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MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

T a g u n g s b e r i c h t 46/1988

Mathematische Modellierung und Simulation elektrischer Schaltungen

30.10. bis 05.11.1988

Die Tagung wurde geleitet von R. Bank (La Jolla, UCSD), R. Bulirsch (TU München) und K. Merten (SIEMENS AG, München).

43 Wissenschaftler aus dem In- und Ausland haben an der Tagung teilgenommen. 9 Teilnehmer kamen aus den USA, des weiteren konnten Gäste aus der DDR, aus Frankreich, den Niederlanden, Irland, Italien, Österreich und der Schweiz begrüßt werden. Dem interdisziplinären Charakter der Tagung entsprach die Zusammensetzung des Teilnehmerkreises: 9 Teilnehmer waren Industriegruppenvertreter, 6 Teilnehmer repräsentierten Arbeitsgruppen der Elektrotechnik, 28 Teilnehmer kamen aus den angewandten Disziplinen der Mathematik.

Der einleitende Übersichtsvortrag (Merten) verknüpfte die Schwerpunkte der Tagung: Schaltkreissimulation, Schaltelementmodellierung, Schaltelementsimulation. Zudem wurden die Verbindungen gezeigt zu möglichen weiteren Forschungsfeldern der Mathematik wie die Ausbeuteoptimierung in der Chip-Produkion (Antreich), die Berücksichtigung von Induktionen der Leiterbahnen (Grabinski) und die Prozeß-Simulation (Rank).

Die vielfältigen physikalischen Effekte, die in den Schaltelementen ablaufen, wurden erläutert (Hänsch), ihre Beschreibung als mathematische Modelle (Jerome, Kerkhoven) vorgestellt. Über eine mögliche Erweiterung dieser Modelle auf Laserdioden wurde berichtet (Ferguson).

Der numerischen Simulation der Transistorgleichungen wurden mehrere Vorträge gewidmet. Die Eigenschaften der Mixed Finite Element Methoden wurden diskutiert (Miller, Pietra, Polak). Iterative Lösungstechniken für die bei Finite Element- bzw. Finite Differenzenmethoden entstehenden großen linearen Gleichungssysteme wurden behandelt (Coughran, Sawatzki). Ein "Nested Iterative" - Verfahren (Rose) wurde vorgestellt. Für die Simulation von 3-D Modellen wurden neue Diskretisierungen (Bank, Bürgler) und ein Softwarepaket (Fichtner) erläutert. Interessant waren der Vortrag über die Zusammenhänge zwischen Transistorgleichungen und der Boltzmanngleichung (Degond), sowie die Ausführungen über die Berücksichtigung des Quantentransports (Ringhofer) und die numerische Behandlung einspringender Ecken in 3-D Modellen (Steger).

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Im weiteren Sinne ließen sich die Vorträge, die grundsätzliche Fragestellungen diskutierten, der Schaltelementsimulation zuordnen: Design eines Simulationsprogramms für die Transistorgleichungen (Seidman), Einsatz von Vektorrechnern (Kiehl), Parallelen in der Modellbildung und Numerik bei Oberflächenspannungen von Tropfen (Mittelmann).

Die Vorträge zur Schaltkreissimulation umfaßten die theoretischen Aspekte: Indexklassifizierung bei DAE's und ihr Zusammenhang mit "Ill-posed" Problemen (März), die Regularisierungstechniken (Griepentrog); sowie zahlreiche numerische Fragestellungen: Berechnung periodischer Lösungen (Zheng), Berücksichtigung der Latenz eines Schaltkreises durch gesplittete Diskretisierung (Schultz), Homotopiemethoden zur Anfangswertbestimmung (Zimmermann), neue numerische Lösungsansätze (Ascher, Rentrop). Die Notwendigkeit zur Entwicklung und Verbesserung der numerischen Methoden in Standard-Softwarepaketen (wie SPICE) wurde sehr eindrücklich dokumentiert (Denk).

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Vortragsauszüge

ANTREICH K.J.

Design Centering and Yield Maximization of Integrated Circuits

Parametric yield is the percentage of manufactured circuits that have parametric performance (e.g., speed or power consumption) within specified limits.

The lecture deals with an advanced formulation of the yield maximization and the design centering problem along with a classification scheme for several problem definitions. Methods for the solution of that problem which can be approached from either a deterministic or a statistical viewpoint are discussed.

ASCHER U.

On Numerical Differential Algebraic Problems with Application to Semiconductor Device Simulation

The talk treats the questions of conditioning of numerical methods for certain differential algebraic equations subject to initial and boundary conditions. The approach taken is that of separating "differential" and "algebraic" solution components, at least theoretically.

This yields conditioning results for differential algebraic boundary value problems in terms of "pure" differential problems, for which existing theory is well-developed. We carry the process out for problems with (global) index 1 or 2.

For semi-explicit boundary value problems of index 1 (where solution components are separated) we give a convergence theorem for a special class of collocation methods. For general index 1 problems we discuss advantages and disadvantages of certain symmetric difference schemes. For initial value problems with index 2 we discuss the use of BDF schemes, summarizing conditions for their successful and stable utilization.

Finally, the present considerations and analysis are applied to two problems involving differential algebraic equations which arise in semiconductor device simulation.

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BANK R. ; J. BÜRGLER

New discretization schemes for the semiconductor current continuity equations

We have developed a new, analytical hybrid finite element method to discretize the semiconductor continuity equations. Contrary to the popular box integration scheme of Scharfetter und Gummel, our technique is rather insensitive to the element geometry, thus avoiding the "obtuse" angle problems usually found in multi-dimensional simulations. Furthermore, a linear ansatz for the current in each element provides higher accuracy. The method works in any dimension and for (n-dimensional) simplexes as well as for quadrilaterals, bricks, prisms, etc. We have successfully tested it on various two- and three-dimensional problems.

COUGHRAN B.

Iterative Methods for Device Simulations

DEGOND P.

Numerical simulations of electron transport in electronic devices using the Boltzmann equation

I would like to present some numerical results that have ben obtained at the "CMAP-Ecole Polytechnique" in Paris, concerning the numerical simulation of hot electron transport in electron devices using the Boltzmann equation. The numerical method is the deterministic particle method described in (1). Results for onedimensional submicronic structures will be presented. Comparisons with the Monte-Carlo method will also be given.

[1] B. NICLOT, P. DEGOND, F. POUPAUD: "Deterministic Particle Simulations of the Boltzmann Transport Equation of Semiconductors". J. Comput. Phys., to appear.

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DENK G.

The Numerical Integration in SPICE2-S:
Analysis and Presentation of a New Implementation

Circuit simulation means - from the mathematical point of view - the solution of a differential-algebraic system (DAS) $F(t,x,\dot{x}) = 0$. This is usually done by discretization, e.g. with a multistep scheme and solving the resulting nonlinear equation by a Newton-Raphson-iteration.

In SPICE2-S, however, a similar DAS is to be solved, namely $\hat{F}(t,x(t),\dot{Q}(x(t))) = 0$, where t denotes the time, x the nodal voltages and Q the charge in the branches. As the local truncation error LTE now depends on the higher derivatives of $Q(x(t))$, this transformation leads to several disadvantages. The most important one is the very expansive calculation of LTE, which has to be done by divided differences.

The main idea for the new implementation is the use of the chain rule $\dot{Q}(x(t)) = \frac{\partial Q}{\partial x} \cdot \dot{x}(t)$, which helps us to transform $\hat{F}(t,x,\dot{Q}) = 0$ back to $F(t,x,\dot{x}) = 0$. this enables us to use well-known results for this type of DAS, e.g. the LTE can be calculated by a simply scaling of the Newton-correction.

The advantages of the new implementation are shown by several simulation results.

FERGUSON W.

Modelling of DH Semiconductor Diode Lasers

A brief overview of the complexities of modelling
1) electrical,
2) thermal, and
3) optical
properties of modern DH semiconductor diode lasers.

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FICHTNER W.

Three-Dimensional Numerical Simulation of Complex Semiconductor Structures

The numerical solution of the semiconductor equations for three-dimensional (3D) structures poses a challenging problem for the scientific computing community.

In this presentation, I shall focus on the numerical aspects of 3D-Simulation. Grid generation and adaption, matrix formulation and linear equation solution shall be discussed in detail.

GRABINSKI H.

Simulation of Signals On Line Systems in a Nonlinear Circuit Environment

An algorithm for the computation of signal propagation in lossy interconnect systems at the chip as well as at the board level is presented. The algorithm allows us to handle effects like delay, dispersion, reflection, and electromagnetic coupling sufficiently. Especially for large systems of lines these effects cannot be treated by existing general purpose network analysis programs because of excessive computer runtime and numerical instabilities.

To be able to handle line systems in a nonlinear circuit environment (e.g. CMOS inverters) the algorithm operates in the time domain. It is implemented in a computer program called LISIM which yields high accuracy, good stability, and small computation time.

Simulation results are given for on-chip line systems of medium size based on the slow-wave mode.

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GRIEPENTROG E.

Transformation of Differential-Algebraic Equations (DAE's) in the Numerical Treatment of DAE's

Considering the autonomous DAE $A(x)x' = f(x)$ (1) in R^m we assume the constraint manifold $S = \{x \in R^m : f(x) \in \text{im}(A(x))\}$ and the manifold of consistent initial vectors $S^c = \{z \in R^m$: there is exactly one solution $x(t)$ with $x(0) = z\}$ to be sufficiently smooth. Obviously $S^c \subseteq S$; if $S^c = S$ the DAE (1) is called an index-1-DAE. For any projector $R(x)$ along $\text{im}(A(x))$, $TS(x) := \ker(D(Rf)(x))$ ($D := \partial / \partial x$) is the tangential space of S in x. Since for each solution $x(t)$ of (1) $x'(t)$ belongs to $TS(x)$ we obtain $x' = Q_s(x)x'$ for each projector $Q_s(x)$ onto $TS(x)$.

Consequently, the "reduction" of (1) to $A_1(x)x' = f(x)$ (2) with $A_1(x) := A(x)Q_s(x)$ does not change the set of solutions, but for the corresponding manifolds we obtain $S^c \subseteq S_1 \subseteq S$. The DAE (1) is called an index-k-DAE, if $k - 1$ reduction steps of this kind produce an index-1-DAE.

Using this concept of S. Reich we can prove, that k transitions from (1) to $\hat{A}_1(x)x' := (A + D(Rf))(x)x' = f(x)$ with $(Rf)(x(0)) = 0$ (3) produce a non-singular matrix $\hat{A}_k(x)$ and therefore an explicit ODE, and that each step reduces the index by 1, too.

HÄNSCH W.

Physical Models for MOSFET Modelling

In the presentation we treat the problem of how to find physical models which are suitable for device (MOSFET) simulation. We will discuss the validity of the chemical semiconductor equations and their possible extension. The modelling of the channel mobility of a MOSFET will be discussed including the quantum - mechanical corrections due to the Si/SiO_2 interface. We will give an evaluation of Monte Carlo methods, especially in the context of the recently discussed approach, which is a hybridization scheme combining MC and PDE methods. Finally we will give a rigorous treatment on how to model the high energy tail of the particle distribution function in an arbitrary field configuration. This will be important for the calculation of the substrate current and the gate oxide injection.

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JEROME J.

Algorithmic Aspects of the Drift-Diffusion and Hydrodynamic Semiconductor Models

KERKHOVEN T.

The One Dimensional Current Driven Semiconductor Equations

We examine the steady state semiconductor equations in one dimension subject to conditions which specify the current through the device supplemented by Dirichlet boundary conditions on one end of the device. We identify solutions to this current driven problem as the fixed points of a mapping T and show uniqueness of solutions for the unipolar problem by demonstrating that T is unconditionally a contraction. Hence we obtain an algorithm for the solution of this problem which is unconditionally convergent to the unique solution if it exists. For both the uni- and the bipolar problem we show existence of solutions close to thermodynamic equilibrium. Thus for the one dimensional unipolar current driven problem the situation is complementary to that for the potential driven problem where it is possible to show existence of solution for arbitrary applied potentials and uniqueness close to thermodynamic equilibrium only. This coincides with physical notions about characteristics of e.g. diodes. From these results we conclude that for the unipolar one dimensional problem the characteristics have to be relatively simple and that no bifurcations can occur.

KIEHL M.

Increasing the Vectorlength for Matrixmultiplication on a Vectorcomputer

The multiplication of two $n \times n$ matrices is of complexity n^3 and is generally done by using 3 nested loops with looplength n at the innermost level.

Here a new storage technique is introduced which allows looplength n^2. This can be essential for optimal performance on a supercomputer.

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MÄRZ R.

Analysis and numerical treatment of differential-algebraic systems

A special concept of canonical subspaces and projectors is proposed for differential-algebraic equations $f(x'(t),x(t),t) = 0$. this concept turns out to become an useful tool for investigating the structure and functional-analytical properties of a large class of equations. In particular, the special nonlinear index 2 and index 3 semi-explicit systems discussed by Brenan, Engquist, Leimkuhler, Gear, Gupta, Petzold and Lötstedt are covered. The proposed subspace/projector technique aims for a (theoretical) decoupling of the different solution components, but it is approved to be very helpful when analyzing the behaviour e.g. of integration methods applied to differential-algebraic equations. In particular, precise informative stability/instability inequalities are derived for the BDF's. Further, convergence results of certain regularizations are obtained via that technique by Hanke, Neubauer and the author.

MERTEN K.

Circuit Simulation in the Semiconductor Industry - State of the Art, Requirements and Future Development

This presentation gives an overview about typical applications in the IC industry. Due to the actual requirements new solutions are discussed in detail. Our approach with the new simulator TITAN which was developed in the SIEMENS Laboratories of Information Technology is presented as a typical implementation made under industrial constraints such as functionality, stability and performance.

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MILLER J.

Numerical solutions of the semiconductor device equations

The stationary behaviour of a semiconductor device can be described by an elliptic system of three coupled nonlinear second order partial differential equations. This consists of a nonlinear Poisson equation for the electrostatic potential and two nonlinear continuity equations, one for conservation of holes, the other for that of electrons.

We consider here mixed finite element methods for solving these equations. An advantage is that the approximation spaces used in these methods are required to have less regularity that those used in standard finite element methods. We also discuss the approximate evaluation of the integrals arising in this formulation. We show that in one space dimension it is possible to obtain the Scharfetter-Gummel scheme as a special case. This means that mixed finite element methods may be regarded as a generalization of exponentially fitted methods, which are useful for solving singularly perturbed problems.

MITTELMANN H.D.

Solving a class of interface problems in 3 dimensions

Capillary surfaces with prescribed volume are determined numerically. The obstacles that confine the given amount of liquid may be planes in space arbitrarily chosen. Parameters of the problem are the Bond number, the contact angle, and the volume. A finite element method is used to approximate the interface and continuation is applied to obtain solutions for given parameter values. A series of examples in different geometries illustrate the power and generality of the proposed algorithm.

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PIETRA P.

Mixed exponential fitting schemes for the current continuity equation

We introduce a class of methods which generalize the Scharfetter-Gummel scheme to 2-D problems for the current continuity equation $\mathrm{div}(\nabla p + p\nabla\psi) - \nu p = R$. The basic idea is the following:

i) write the equation in the form $\mathrm{div}\,(e^{-\Psi}\nabla\varrho) - \nu e^{-\Psi}\varrho = R$ through the change of variable $p = e^{-\Psi}\varrho$;
ii) discretize the asymmetric equation via low order mixed finite element schemes;
iii) go back to p via some discrete version of the transformation $p = e^{-\Psi}\varrho$ and solve for p. If you make the proper choices of mixed finite element spaces, an M-Matrix is produced.

POLAK S.J.

Device modeling Magnetic field simulation

Device modeling is governed by three equations, all three of the form $\nabla\cdot\alpha_i(u)\nabla u_i = f_i(u)$ $i = 1,2,3$, where u is the vector (u_1,u_2,u_3) of unknown functions. The requirements for two of the three equations, the so called continuity equations, posed by the device physics are such that (current conservation) almost all practical applications are using a so called box method which is an extension of a method for a 1-dimensional, homogeneous singularly perturbed problem (see [1]). However, this is a very unflexible method with only limited mathematical basis. Recently [2] shows that a mixed FEM is an extension or rather includes the 1-D scheme and satisfies the usual other requirements. However, the paper only analyses the situation where $f_i(u) = 0$. This is essentially unrealistic. Moreover $f_i(u) \neq 0$ gives essential problems. This talk will discuss a solution for those problems. The solution boils down to lumping the mass matrices involved. However this is not as straight forward as for conforming FEM. There are also some problems to be solved still at the time this summary is written.

[1] S.J. Polak, C. den Heijer, W.H.A. Schilders, P.A. Markowich: Semiconductor device modeling from the numerical point of view, Int.J.Num. Meth. Engng., vol. 24, pp. 763-838 (1987)

[2] F. Brezzi, L.D. Marini, P. Pietra: Two-dimensional exponential fitting and application to semiconductor device equations (to appear)

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RANK E.

Local oxidation of silicon - a finite element approach

Local oxidation of silicon is an important step in processing highly integrated semiconductor devices. Oxygen diffuses through a layer of silicon-dioxid to the interface with pure silicon below the dioxid. There the oxygen reacts with silicon to new dioxid which has more than twice the volume of the original silicon. Thus silicon is consumed away and the dioxid layer is lifted up.

In the standard finite element approach for simulation of this local oxidation the interface is modelled as a sharp line, making it necessary to remesh the dioxid-range after each time step. The new method presented in this paper models the interface as a smooth transition zone and the dioxid is characterized by a density function over the domain of computation. Thus it is possible to solve on a topologically invariant finite element mesh in a time stepping procedure a coupled system of equations for the oxygen diffusion, the chemical reaction and the structural displacement. Several numerical examples show the advantages of the new approach.

RENTROP P.

ROW-Type Methods for the Integration of Electric Circuits

Two examples for a nodal analysis of electric circuits are presented. The mathematical model leads to linearly implicit initial value problems of ordinary differential equations:

$$C\,U'(t) = F(U,t), \quad U(t_0) = U_0$$

U: n-vector, C: singular (n×n)-matrix.

Three problems in the numerical simulation of the circuits are discussed:

i) Which modifications of standard stiff ROW-solvers - assuming C to be a regular matrix - are necessary?

ii) What are consistent initial values?

iii) How to implement an Index-Monitor?

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RINGHOFER CH.

Simulation of Quantum Transport in Solid State Semiconductors

Simulations via the Basic Semiconductor Equations, or even the Boltzmann Equation, do not adequatly describe the transport picture in devices, such as HEMT transistors or very small tunneling diodes, since they neglect quantum mechanical effects. These effects occur in narrow channels close to pinch-off and in ultra submicron devices. In this talk the analytical and numerical treatment of a model describing quantum transport in solid state semiconductors is discussed. The governing equation is a nonlocal pseudo differential equation and is derived from the Liouville equation of quantum mechanics. It describes the time evolution of the Wigner distribution function. A highly parallelizable spectral collocation technique for the solution of the Wigner equation is presented and a stability and convergence analysis is given. It is discussed to what extent the solutions can be regarded as quantum mechanical corrections to the ones obtained from the classical Boltzmann- or Vlasov equation.

ROSE D.

Convergence of Nested Iterative Methods for Linear Systems

SAWATZKI R.

Influence of the Device Size on the Convergence of the Gummel Algorithm

SEIDMAN T.

An Algorithmic Velocity Approach to Device Modelling

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SCHULTZ R.

Local Timestep Control for Simulating Electrical Circuits

For circuit simulation in the time domain the classical direct integration algorithm using Backward Differentiation Formulas, Newton-Raphson procedure and sparse Gaussian linear solver has proved to be accurate and efficient. By introducing local timestep control, circuit latency is exploited and computational expense is saved. Local timesteps mean that for every part of the circuit an adequate integration stepsize is chosen. Electrical interdependencies between circuit parts having different integration stepsizes are fully taken into account by defining an extrapolation mode for latent circuit parts. Applications are given, demonstrating that the algorithm works well and is able to achieve computational savings without loss of universality, accuracy and reliability.

STEGER K.

Corner Singularities of Solutions of the Potential Equation in Three Dimensions

Solutions of elliptic boundary value problems have singularities at irregular boundary points. Some higher order derivatives are not L_2 - integrable. Numerical approximations of these problems are affected by these singularities unless they are taken into account by e.g. local grid refinement.

In two dimensions the singularity of the solution depends essentially on the inner angle at the corner point. In three dimensions the critical parameter to describe the singularity at a corner point is given by the smallest eigenvalue of the Laplace-Beltrami-Operator defined on a region of the two-dimensional sphere. A FE-method is presented to estimate this parameter. It will be demonstrated that this method is efficient enough to be included in a grid generation program.

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ZHENG Q.

Einige systemtheoretische Bemerkungen zu Algebro-Differentialgleichungen

Zur Analyse asymptotischen Verhaltens eines elektrischen Netzwerkes sind die systemtheoretischen Aussagen für die Lösungen der Algebro-Differentialgleichungen von Bedeutung. Im Vergleich zum breiten Spektrum der numerischen Verfahren zur Lösung der Algebro-Differentialgleichungen ruhen Aktivitäten in diesem Bereich.

Der Autor zeigt, daß einige wichtige Ergebnisse beim dynamischen System, z.B. der fundamentale Satz von Hopf, auf die Algebro-Differentialgleichungen verallgemeinert werden können. Die Bedeutung solcher Verallgemeinerungen werden an konkreten Beispielen veranschaulicht.

ZIMMERMANN H.G.

Homotopy Methods in Circuit Analysis

In dc-analysis of electrical circuits, one is interested in stationary solutions. Today circuits with 5000 and more elements are of interest. This leads to nonlinear algebraic systems of similar dimensions. Normally this is solved by an iteration method or by pseudo-transient analysis. The described homotopy method can be interpreted as a generalization of both. It should be more reliable than the first and faster than the second algorithm. It is based on a predictor / corrector technique, includes a handling of turning points and bifurcations such that it is well suited for circuits with very high gain and branching. Finally a special imbedding is discussed, which is physically interpretable and takes sparsity of electrical circuits into account.

Berichterstatter : P. Rentrop

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