equations for the Slotboom variables are usually discretized by the well-established box method. This box method can be considered as a Petrov-Galerkin method for a piecewise linear approximation with piecewise constant test-functions. On the Delaunay triangulation in two dimensions the commonly employed box method discretization yields a discretized system with a maximum principle for the Slotboom variables.

Because the piecewise constant test-functions are not of $H^1$ regularity complications arise in applying standard finite element error analysis to this Petrov-Galerkin method. These complications can be circumvented by the following observations. The drift-diffusion model for the Slotboom variables is described by an elliptic gradient equation. Through Gauss's law we show that the Petrov-Galerkin discretization of an elliptic gradient equation for a piecewise linear approximation function depends only on the size of the integrals of the test functions over the faces of the elements, and on the regularity of the coefficients in the elliptic gradient equation. We demonstrate that this observation implies immediately that in two dimensions a box method in which the boxes bisect the finite element faces is equivalent to the piecewise linear finite element method. Hence, regularity complications can be avoided.

However, in three dimensions a box method is only equivalent to the piecewise linear finite element discretization if the boxes partition the faces of the elements in three equal parts. This implies that the box method based on perpendicular bisecting planes and the piecewise linear finite element method need not generate identical stress matrices for the Laplacean in three dimensions.

However, the box method based on perpendicular bisectors yields a maximum principle on a Delaunay tetrahedrization whereas the piecewise linear finite element method need not. We introduce an alternative Petrov-Galerkin method which is equivalent to the box method based on perpendicular bisecting planes but which circumvents problems with reduced regularity.

10:30 am  Coffee Break  Reception Room EE/CS 3-176

11:00 am  M. Rudan  Integrated tools for device design
University of Bologna

226
Abstract: Process and device simulators have found a wide acceptance among designers; these tools are providing reliable results that allow one to cut the cost associated with the laboratory experiments required to investigate different tradeoffs. Even though the software environment to support device design has had a steady improvement in the last few years, the tuning of the process parameters is usually left to the process designer who, on his own, has to choose the tradeoff among many objectives in competition with one another. From this point of view, the availability of an integrated synthesis system that supports an optimized design of semiconductor devices is likely to be an useful tool for a timely and high-quality design development.

The first part of the talk will outline the development of an optimization tool based on our two-dimensional device-analysis code IFIELDS. The activity is carried out in the frame of an EEC-sponsored Project, STORM. The main objective of the optimization part of the Project is the development of an automatic optimizer for process and device design, whose goal is computing optimal values for the process parameters according to given targets and constraints.

In the second part, a brief description is given of how the optical-generation phenomena have been incorporated into IFIELDS. This goal has been achieved by introducing a number of optical windows and interleaved material layers through which a radiation with arbitrary spectrum, incidence angle, and polarization state enters the crystal, and by evaluating the corresponding generation rate at each node of the discretization grid. The code equipped with this new capability makes the description of realistic semiconductor optical sensors feasible.

Joint work with M. C. Vecchi, G. Versellesi and Zs. M. Kovács.

2:00 pm Henry H.K. Tang IBM, East Fishkill Transport theoretic foundation of generalized hydrodynamics

Abstract: Some of the central issues of modeling submicron devices, both theoretical and computational, are examined from the viewpoint of two complementary approaches. 1. A macroscopic theory of generalized hydrodynamics is derived from a Boltzmann-Vlasov-type (BV) transport equation. 2. A finite-difference method is developed to solve the time-dependent BV equation.

The non-equilibrium dynamics of hot electrons in strong fields is studied from the framework of a microscopic BV equation. We reformulate the collision integrals of the BV equation by means of a relaxation-time representation. Each type of integral - due to electron-electron, electron-phonon or electron-impurity scattering - is rewritten as a series of relaxation-time-like terms, analogous to a partial-wave decomposition of the underlying scattering matrix. Truncation of these series leads to a class of generalized relaxation-time models which incorporate much of the salient features of the original collision integrals, but which can be more readily solved.

Generalised hydrodynamics is formulated in terms of the hierarchy of moment equations of the BV equation. The simplest version consists of a continuity equation, a generalized momentum equation and equations of the temperature tensor. It reduces to the standard drift-diffusion model and classical hydrodynamics under the restrictive assumption of local equilibrium of the electrons. We emphasize the significance of the temperature tensor field which characterizes non-equilibrium. The fundamental problems of closing the moment equations and computing the transport coefficients are transparent and can be solved readily in a class of relaxation-time models. Our approach is novel in several respects. First, the essential physics of microscopic non-equilibrium processes is included. Second, no explicit assumption about short mean free paths of the electrons is invoked. The formalism applies even in the ballistic regimes where the collisional frequency is low. Third, our analysis leads to new computational schemes for the intrinsically non-local transport parameters (such as mobility and thermal conductivity), which go beyond the confines of the classic Hilbert-Chapman-Enskog-type methods.

Many important physics issues of electron transport over small spatial dimensions and time scales require detailed information of the electron distribution. A finite-difference technique is developed to solve the time-dependent BV equation. This method is based on an accurate and efficient solver which solves the collisionless Boltzmann-Vlasov equation. In the general problem, with the help of the relaxation-time representation, the collision integrals are expressed as simple integral operators over the momentum space. Regarded as "pseudo-potentials", the collision terms (on the right side of the BV equation) and the self-consistent coulomb field (on the left side) are treated numerically on an equal footing. These ideas are tested in a transport
model in 1-dimensional coordinate space and 3-dimensional momentum space. We discuss the prospects of applying this scheme to problems in 2-dimensional coordinate space and for realistic devices.

3:30 pm Emad Fatemi IMA Simulation of $n^+nn^+$ channel using finite difference techniques for Boltzmann equation

Abstract: In this talk we discuss simulation of a $n^+nn^+$ channel using finite difference discretization of the Boltzmann-Poisson system in 1D(space)-1D(velocity). We use a first order upwind method. The collision operator is approximated by relaxation to a Maxwellian. The simulation is compared with the Hydrodynamic model. Also a numerical investigation is done with respect to the heat conduction term in the Hydro model.

5:30 pm Semiconductors BBQ Picnic Courtyard between Vincent and Murphy Halls

Friday, July 26

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am P. Degond ENS-Cachan, France On the Child-Langmuir law for semiconductors

Abstract: The Child-Langmuir injection law is widely used in vacuum diodes modelling. It describes the emission of an electron beam at a cathode when the energy of the emitted particles is small compared with the applied potential. In the early eighties, the physicists M.S. Shur and L.F. Eastman proposed a model of ballistic transistor based on the Child-Langmuir model. Such models can be mathematically obtained by means of an asymptotic analysis of a singular perturbation problem for the stationary Vlasov-Poisson equation (in the vacuum diode case) or the Vlasov-Poisson-Boltzmann equation (in the semiconductor case). These models produce an accurate description of the behaviour of the carriers close to the cathode contacts and can be used to design precise boundary conditions especially for particle or Monte-Carlo calculations.

10:30 am Coffee Break Reception Room EE/CS 3-176

11:00 am Michael Sever Hebrew University Symmetric forms of energy-momentum transport models

Abstract: The energy-momentum transport models of carrier flow in a semiconductor admit entropy functions and thus a generalized symmetric form. A simpler such form can be obtained for the reduced "mass-momentum" system, thinking of the energy equation as essentially determining the carrier temperature distribution. The use of such a symmetric form leads naturally to suitable choices for boundary conditions, discretization schemes, and regularization when discontinuous solutions appear.

2:00 pm Joseph W. Jerome Northwestern University Energy models for one-carrier transport in semiconductor devices

Abstract: Moment models of carrier transport, derived from the Boltzmann equation, have made possible the simulation of certain key effects through such realistic assumptions as energy dependent mobility functions. This type of global dependence permits the observation of velocity overshoot in the vicinity of device junctions, not discerned via classical drift-diffusion models, which are primarily local in nature. It has been found that a critical role is played in the hydrodynamic model by the heat conduction term. When ignored, the overshoot is inappropriately damped. When the standard choice of the Wiedemann-Franz law is made for the conductivity, spurious overshoot is observed. Agreement with Monte-Carlo simulation in this regime has required empirical modification of this law, as observed by IBM researchers, or nonstandard choices. In this lecture, simulations of the hydrodynamic model in two dimensions, as well as simulations of a newly developed energy model, the RT model, will be presented. These simulations have been carried out by Chi-Wang Shu of Brown University. The RT model, intermediate between the hydrodynamic and drift-diffusion model, was developed at the University of Illinois to eliminate the parabolic energy band assumption, and to reduce the spurious overshoot with physically consistent assumptions. The algorithms employed for both models are the essentially nonoscillatory shock capturing algorithms, developed at UCLA during the last...
decade. Some mathematical results will be presented, and contrasted with the highly developed state of the drift-diffusion model.

Monday, July 29

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am  Michael Ward  Stanford University  Some examples of singular perturbation methods in device modeling

10:30 am  Coffee Break  Reception Room EE/CS 3-176

11:00 am  William Coughran  AT&T Bell Labs  The role of numerical algorithms and visualization in complex semiconductor simulation

2:00 pm  Herbert S. Bennett  NIST  Physics for device simulations and experimental verification

Abstract: The motivations for using computers to simulate the electrical characteristics of transistors are discussed. Our work and that of others in the area of device physics and modeling are described. We compare conventional device physics with an alternative approach to device physics that is more directly traceable to quantum-mechanical concepts. We then apply this new approach to quasi-neutral regions, space-charge regions, and regions with high levels of carrier injection. Examples of applying quantum-mechanically-based device physics to energy band diagrams for bipolar transistors are given. The limits for using theoretical results from uniform media in numerical simulations of devices with large concentration gradients are discussed. Calculations of the effective intrinsic carrier concentrations for gallium arsenide and silicon are also given along with published data. In addition, calculations of the mobilities for GaAs that are based in part on quantum-mechanical phase shifts are compared with published data. We then conclude with a discussion of the requirements for verifying and calibrating device simulators for the submicrometer domain.

Joint work with Jeremiah R. Lowney.

3-3:30 pm  Tom Seidman  U. of Maryland, Baltimore Cty.  Mathematical treatment of the time-dependent drift/diffusion model

Abstract: The drift/diffusion model is considered under general enough conditions to include, e.g., "standard" impact ionization source terms. Existence is shown for the general model and then, under somewhat more restrictive conditions, a constructive (contractive iteration) argument gives both existence and uniqueness.

Tuesday, July 30

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

10:30 am  Coffee Break  Reception Room EE/CS 3-176

9:30 am  Thomas Kerkhoven  University of Illinois, Urbana  Numerical simulation of quantum wires in periodic heterojunction structures

Abstract: Electron confinement in quantum planes, wires, and dots is modeled by Schrödinger's equation coupled with Poisson's equation for the electrostatic potential. A self-consistent solution to this system of equations is obtained as follows. Schrödinger's equation is solved by subspace iteration. Poisson's equation is solved by a suitably preconditioned conjugate gradient algorithm. Self consistency of the coupled model is obtained by a Jacobian-free implementation of Newton's method.
The periodic structure can only be employed for the design of quantum wires if the following conditions can be met. The periodic structure allows a ground state wave function which is bound. The occupancy of the non-bound states can be made negligible with respect to the occupancy of the bound ground state. This second condition requires again that the separation between the bound state and the lowest non bound state is sufficient.

We briefly describe our algorithm and proceed to discuss in detail the design of the periodic heterojunction structure which satisfies the requirements mentioned above.

11:00 am Peter Szmolyan
Technical University Vienna

Abstract: If a constant voltage above a certain threshold is applied to a piece of semiconductor material with negative differential resistance periodic current oscillations are observed. The current peaks are due to dipole waves which are generated periodically at one contact he device and leave at the other contact. We give a refined analysis of the classical explanation of the Gunn effect as traveling waves on an infinite domain. We show that under appropriate boundary conditions periodic solutions on a finite domain are generated by a Hopf bifurcation. We give an asymptotic analysis of the periodic generation, propagation, and destruction of the dipole waves.

2:00 pm Patrick S. Hagan
Los Alamos National Lab

Abstract: Semiconductors are commonly modeled and analyzed at two different levels of description. At the macroscopic level, the Basic Semiconductor Equations (BSEs) are a system of diffusion-drift equations which describe the densities of electrons and holes in real space. At a much more fundamental level, Boltzmann equations describe the densities of electrons and holes in phase-space. Although the BSEs are quite accurate when electric forces are not too large, it is well-known that the BSEs become increasingly inaccurate as the strength of the electric field increases. Unfortunately, electric field strengths generally increase as devices get smaller, with the BSEs becoming essentially worthless for predicting the performance of sub-micron devices.

We have recently used singular perturbation techniques to analyze the Boltzmann equations for semiconductors. This analysis shows that the BSEs are an asymptotically correct "outer solution" to the full Boltzmann equations for moderate electric field strengths. However, as devices become smaller and electric field strengths increase, the Boltzmann equations enter the strong force regime, which renders the BSEs incorrect. In this regime our analysis yields a new system of equations in which the drift velocities and diffusivities are nonlinear functions of the electric field. Unlike the BSEs, we expect these new High Field Semiconductor Equations to remain accurate regardless of the electric field strength. Remarkably, these equations show that Einstein's relation is satisfied in the high field regime, even though the system responds nonlinearly to the electric forces.

We will also derive the 3-dimensional analogue of the high field equations, and analyze the asymptotic and quantum mechanical corrections to these equations.

3-3:30 pm Leonid V. Kalachev
Moscow State University

Abstract: The numerical treatment of the drift-diffusion model using a Gummel-type iteration process often involves the solution of nonlinear equations by the Newton iteration methods. The speed of convergence and sometimes the convergence itself depend crucially on the right choice of the initial iterate. Asymptotic methods show their effectiveness when used to construct such initial iterates as asymptotic approximations for solutions of some of the drift-diffusion equations when a small parameter enters the system. We discuss the construction of the asymptotics for the singularly perturbed Poisson equation in a rectangular semiconductor device. Explicit expressions for the terms of the asymptotic approximation significantly provide a way to use asymptotics in numerical processes and to reduce the time for simulations.

We also discuss the asymptotic analysis of Gunn effect in a bounded domain modeling the Gunn diode. The asymptotic approach allows one to construct the approximation of the moving pulse-type solution and to obtain some characteristics of the device.
We give a short survey of some other results concerned with applications of asymptotic methods to semiconductor device modeling.

**IMA Postdoc Seminar**

4:00 pm  Chao-Nien Chen  
IMA  
**Bifurcation for prescribed mean curvature problems**

*Abstract:* We discuss bifurcation and existence results for a class of prescribed mean curvature problems which admit zero as a trivial solution.

The SEMINAR meets in Vincent Hall 570

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**Week 3 - Quantum Effect**: (½ week), July 31 – Aug. 2, 1991  
(Farouk Odeh and Bill Coughran will be in residence and in charge of weeks 2 and 3)

As the dimensions of modern devices decrease to ultrasmall levels, quantum effects begin to play a major role. Examples are the quantization of states in confined regions—thin channels, quantum-wires etc.—and tunneling phenomena in resonant diodes. This involves a coupling of electromagnetics directly to quantum mechanics, i.e., to eigenfunctions of the Schrödinger equation. New transport models, such as the Wigner pseudo-differential equation and/or what may be loosely called quantum-Boltzmann have to be applied for an adequate description of “quantum devices.” Path integrals, pseudo-differential operators and numerical techniques for eigenvalues and eigenfunctions are expected to provide the mathematical tools for this area.

**Wednesday, July 31**

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am  Harold L. Grubin  
Scientific Research Associates  
**Small devices and the Boltzmann equation in quantum mechanics**

10:30 am  Coffee Break  
Reception Room EE/CS 3-176

11:00 am  Christian Ringhofer  
Arizona State University  
**Numerical methods for quantum transport phenomena in semiconductor devices**

2:00 pm  H.C. Liu  
National Research Council Canada  
**High frequency quantum transport**

*Abstract:* A scattering model is formulated for quantum transport under both dc and ac applied voltages. Analogous to the scattering model for the time-independent quantum transport, the present approach views a quantum device as a scattering target connected to electron reservoirs in thermal equilibrium. Such a model is therefore applicable only to the extreme quantum cases, e.g., tunneling through double-barriers and ballistic conduction through constrictions or quantum point contacts. The goal is to investigate (a) how an electron interacts with a high frequency ac field when traversing a quantum structure, (b) what is the frequency scale at which a quantum device characteristics deviate from its low frequency values, and (c) what is the device high frequency characteristic, e.g., device impedance as a function of frequency. A physical insight into these issues is of great relevance to the frequency limits of quantum devices. The double-barrier resonant tunneling diode and the ballistic constriction are discussed as examples.

3-3:30 pm  Daniel C. Cole  
IBM GTD  
**The thermodynamics of Casimir forces between conducting parallel plates**

*Abstract:* The bulk of this talk is related to a recent emerging field of physics called cavity quantum electrodynamics. However, Casimir forces, as well as the underlying van der Waals forces, also play a role in semiconductor physics and devices, which is the main theme of this conference. This role is briefly discussed as well as speculated upon. The talk then turns to the following two idealized operations: (1) quasistatically displacing two parallel conducting plates immersed in thermal radiation, and (2) slowly changing the temperature of the radiation. By imposing the condition that no heat must flow at $T = 0$ during a reversible...
thermodynamic operation, the functional form of the quantum zero-point radiation spectrum is deduced. Turning to thermodynamic operations on the plates at \( T \neq 0 \), and imposing that the second law of thermodynamics must hold, then results in a generalized derivation of Wien's displacement law. The calculations involve changes in singular energy expressions and cancellations between singular forces.

3:30 pm  Akerman Hall 130D  Tour of Dan Joseph's Lab

We will show experiments on water lubricated pipelining with bamboo waves and corkscrew waves, two dimensional cusped interfaces which violate Laplace's law, rollers, drafting, kissing and tumbling of fluidized particles, non linear stabilization of fingering instabilities in porous media, drag reduction using riblets. The tour probably will last 30 or 40 minutes.

Thursday, August 1

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am  Antonio Gnudi  Some applications of the hydrodynamic model and Boltzmann transport equation in semiconductor device simulation
University of Bologna

Abstract: Phenomena related to high energy carriers in semiconductors play an important role in the design of submicrometer devices. Some models have been devised to take such effects into account in engineering simulation tools both at macroscopic (Hydrodynamic model) and microscopic level, by means of a more careful examination of Boltzmann Transport Equation (BTE).

In this talk we review some applications of the hydrodynamic model to the simulation of MOSFET's, with emphasis on the ways impact ionization can be incorporated in the model in a physically sound yet simple way. Comparison with measured substrate currents will be discussed.

In order to extract more detailed information from BTE, a method will be outlined based on expansion of the distribution function in Spherical Harmonics in momentum space. This method is applied to both the homogeneous transport problem, with comparison to Monte Carlo, and to a one-dimensional bipolar transistor.

Joint work with Farouk Odeh.

10:30 am  Coffee Break
Reception Room EE/CS 3-176

11:00 am  Erasmus Langer  Numerical simulation of MOS transistors
Technical University Vienna

Abstract: This contribution is intended to review the international state-of-the-art in numerical simulation of MOS devices. Much emphasis is laid on the discussion of recent refinements to carrier transport models, e.g. drift-diffusion model, enhanced drift-diffusion equations, hydrodynamic model, and Monte Carlo simulation. Adequate models for the physical parameters are reported with suitable parameter values, e.g. carrier mobilities taking into account the various scattering mechanisms, and carrier generation-recombination including impact ionization. Examples are presented for two different types of MOS devices: on the one hand, three-dimensional simulation results of a miniaturized MOS transistor are discussed which have been obtained by our simulator MINIMOS 5.0, and on the other hand, simulation results concerning a power MOS transistor are shown which has been investigated by our device simulation program BAMB1 2.1.

2:00 pm  Bernardo Cockburn  Discontinuous approximations for the drift-diffusion and the hydrodynamic models
University of Minnesota

Abstract: A fully parallelizable method, initially devised for numerically solving nonlinear conservation laws in several space dimensions, is extended to the drift-diffusion and to the hydrodynamic models. The method is combined with a mixed finite element that provides directly an approximation of the electric field. Stability results and error estimates are obtained for a one-dimensional version of the drift-diffusion
model. Preliminary numerical results showing the performance of the methods are shown for both the 
(one-dimensional) drift-diffusion and hydrodynamic models.
Joint work with J. Jerome and I. Triandaf.

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**Friday, August 2**

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

This day is set aside for contributed talks and discussions

10:30 am Coffee Break

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Week 4 - Circuit Analysis, August 5-9, 1991

(Jacob White will be in residence and in charge of week 4)

The high cost of integrated circuit fabrication, both in time and materials, forces designers to simulate their complete designs in as much detail as possible. Typically, the approach of choice is to construct a differential algebraic (DAE) system that describes the circuit, and solve that system numerically for a given set of inputs. More specifically, the circuit is assumed to be an interconnection of lumped elements (e.g. resistors, capacitor, inductors and transistors), characterized by a relation between the terminal voltages and terminal currents. The equation system that describes such a network is then constructed using the Kirchoff voltage and current laws, and this leads to an index 1 system of differential-algebraic equations where the state variables are not always readily identified. In general, the system of equations generated from most circuits is very stiff, even if the algebraic equations are not present. Also, the system is quite nonlinear, and this makes finding an initial solution which satisfies the initial conditions and the algebraic constraints rather difficult.

The circuit simulation problem can be broken into two classes: solving large initial value problems, with as many as 10,000 unknowns, efficiently; and computing periodic or quasi-periodic solutions for smaller problems, with 10 to 100 unknowns. For solving the large initial value differential-algebraic systems, the topics of interest are techniques for stiff systems; techniques for solving large nonlinear systems where the Jacobian can be much more than one rank deficient; multirate integration methods; and iterative techniques for very nonsymmetric problems. For computing periodic or quasi-periodic solutions to these DAE systems, topics of current interest are existence and uniqueness of solutions, high order methods for very stiff problems, spectral methods, mixed time-frequency methods and other types of collocation methods.

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**Monday, August 5**

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am Welcoming Remarks

9:40 am Sally Liu & Kishore Singhal

**Abstract:** Recent progress in circuit simulation will be reviewed. Bottlenecks in applying current state-of-the-art circuit simulation capabilities to VLSI and high-performance design methodologies will be presented. We will also identify some open issues to facilitate discussions at the workshop.

10:40 am Coffee Break

11:00 am Linda R. Petzold

**University of Minnesota**

**Abstract:** In recent years there has been much progress in the analysis and development of numerical methods and software for the solution of differential-algebraic equation (DAE) systems. However, many of these
results implicitly assume that the underlying differential system is nonstiff. In this lecture, we outline recent developments in theory, methods and software which have implications for the solution of stiff DAEs. In particular, we give conditions under which a DAE is well-conditioned, and examine formulations of the DAE which preserve the stability and which lead to stable discretisations. For initial and boundary value DAEs requiring symmetric discretizations, we describe a class of collocation methods which overcome stability and accuracy limitations of previously-defined symmetric methods. Finally, for large-scale stiff initial value DAEs, we discuss the status of available software.

2:00 pm  Bob Melville
AT&T Bell Labs
Globally convergent homotopy methods for the operating point and steady-state problems

Abstract: Robust computation of the DC operating point(s) of an integrated circuit is crucial for simulation. An operating point is of interest in its own right, and is needed as a starting point for transient analysis and as a bias point for small-signal or noise analysis. The operating point problem may be formulated as a system of non-linear equations to be solved for a zero, in which the unknowns are node voltages and/or branch currents. In some cases, the system of equations may have more than one solution, corresponding to multiple possible bias solutions for the circuit which they model.

The following three methods seem to be the most popular approaches to the computation of an operating point in SPICE-class programs:
1. Norm-reducing variations of Newton’s method;
2. Transient methods which simulate the dynamics of the circuit as the power supply comes on;
3. Numerical continuation which tracks the state of the circuit for different values of the power supply voltage (not as a dynamical system as in (2) above).

Our presentation makes a case for homotopy (continuation) parameters other than supply voltage. In particular, for bipolar networks, the use of transistor current gain (forward and reverse alpha) as a homotopy parameter gives excellent results. Concepts from circuit theory are used to establish a coercivity condition so that the zero set of our various homotopies must be bounded. However, the zero set can still exhibit undesirable singularities such as bifurcations and cusps. Such singularities can be eliminated by the introduction of an appropriate randomization vector. Mathematical justification for this procedure will be given based on a version of Sard’s theorem.

Timing results on a set of benchmarks support our claim that genuine global convergence can be enjoyed at a computing cost which is easily within a factor of five of other, less widely convergent techniques.

The steady-state response of a non-linear network driven by a single periodic source can be obtained as the solution of a two-point boundary value problem on a discrete mesh of time points. In fact, the time-point equations can be viewed as operating point equations of a DC network. A coercivity result will be given for these equations which lets us claim global convergence of a homotopy method for their solution.

Time permitting, we will discuss multiple solutions of operating point equations and qualitative stability analysis of the solutions.

Various parts of the work to be presented have been joint with Ljiljana Trajkovic at BellCore, and Mike Fang, Peter Doyle, and of Jeff Lagarias at AT&T.

4:00 pm  Vincent Hall 502
(The IMA Lounge)
IMA Tea (and more!)

Tuesday, August 6

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9.30 am  Albert Ruehli
IBM
Serial and parallel waveform relaxation algorithms

10:30 am  Coffee Break
Reception Room EE/CS 3-176

234
Newton-iterative and iterative-Newton methods for nonlinear systems

Abstract: We discuss two generic methods for solving nonlinear algebraic or operator systems of equations. Newton-iterative methods solve successive linearized systems by an inner iterative method, i.e., Newton-Gauss-Seidel. Iterative-Newton methods, as in Gauss-Seidel-Newton, solve smaller sets of nonlinear equations approximately, usually using one step of Newton's methods. We compare these methods with an eye toward computational efficiency; in particular, memory requirements, function evaluations, arithmetic operations, and ease of implementation. Circuit and device simulation motivate our discussion.

Gradient-descent acceleration for waveform relaxation

Abstract: A new algorithm for accelerating dynamic iterations for DAE systems is developed. The algorithm is based on extend, i.e., the generalized conjugate-residual algorithm for matrix problems to function spaces. Experimental results for the method used to solve time-dependent drift-diffusion plus Poisson equation is given to demonstrate the effectiveness of the acceleration.

Estimating waveform relaxation convergence

Abstract: The waveform relaxation method is considered as a method for decoupling systems of ODEs or DAEs for parallel implementation. Ultimately, waveform relaxation converges superlinearly in finite intervals. In the early sweeps, this is typically not observed, and it has been proposed that the practical convergence is linear until the late stages of the iteration. Taking this viewpoint, the author obtains an estimate for a window length wherein waveform relaxation converges like \( \omega^n \) by looking in the Laplace domain. The results are stated in terms of a quantity called the speed of a splitting which measures the extent to which subsystems are decoupled. A numerical experiment is presented.

Wednesday, August 7

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

Moment-matching approximations for linear(ized) circuit analysis

Abstract: Moment-matching approximations appear to be a promising approach for linear circuit analysis in several application areas. Asymptotic Waveform Evaluation (AWE) uses moment-matching to approximate the time- or frequency-domain circuit response in terms of a reduced-order model. AWE has been demonstrated as an efficient means for solving large, stiff, linear circuits. However, since it is based upon moment-matching, which has been shown to be equivalent to a Pade' approximation, AWE is prone to yielding unstable waveform approximations for stable circuits. In addition, it is difficult to quantify the time domain error for moment-matching approximations. We address the issues of stability and accuracy of moment-matching approximations as they apply to linear circuit analysis.

Multipole-accelerated 3-D capacitance extraction

Abstract: In this talk we will describe a fast method for computing the capacitance matrix of a general 3-dimensional geometry of ideal conductors in free space. The method is an acceleration of the standard boundary-element approach to solving the first-kind integral equation for conductor surface charge. In this accelerated approach, the dense matrix problem generated from the boundary-element discretization is solved with a preconditioned generalized conjugate-residual method, where a multipole approximation is used to compute the iterates, and the preconditioner is matched to the multipole algorithm. A novel adaptive scheme for the 3-dimensional multipole algorithm will be presented, along with results indicating the effectiveness of
the approach on engineering problems. Finally, numerical evidence is presented indicating that the number
of GCR iterations does not increase with increasing geometric complexity, demonstrating that in practice
the algorithm is order($N$), where $N$ is the number of boundary elements.

2:00 pm Olgierd A. Palusinski
University of Arizona, Tucson

Abstract: Waveform Relaxation (WR) is an attractive way to reduce CPU time needed for simulation of
transients in integrated circuits. One of the problems associated with WR is a need for storage of intermediate
solutions for coupling variables and exchange of those variables between appropriate subcircuits. Spectral
technique based on Chebyshev polynomials offers the most compact representation of variables and has
many features facilitating computation and exchange of data which is necessary in WR. The technique will
be briefly described and some results of application to MOS circuits given.

Thursday, August 8

Unless otherwise stated, the talks today are in Conference Hall EE/CS 3-180

9:30 am Jiri Vlach
University of Waterloo

Abstract: A special integration method, based on numerical Laplace inversion, was developed for the analysis
of switched networks. The method can
(a) find correct time domain response in the presence of Dirac impulses
(b) find consistent initial conditions after switching, even if at the time of switching the conditions are inconsistent
and Dirac impulses may be present.
(c) Discover not only the absence or presence of the Dirac impulse, but also its area and perform correct switching
of other elements in the network.

The method was used for the development of:
(a) Program for analysis of periodically switched analog networks (with all linear elements).
(b) Program for analysis of networks with internally controlled switches, as needed for analysis of switched power
supplies.

The lecture will explain basis of the integration method and will show examples solved by our programs.

10:30 am Coffee Break
Reception Room EE/CS 3-176

11:00 am Michael E. Henderson
IBM, Watson Research Center

Abstract: It has become fairly standard to compute periodic solutions in systems of ODE's, and to track the
solutions and their bifurcations as some parameter in the equations is varied. I will describe the equations
used and some of the considerations which arise when the method is implemented. Finally, I will describe
one application, where these techniques have been used to compute periodic solutions in a pair of coupled
Josephson junctions.

2:00 pm Ken Kundert
Cadence Design Systems

Abstract: Analog circuits like switching filters are typically driven with a clock which is at a much higher
frequency than the signals the circuit is intended to process. Designers of such circuits are often interested
in steady-state distortion due to both static effects, such as nonlinearities in the capacitors, and dynamic
effects, such as the charge injection during MOS transistor switching or slow operational amplifier settling.
Steady-state distortion can be computed using the circuit simulation program SPICE, but this approach is
computationally very expensive. Specialized programs for switched capacitor filters can be used to rapidly
compute steady-state distortion, but do not consider dynamic effects. In this talk we present a new mixed
frequency-time approach for computing both steady-state distortion. The method is both computationally
Efficient and includes both static and dynamic distortion sources. The method has been implemented in a C program, *Nitswit*, and results from several examples will be presented.

3:00 pm Werner Liniger IBM Yorktown Heights On sparse factorization methods for Poisson's equation

*Abstract:* We discuss fast algorithms for solving Poisson's (or other elliptic) equations on general regions with arbitrary mixed boundary conditions. These algorithms create preconditioners which are second-order, both in the interior of the region and near the boundary. The associated iterative scheme has interesting and novel convergence properties.

5:30 pm 502 & 570 Vincent Hall Giant Hoagie Party (sandwiches, salad, fruit, desert)

Friday, August 9

The talk today is in Vincent Hall 570

9:30 am Paul Cox Texas Instruments Circuit simulation algorithms

*Abstract:* Circuit simulators are one of the most widely used and essential tools used in the design of integrated circuits. To satisfy these requirements two conflicting requirements must be satisfied. The circuit simulation must provide the accuracy and robustness required for critical memory and analog circuit designs and it must be efficient enough to simulate large VLSI circuit designs. We have been involved for some time in the development and refinement of the circuit simulator SUPPLE at Texas Instruments. The objective of this work was to provide a circuit simulator with all of the capabilities and robustness of SPICE but with enhanced performance from the exploitation of multi-rate behavior and parallel processing.

The algorithms developed for use in SUPPLE have improved the efficiency to simulation, however, a number of issues need to be resolved in order to support the design of larger VLSI designs. These issues include:

- DC convergence. A DC solution of the circuit matrix is the first step in any type of circuit simulation. However, no efficient methods exist which can guarantee a DC solution.
- Matrix partitioning. Efficient methods of partitioning need to be developed for exploitation of multi-rate behavior and parallel processing.
- Transient time step control. New algorithms need to be developed to provide better a priori truncation error estimation.
- Matrix solution algorithms. New matrix solution techniques are required which can provide the robustness of direct solution methods but are efficient enough to be used on very large sparse matrix systems.

10:30 am Coffee Break Vincent Hall 502

The rest of this day is set aside for discussions

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**CURRENT IMA PARTICIPANTS**

**POSTDOCTORAL MEMBERS FOR 1990-91 PROGRAM YEAR**

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<tr>
<th>NAME</th>
<th>PREVIOUS/PRESENT INSTITUTION</th>
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<tr>
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**POSTDOCTORAL MEMBERSHIPS IN INDUSTRIAL MATHEMATICS FOR 1990-91 YEAR**

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**LONG-TERM VISITORS IN RESIDENCE**

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<td>June 1 - Nov 30</td>
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<td>Li, Tong</td>
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<td>Aug 27 (90) - Aug 26, (91)</td>
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**SUMMER PROGRAM PARTICIPANTS IN RESIDENCE**

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