

ARCHIEF

# CONFERENTIE VAN NUMERIEK WISKUNDIGEN

*30 september — 2 oktober 1985*

CONFERENTIEOORD WOUDSCHOTEN  
ZEIST



Werkgemeenschap Numerieke Wiskunde

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## TIENDE CONFERENTIE NUMERIEKE WISKUNDE

### Doel van de conferentie

De Conferentie Numerieke Wiskunde wordt eenmaal per jaar gehouden onder auspiciën van de Werkgemeenschap Numerieke Wiskunde. Het doel van de conferentie is om kennis te nemen van recente ontwikkelingen binnen de numerieke wiskunde. Hiertoe worden jaarlijks twee thema's vastgesteld. Lezingen over deze thema's worden normaliter verzorgd door uitgenodigde buitenlandse en binnenlandse deskundigen.

### Thema's

1. *Numerieke methoden voor halfgeleiderproblemen.*
2. *Meerdimensionale approximatie en ijle kleinste-kwadratentechnieken.*

### Organisatie

De organisatie is in handen van de voorbereidingscommissie bestaande uit de heren van Veldhuizen (VU) (voorzitter), Boerstool (NLR), Traas (THT) en Verwer (CWI) (secretaris), en van het Centrum voor Wiskunde en Informatica.

Thema 1. W. Fichtner, ETH Zürich (voorheen AT & T Bell. Labs., Murray Hill)  
P. Markowich, TU-Wien  
G. de Mey, Rijksuniversiteit Gent  
S. Polak, Philips, Eindhoven

Thema 2. W. Dahmen, Universität Bielefeld  
B.N. Parlett, University of California, Berkeley  
Ph.L. Toint, Université de Namur

Een korte voordracht zal worden gegeven door R.H.J. Gmelig Meyling, P. de Groen, C. den Heyer  
en S. Polak, J. ter Maten & W. Schilders.

## Programma

### *Maandag 30 september*

9.45-10.40	aankomst, koffie	15.15-15.45	thee
10.40-11.45	opening, Parlett	15.45-16.15	Gmelig Meyling
11.45-12.45	Polak	16.15-17.15	Fichtner
12.45	lunch	18.00	diner
14.15-15.15	Dahmen		

### *Dinsdag 1 oktober*

8.00- 9.00	ontbijt	12.45	lunch
9.00-10.00	Toint	14.15-15.15	Fichtner
10.00-10.30	koffie	15.15-15.45	thee
10.30-11.30	Markowich	15.45-16.15	de Groen
11.30-12.30	de Mey	16.15-17.15	Parlett

### *Woensdag 2 oktober*

8.00- 9.00	ontbijt	12.45	lunch
9.00-10.00	Dahmen	13.45-14.45	Markowich
10.00-10.30	koffie	14.45-15.45	de Mey & Cuypers
10.30-11.00	Polak, ter Maten, Schilders	15.45	sluiting, thee, vertrek
11.00-11.30	den Heyer		
11.30-12.30	Toint		

De bar is geopend van 17.00-18.00 uur en van 20.30-24.00 uur.

**Maandag 30 september**

10.45	opening B.N. Parlett	<i>Matrix Functions and their Computation.</i>
11.45	S. Polak	<i>The Equations and Unknowns in Semiconductor Device Analysis</i>
14.15	W. Dahmen	<i>Approximation by Polyhedral Splines</i>
15.45	R.H.J. Gmelig Meyling	<i>On the Use of Bivariate B-Splines in Least Squares Approximation Problems</i>
16.15	W. Fichtner	<i>Numerical Methods for Semiconductor Device Simulation</i>

**Dinsdag 1 oktober**

9.00	Ph.L. Toint	<i>Solution of Large Scale Linear Least Squares Problem in Geodetic Doppler Positioning</i>
10.30	P. Markowich	
11.30	G. de Mey	<i>Possibilities of the Boundary Element Method for Semiconductor Device Modelling</i>
14.15	W. Fichtner	<i>Numerical Methods for Semiconductor Device Simulation</i>
15.45	P. de Groen	<i>Fitting Data by Sums of Exponentials</i>
16.15	B.N. Parlett	<i>Recent Developments in the Computation of <math>\exp(Bt)</math></i>

**Woensdag 2 oktober**

9.00	W. Dahmen	<i>Subdivision Techniques for the Generation and Interrogation of Spline Surfaces</i>
10.30	S. Polak, J. ter Maten & W. Schilders	<i>The Discretization of the Semiconductor Equations</i>
11.00	C. den Heijer	<i>Preconditioned Iterative Methods for Nonsymmetric Linear Problems that Occur when Solving the Coupled Semiconductor Equations</i>
11.30	Ph.L. Toint	<i>Solution of Large Nonlinear Least Squares Problems Using the Concept of Partial Separability</i>

13.45 P. Markowich

14.45 G. de Mey & F. Cuypers

*ALDEP: a 2-D Boundary Element Method  
Analysis of Semiconductor Components Using  
the Abrupt Depletion Approximation*

Abstract: We review some recent developments in the theory of multivariate splines centering upon the notion of so-called polyhedral splines. In analogy to Schoenberg's geometric interpretation of univariate B-splines  $n$ -dimensional polytopes are used to generate  $s$ -variate smooth piecewise polynomials of degree  $n-s$  which in particular have compact support. Such generalized B-splines can be employed as basis functions for interpolation, least squares fits or finite element approximations. In this context, the central issues are the numerical evaluation of such splines, the construction of stable bases and to determine the approximation rates of linear combinations of polyhedral splines. It turns out that different choices of the underlying polytopes require to develop tools from quite different mathematical fields such as combinatorial topology or Fourier analysis.

SUBDIVISION TECHNIQUES FOR THE GENERATION AND INTERROGATION OF SPLINE SURFACES

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Abstract

So called subdivision algorithms serve as powerful tools for interrogation and definition of surfaces in the context of Computer Aided Geometric Design. When dealing e.g. with surface representations in terms of Bernstein Polynomials B-splines or box splines the objective of such techniques is to convert a given polynomial or spline expansion into one with respect to a "refined" basis. If the basis functions are nonnegative and form a partition of unity the new coefficients in the refined expansion (forming the refined control net) are convex combinations of the original ones. The potential merit of such techniques with regard to the above mentioned applications relies on the following facts: The generation of the refined control nets is typically computationally more efficient than usual point evaluations. The refined control nets converge to the underlying surface.

We discuss the complexity and convergence properties of subdivision algorithms for a general setting of multivariate splines and piecewise polynomials. In particular, the typical and in general best possible rate of convergence turns out to be quadratic.

# Numerical Methods for Semiconductor Device Simulation

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At AT&T Bell Laboratories, we have developed a program package called DEVICE (**D**evice **E**ngineering for **V**LSI **C**ircuit **E**lements). DEVICE allows the steady-state and transient solution of the basic semiconductor equations on arbitrarily shaped twodimensional regions. External circuit elements can be included in the simulations. Typical applications range from the analysis of submicron MOSFET structures to high voltage bipolar devices and complex parasitic coupled elements in VLSI CMOS. In the development of the program, we have experimented with different approaches to the numerical equation solution ranging from various nonlinear iteration strategies, different sets of variables to a variety of linear equation solution schemes.

In the first talk, I shall concentrate on the numerical methods used inside DEVICE for robustness and speed. Among the topics treated are grid generation for nonplanar structures, nonlinear iteration strategies, solution of large sparse linear systems, and temporal discretization.

In the second talk, I shall illustrate the performance of the algorithms with a series of examples. In addition, I shall present a computer-generated color movie on the switching behavior of semiconductor devices.

# ON THE USE OF BIVARIATE B-SPLINES IN LEAST SQUARES APPROXIMATION PROBLEMS

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In this talk we consider the space of  $C^1$ -smooth quadratic B-splines [1] defined by certain knot sets in the plane. We discuss some problems related to the construction of suitable knot set configurations [2] and the computation of linear combinations of B-splines by certain recurrence relations. We study least squares approximation of a given function on some polygonal domain to illustrate the practical use of these B-splines.

## References:

- [1] Dahmen, W., Micchelli, C.A., *Multivariate splines - a new constructive approach*, in *Surfaces in Computer Aided Geometric Design*, ed. R.E. Barnhill & W. Böhm, North-Holland, Amsterdam, 1983, 191-215.
- [2] Gmelig Meyling, R.H.J., *An algorithm for constructing configurations of knots for bivariate B-splines*, Report 85-06, University of Amsterdam, 1985.

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An important problem in (among others) chemistry and biology is the fit of a weighted sum of exponentials

$$f(t) := \sum_{i=0}^n c_i \exp(\alpha_i t)$$

with unknown  $c_i$  and  $\alpha_i$  to a given set of  $m \geq 2n$  data pairs

$$\{(t_j, y_j) \mid j = 1 \dots m\}.$$

Several times I have been asked by people working in those domains for a good algorithm to do this job.

Among numerical analysts the problem generally is recognized as a hard and badly conditioned problem, cf [1].

The landscape of the object function

$$\sum_{j=1}^n (f(t_j) - y_j)^2,$$

for which a minimum has to be found, contains very flat valleys and very steep slopes; moreover, each iterative minimization procedure has to face the problem that the interchange of pairs of unknown  $(c_i, \alpha_i)$  does not change the object function. However, for the case where the data are sampled at equidistant times ( $t_j = t_0 + jh$ ,  $j = 1 \dots m$ ), a simple and very elegant algorithm has been published recently, cf [2]. In that case the data can be considered as the outputs of a linear  $n$ -dimensional system, which can be ‘realized’ quite easily. We shall show that this yields an approximation which is near to the least squares minimum.

**References:**

- [1] J.M. Varah, *On fitting exponentials by nonlinear least squares*, SIAM J. Scientific & Statistical Comp. **6** (1985) pp. 30-44.
  
- [2] B. de Moor & J. Vandewalle, *A numerically reliable algorithm for fitting a sum of exponentials or sinusoids to noisy data*, to appear in the Proceedings of the 3rd IFAC/IFIP Internat. Symposium on Computer Aided Design in Control and Engineering Systems, Copenhagen, 1985

PRECONDITIONED ITERATIVE METHODS FOR NONSYMMETRIC LINEAR PROBLEMS THAT  
OCCUR WHEN SOLVING THE COUPLED SEMICONDUCTOR EQUATIONS

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In this paper we consider a class of iterative methods (projection methods) for the solution of linear equations. This class contains among others Conjugate Gradients, Bi-Conjugate Gradients and Orthomin. It appears that a variant of Bi-Conjugate Gradients (CG-squared), when used with a so-called "incomplete line block factorization" as preconditioning, is a robust and efficient method for the solution of the nonsymmetric linear systems arising in the numerical solution methods for the coupled semiconductor equations.

POSSIBILITIES OF THE BOUNDARY ELEMENT METHOD FOR SEMICONDUCTOR DEVICE  
MODELLING

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Until now the solution of the fundamental non linear equations of semiconductor devices has been performed by finite difference and finite element techniques [1]. The boundary element techniques was only used in some particular cases where the equations can be simplified to linear potential equations such as Hall plates [2], pn junctions [3], solar cells [4][5], high voltage transistors [6]. At first sight, the boundary element method seems not to be suited because the equations are extremely non linear due to the exponential function  $\exp(q\phi/kT)$ . The boundary element method can only be applied to a linear operator with a known Green's function. Nevertheless the boundary element method has been introduced by using a suitable iteration procedure in order to handle the non linear terms. One of the main advantages of the boundary integral equation method, i.e. the reduction of the dimension, is lost partially. A 2-D problem is replaced by a 1-D integral equation but still a 2-D numerical integration is required.

The method will firstly be illustrated on the so-called zero current approximation for semiconductor devices. Using this approximation, the current continuity equations can be neglected and only the Poisson's equation has to be solved in a 2-D domain  $S$  with boundary  $C$

concentration,  $N_A$  the substrate doping (assumed p-type). All distances were normalised to the Debye length. Note the numerical values  $q/kT = 40$  and  $\Phi = 1, \dots 5$  Volts so that the exponentials can attain very high values.

In order to construct a boundary integral equation, the Green's function  $G(\bar{r}|\bar{r}') = \frac{1}{2\pi} \ln|\bar{r}-\bar{r}'|$  of the Laplace operator is used :

$$\nabla^2 G(\bar{r}|\bar{r}') = \delta(\bar{r}-\bar{r}') \quad (2)$$

Applying Green's theorem on (1) and (2), one obtains :

$$\begin{aligned} \phi(\bar{r}') = & - \oint_C [G(\bar{r}|\bar{r}') \nabla \phi \cdot \bar{u}_n - \phi(\bar{r}) \nabla G(\bar{r}|\bar{r}') \cdot \bar{u}_n] dC \\ & + \iint_S (-e^{-\phi(\bar{r})} + \frac{n_i}{N_A^2} e^{\phi(\bar{r})} + 1) G(\bar{r}|\bar{r}') dS \end{aligned} \quad (3)$$

The point  $\bar{r}'$  can be placed everywhere inside  $S$  or on the boundary  $C$ . In the latter case some rules should be taken into account to handle singularities. If  $\bar{r}'$  is placed on the boundary  $C$ , (3) is reduced to an integral equation. The unknown function being the potential  $\phi$  or its normal derivative  $\nabla \phi \cdot \bar{u}_n$  depending upon the kind of boundary condition. However, the surface integral in (3) also requires the knowledge of the potential  $\phi$  in the domain  $S$ . Therefore the following iteration technique has been set up. Suppose at a given iteration step  $k$ , approximate  $\phi$ -values are known in  $S$  :  $\phi^k$ . Putting  $\phi^k$  in the surface integral of (3), the linear integral equation can be solved yielding  $\phi$  and  $\nabla \phi \cdot \bar{u}_n$  along the boundary. Using (3) again with  $\bar{r}'$  inside  $S$ , new  $\phi$ -values in  $S$  can be calculated denoted by  $\phi^*$ . Then the following algorithm is used :

$$\phi^{k+1} = \phi^k + \lambda(\phi^* - \phi^k) \quad (4)$$

giving the  $\phi$ -values inside  $S$  at iteration step  $k+1$ .

It was found experimentally that no convergence was obtained for  $\lambda > 0.5$ . For  $\lambda = 0.1$  to  $0.2$  good convergence results were obtained. The

formula (4) can be seen as an underrelaxation method with  $\lambda$  being the relaxation parameter.

The previous described method has been applied to a simple rectangular geometry which offers us the opportunity to compare the numerical results with a 1-D analytical model using the abrupt depletion approximation. A second application involves a MOS transistor working under subthreshold conditions. These results were compared with simulations done with the CADDET program, a simulation tool based on finite difference approximation [8].

The next step in the research is to include a current continuity equation for the minority carriers. Using normalised potential  $\phi$  and normalised quasi Fermi potential  $\phi_n$  for the electrons one has to solve the following equations :

$$\nabla^2 \phi = \frac{n_i}{N_A} e^{\phi - \phi_n} - \frac{n_i}{N_A} e^{\phi - \phi_p} + 1 \quad (5)$$

$$\nabla^2 \phi_n = \nabla(\phi_n - \phi) \cdot \nabla \phi_n \quad (6)$$

where the quasi Fermi level  $\phi_p$  for the holes is assumed constant. A similar iterative boundary element technique was used to solve (5) and (6) numerically. Different relaxation parameters  $\lambda$  and  $\lambda_n$  were used for the Poisson (5) and the continuity equation (6). Some results were obtained but the convergence of the continuity equation was very poor so that new and better iteration techniques have to be found in order to make the BEM usefull for semiconductor device modeling.

2) G. De Mey :

"Potential calculations in Hall plates"

Advances in Electronics and Electron Physics, 1983, vol. 61, p. 1-62.

3) P. Devisschere and G. De Mey :

"Integral equation approach to the abrupt depletion approximation in semiconductor components"

Electronics Letters, 1977, vol. 13, p. 104-106.

4) G. De Mey :

"An integral equation method to calculate the transient behaviour of a photovoltaic solar cell"

Solid State Electronics, 1978, vol. 21, p. 595-596.

5) G. De Mey and P. Devisschere :

"Grid contacts on solar cells"

Nieuw Archief voor Wiskunde, 1983, vol., p. 270-289.

6) G. De Mey, D. Loreet and A. Van Calster :

"Modeling of DMOS transistors"

Colloquium Topics in Applied Numerical Analysis,  
(ed. : J.G. Verwer), CWI Syllabus 4, p. 297-311.

7) G. De Mey

"The boundary element method for modeling semiconductor components under low current approximation"

NASECODE 4 Conference, Dublin, 1985.

8) "CADET - Computer Aided Device Design in two dimensions"

Internal document, Hitachi Central Research Laboratory.

# ALDEP: A 2-D BOUNDARY ELEMENT METHOD ANALYSIS OF SEMICONDUCTOR COMPONENTS USING THE ABRUPT DEPLETION APPROXIMATION

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The basic equations used for semiconductor device modeling are extremely non linear. In some cases such as MOS transistor under subthreshold conditions (i.e. very low drain current) only the Poisson's equation needs to be solved. This (still non linear) equation can be simplified furtheron by using the abrupt depletion approximation. The semiconductor device is then divided into two zones : a neutral and a depleted one. In the neutral zone the charge density is zero. In the depleted zone however, no free charge carriers are available and the charge density is then  $-qN_A$  for a p-type substrate with doping  $N_A$ . One has the following equation for the electric potential  $\Phi$  :

$$\nabla^2 \Phi = \begin{cases} 0 & \text{neutral zone} \\ \frac{qN_A}{\epsilon_0 \epsilon_S} & \text{depleted zone} \end{cases} \quad (1)$$

where  $\epsilon_0 \epsilon_S$  denotes the dielectric constant of the semiconductor.

The main problem is now to determine the boundary between the depleted and the neutral area :  $\partial B$ . If the potential  $\Phi = 0$  at the sub-

but in our case the position of the boundary  $\partial B$  is not a priori fixed which provides us an additional degree of freedom.

An iteration technique has been set up to determine  $\partial B$  iteratively. Using an initial guess  $\partial B$  the equations (1) can be solved using the boundary element method. The potential  $\Phi$  and its normal derivative  $\partial\Phi/\partial n$  along  $\partial B$  can then be calculated. From the (non zero) value of  $\partial\Phi/\partial n$  in a particular point of  $\partial B$  a new position can be calculated by using Gauss theorem. This procedure is repeated until convergence is obtained.

The previous described method has been implemented in a program ALDEP. It has been applied to rough shaped  $\text{Cu}_2\text{S}-\text{CdS}$  solar cells and MOS transistors. From the MOS simulations it was also possible to calculate the subthreshold drain current using a saddle point technique. The results were also compared with CADDET simulations of the same transistor and good agreements were found.

#### References.

1) F. CUYPERS and G. DE MEY :

"Boundary element method for calculation of depletion layer profiles"

Electronics Letters, 1984, vol. 20, p. 229-230.

2) "CADDET - Computer aided device design in two dimensions"

Internal document, Hitachi Central Research Lab.

MATRIX FUNCTIONS AND THEIR COMPUTATIONS

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We introduce  $\exp(Bt)$  and mention a few applications and properties, such as its sensitivity to perturbations.

Ways to compute  $\sqrt{B}$  and  $\log(Bt)$  will be described including recent work of Nick Higham on  $\sqrt{B}$ . Applications of these functions will be mentioned.

Some traditional approaches to the computation of  $\exp(Bt)$  will be reviewed: series, rational approximation, scaling and squaring. Examples of difficulties will be presented.

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The weakness of the Jordan form.

Advantages of the Schur form  $S$ .

Block Diagonalization

A recurrence among the elements

of  $f(S)$

The Newton form of interpolation

Accurate divided differences for  $\exp$

The clustering of eigenvalues

An accurate program.

### References

Bjorck, A. and Hammarling, S. (1983) "A Schur Method for the square root of a matrix," Lin. Alg. Appls. vol 52/53, pp.127-140.

McCurdy, A.; Ng, K.C.; Parlett, B.N. (1984), "Accurate computation of Divided Differences of the Exponential Function," Math. Comp., vol 43, pp.501-528.

Moler, C.B. and Van Loan, C.F. (1978), "Nineteen Dubious Ways to Compute the Exponential of a Matrix," SIAM Review vol 20, pp.801-836.

Parlett, B.N. (1976), "A Recurrence Among the Elements of Functions of Triangular Matrices," Lin. Alg. Appls. vol 14 pp.117-121.

Singer, B. and Spilerman, S. (1976), "The Representation of Social Processes by Markov Models," Amer. J. Sociology, vol 82, pp.1-54.

Wragg, A. and Davies, C. (1973, 1975), "Computation of the Exponential of a Matrix," Part I in JIMA, vol 11, pp.369-375, Part II in JIMA vol 15, pp.273-278.

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In this lecture we discuss the equations and the choice of unknowns used in semiconductor device analysis. Basically there are four equations involved. In the simplest form they are formulated in terms of the four unknown functions

$u$ , electrostatic potential,  
 $p$ , positive carrier density,  
 $n$ , negative carrier density and  
 $T$ , temperature.

The equations are

$$(1) \operatorname{div} \operatorname{grad} u = p - n + d$$

$$(2) \partial n / \partial t = \operatorname{div} (\mu_n n \operatorname{grad} u + D_n \operatorname{grad} n) - R$$

$$(3) \partial p / \partial t = \operatorname{div} (\mu_p p \operatorname{grad} u + D_p \operatorname{grad} p) + R$$

(4) temperature equation, this equation still is rarely solved together with the other equations so we leave it out of the rest of the discussion.

$D = D(x, y, z)$ ,  $R = R(p, n, u)$ ,  $\mu_n = \mu_n(p, n, u)$ ,  $D_n = D_n(p, n, u)$ ,  
 $D_p = D_p(p, n, u)$ .

First we discuss the choice of unknown functions. Basically there is a trade off between nonlinearity and variation of the unknown. We may choose the unknown functions such that the problem is rather linear but then these functions will vary extremely. In fact they may vary so rapidly that, in very thin spatial areas they will be far out of the exponential range of any computer. On the other hand we may choose unknowns that are far less varying but the equations then will be extremely nonlinear.

Most used are four choices of unknowns,

- (A)  $u, p, n$ , as shown above,
- (B)  $u, \phi_p, \phi_n$   
where  $\phi_p = pe^{\alpha u}$ ,  $\phi_n = ne^{-\alpha n}$ .
- (C)  $u, \phi_p, \phi_n$   
where  $\phi_p = (\log \phi_p) / \alpha$ ,  $\phi_n = -(\log \phi_n) / \alpha$
- (D) stream functions

We discuss the different choices and show the accompanying equations. Furthermore there are four levels of simplification to be distinguished,

- (I) zero current, there is only the Poisson equation,
- (II) steady on state, the Poisson and the continuity equations but  $\partial p / \partial t = \partial n / \partial t = 0$ .
- (III) transient on state, the last with non zero time derivatives,
- (IV) temperature included, plus temperature equation.

Of course these models are considered in one, two and three dimensions. We may classify the problems according to the Estimated Computational Feasibility Ratio In Percentages, (ECFRIP), giving the following table.

model				
space dim	I	II	III	IV
1	100	100	50	50
2	100	100	25	0

Some examples of typical spatial configurations will be shown, together with function  $D(x,y,z)$ . Usually the outside boundary is rectangular with Neumann type boundary conditions. However there are interfaces inside the rectangle possible with Dirichlet and Neumann boundary conditions. Some of the unknowns and equations then are only present in part of the problem. The existence and uniqueness problems will be briefly discussed. The model I case, giving a Poisson equation, involves a monotone operator. So then the existence and uniqueness problems are practically solved. In further cases only limited answers to existence and uniqueness problems are known. Mostly they depend upon the nonlinearities of  $\mu_n$ ,  $\mu_p$ ,  $D_n$ ,  $D_p$  and  $R$ . A brief survey of the algorithms we use will be given. The discretisation and the linear algebra problem will be treated separately in short lectures.

THE DISCRETISATION OF THE SEMICONDUCTOR EQUATIONS

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In this lecture we treat the discretisation of the semiconductor equations. As the Poisson equation is monotonic we can use a FEM. The continuity equations are strongly singularly perturbed. This is so because the  $\epsilon, D(x, y, z)$  and the boundary conditions of the Poisson equation cause a locally large  $\text{grad } u$ . The region where this is the case is termed the depletion region. In this region the ~~term~~  $\text{grad } u, \text{grad } n$  and  $\text{grad } u, \text{grad } p$  will be dominant in the continuity equations. In the one dimensional case with constant coefficients and constant (unrealistic)  $\text{grad } u$  this is exactly the convection diffusion equation. It is easy to understand how an exponential fitting scheme will give a stable discretisation in that case. This scheme is termed the Gummel discretisation in semiconductor analysis. However it essentially uses the fact that the solution space for the linear homogeneous case in one dimension is spanned by a constant and one exponential function. In more dimensions this is not the case, so a generalisation is not straightforward. We shall discuss some two dimensional generalisations. On the one hand one may use upwind FEM schemes, on the other hand box schemes are much used in this field. As far as we know a completely satisfactory scheme is not yet known.

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The purpose of the talk is to describe some new algorithms for the numerical solution of large scale linear least squares calculations. The origin of the developments presented is in the Doppler positioning problem in geodesy, where respective positions of ground stations have to be deduced from observations on the Doppler shift of radio waves emitted by artificial satellites. Advantage is taken of the structure of the set of equations to propose solutions methods that cope with very large systems. Both direct and iterative methods are considered, and a comparison made between them with respect to such parameters as CPU time for solution, input/output and storage requirements. Extension of the methodology to more general problems is also discussed.

(The material of this talk is resulting from a joint research with G.H. Golub, P. Mäanneback and Ch. Murigande.)

SOLUTIONS OF LARGE NONLINEAR LEAST SQUARES PROBLEMS USING THE CONCEPT  
OF PARTIAL SEPARABILITY

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The practical numerical procedures for solving nonlinear least squares problems are considered, and extensions based on the concept of partially separable optimization are proposed, to deal with the case where the number of variables is high. The solution of problems involving several hundreds of nonlinear variables is shown to be feasible at a reasonable cost, and numerical experience is reported to support this claim as well as some of the algorithmic choices that have to be made in this context. Model choice and updating is discussed with some detail, and the efficiency of merging procedures examined.

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