

Weierstraß-Institut für Angewandte Analysis und Stochastik

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SCEE Workshop "Scientific Computing in Electrical Engineering"

September 30 - October 2, 1998 Berlin, Germany

Peter Deuflhard,¹ Herbert Gajewski,² Georg Hebermehl,² Wolfgang Heinrich,³ Arnulf Kost,⁴ Ulrich Langer,⁵ Thomas Weiland⁶ (eds.)

submitted: 24 August 1998

- ¹ Konrad-Zuse-Zentrum für Informationstechnik Berlin
- Weierstraß-Institut für Angewandte Analysis und Stochastik
- Ferdinand-Braun-Institut für Höchstfrequenztechnik

- ⁴ Brandenburgische Technische Universität Cottbus
- Johannes-Kepler-Universität Linz
- Institut für Hochfrequenztechnik der TU Darmstadt

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Co-Sponsor: German Chapter of the IEEE Microwave Theory and Techniques Society.

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SCEE

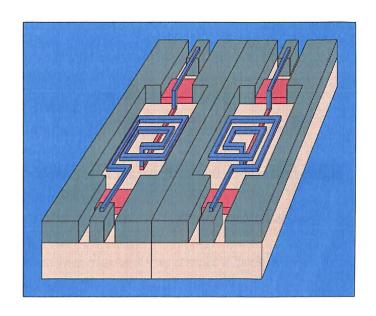
Workshop Scientific Computing in Electrical Engineering

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German Chapter of the IEEE Microwave Theory and Techniques Society

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1 Programme

The workshop will bring together mathematicians, computer scientists, and engineers from research institutes, universities, and industry who work on modeling and numerical simulation on the field of electromagnetics and electronics.

- Microwave Circuits (No. 1)
- Integrated Optics (No. 2)
- Optoelectronical Devices (No. 3)
- Electromagnetic Compatibility (No. 4)
- Quasistatic Magnetics (No. 5)

The programme of the workshop will consist of

- invited lectures and
- contributed presentations in lecture and poster format

Scientific Committee:

Peter Deuflhard

Konrad-Zuse-Zentrum für Informationstechnik Berlin

Herbert Gajewski

Weierstrass Institute for Applied Analysis and Stochastics

Wolfgang Heinrich

Ferdinand-Braun-Institut für Höchstfrequenztechnik

Arnulf Kost

Brandenburgische Technische Universität Cottbus

Ulrich Langer

Johannes Kepler Universität Linz

Thomas Weiland

Institut für Hochfrequenztechnik der TU Darmstadt

Local Organizing Committee:

Georg Hebermehl

Weierstrass Institute for Applied Analysis and Stochastics

Wolfgang Heinrich Ferdinand-Braun-Institut für Höchstfrequenztechnik

Time for presentation, including discussion:

Contributed Presentations 30 minutes Invited Lectures 45 minutes

Wednesday, September 30, 1998

from 10.00	Registration						
13.00-13.15	Opening						
13.15-14.00	Hans-Christoph Kaiser, Herbert Gajewski						
	Weierstrass Institute for Applied Analysis and Stochastics,						
	Berlin, Germany						
3	$Transversal\ modelling\ of\ semiconductor\ lasers\ with\ ToSCA$						
14.00-14.30	Carl M. Weinert, C. Caspar, HM. Foisel, B. Strebel, L.						
	Molle						
	Heinrich-Hertz-Institut für Nachrichtentechnik Berlin						
	GmbH, Germany						
3	Numerical simulation of optical transmitters and optoelec-						
	tronic transponders in optical networks						
14.30-15.00	Uwe Bandelow, Hans-Christoph Kaiser, Hans-Jürgen						
	Wünsche						
	Weierstrass Institute for Applied Analysis and Stochastics,						
	Berlin, Germany						
	Institut für Physik der Humboldt-Universität zu Berlin,						
	Germany						
3	Energy Calculations for Localized Multiparticle Stats in						
	Quantum Wells						

15.00-15.30	Jan Sieber, Mindaugas Radziunas						
	Weierstrass Institute for Applied Analysis and Stochastics,						
	Berlin, Germany						
3	Numerical Simulation of Self Pulsating Semiconductor						
	Lasers						
15.30-16.15	Frank Schmidt						
	Konrad-Zuse-Zentrum für Informationstechnik Berlin,						
	Germany						
2	Transparent Boundary Conditions for the Numerical Solu-						
	tion of Scattering Problems in Integrated Optics						
16.15-16.45	Break						
10.10	Dicar						
16.45-17.30	Reinhard März						
	Reinhard März						
16.45-17.30	Reinhard März Siemens AG, Corporate Technology, Munich, Germany						
16.45–17.30 2	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics						
16.45–17.30 2	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics Matthias Ehrhardt, Anton Arnold						
16.45-17.30 2 17.30-18.00	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics Matthias Ehrhardt, Anton Arnold Technische Universität Berlin, Germany						
16.45-17.30 2 17.30-18.00	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics Matthias Ehrhardt, Anton Arnold Technische Universität Berlin, Germany Discrete Transparent Boundary Conditions for General						
16.45-17.30 2 17.30-18.00 2	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics Matthias Ehrhardt, Anton Arnold Technische Universität Berlin, Germany Discrete Transparent Boundary Conditions for General Schrödinger-Type Equations						
16.45-17.30 2 17.30-18.00 2	Reinhard März Siemens AG, Corporate Technology, Munich, Germany Design and Modeling for Integrated Optics Matthias Ehrhardt, Anton Arnold Technische Universität Berlin, Germany Discrete Transparent Boundary Conditions for General Schrödinger-Type Equations Gunther Schmidt						

Thursday, October 01, 1998

08.30-09.15	Peter Rentrop, Michael Günther, Markus Hoschek					
	TU Darmstadt, Fachbereich Mathematik, Germany					
1	Differential-Algebraic Equations in Electric Circuit Simu-					
	lation					
09.15-09.45	Daniel N. E. Skoogh					
	Department of Mathematics, Chalmers University of Tech-					
	nology, Sweden					
1	Model Reduction by the Rational Krylov Method					
09.45-10.15	Alain Bossavit					
	Electricité de France, France					
1	Revisiting Spurious Modes					
10.15-10.45	Break					
10.45-11.30	Wolfgang Heinrich					
	Ferdinand-Braun-Institut für Höchstfrequenztechnik					
	(FBH), Berlin, Germany					
1	The Finite-Difference Method in Frequency Domain - An					
	Indispensable Tool for the Electromagnetic Analysis of Mi-					
	crowave Integrated Circuits and Multi-Chip Modules					
11.30-12.00	Georg Hebermehl, Rainer Schlundt, Horst Zscheile,					
	Wolfgang Heinrich					
	Weierstrass Institute for Applied Analysis and Stochastics,					
	Berlin, Germany					
	Ferdinand-Braun-Institut für Höchstfrequenztechnik,					
	Berlin, Germany					
1	Computation of Eigen Modes for Transmission Lines					
12.00-12.30	Thomas Schnelle, Torsten Müller, Günter Fuhr					
	Humboldt University, Dept. Biology, Germany					
4	High frequency electric fields in microstructures - simula-					
	tion and biological applications					
12.30-14.00	Lunch-break					
14.00-14.45	Thomas Weiland					
	TU Darmstadt, FB18, FG TEMF, Germany					
4	Maxwell's Grid Equations as Basis for EMC Computations					
	in Time and Frequency Domain					

14.45-15.30	Gerhard K. M. Wachutka						
14.45-15.50	Institute for Physics of Electrotechnology, Munich Univer-						
	sity of Technology, Germany						
4							
4	Numerical Analysis of Distributed Inductive Parasitics in						
	High Power Bus Bars						
15.30-16.45	Poster session & Break						
	Henning Glasser, Thomas Schnelle, Günter Fuhr						
	Humboldt University, Dept. Biology, Germany						
4	THE TOLERANCE OF ADHERENTLY GROWING						
	CELLS TO PERMANENT HIGH FREQUENCY ELEC-						
	TRICAL FIELDS						
	Wolfgang Hackbusch, Steffen Börm						
	Universität Kiel, Germany						
4	Computation of axisymmetric Eigenmodes of Maxwell's						
	Equation						
	Arnim Nethe						
	Brandenburgische Technische Universität Cottbus,						
	Lehrstuhl Theoretische Elektrotechnik, Germany						
5	Simulation of the electromagnetic field of an induction						
	hardening set-up						
	Michael Schinnerl						
	Johannes Kepler University Linz, Austria						
5	Multigrid Methods for Coupled Nonlinear Magneto-						
	Mechanical Problems						
1	Rainer Schlundt, Georg Hebermehl, Horst Zscheile,						
	Wolfgang Heinrich						
	Weierstrass Institute for Applied Analysis and Stochastics,						
	Berlin, Germany						
	Ferdinand-Braun-Institut für Höchstfrequenztechnik,						
	Berlin, Germany						
1	On the Computation of Systems of Linear Algebraic Equa-						
	tions for Monolithic Microwave Integrated Circuits						

	Manfred Uhle, Dietmar Hömberg, Jürgen Fuhrmann Weierstrass Institute for Applied Analysis and Stochastics,					
	Berlin, Germany					
5	Numerical simulation of induction hardening of steel					
16.45-17.30	Arnulf Kost					
	Brandenburgische Technische Universität Cottbus, Ger-					
	many					
4	Electromagnetic Field Computation for Linear and Nonlin-					
	ear Shielding by Thin Magnetic Layers in EMC					
17.30-18.00	Markus Clemens, Thomas Weiland					
	TU Darmstadt, FB18, FG TEMF, Germany					
5	Numerical Calculation of Slowly Varying Electromagnetic					
	Fields Using the Finite Integration Technique					
from 20.00	Welcome Party					

Friday, October 02, 1998

08.30-09.15	Roland H. W. Hoppe					
00.00 00.10	Institute of Mathematics, University of Augsburg, Ger-					
	, , , ,					
5	many Numerical Solution for Interior and Enterior Demain					
5	Numerical Solution for Interior and Exterior Domain					
20 15 20 15	Problems in Electromagnetic Field Computation					
09.15-09.45	Ralf Hiptmair					
	Institute of Mathematics, University of Augsburg, Ger-					
	many					
5	Multigrid Method for Eddy Current Problems					
09.45-10.15	Andrea Toselli					
	Courant Institute, New York University, USA					
5	OVERLAPPING SCHWARZ METHODS FOR					
	MAXWELL'S EQUATIONS IN CONDUCTIVE MEDIA					
10.15-10.45	Break					
10.45-11.30	Oszkar Biro					
13013	IGTE, Technical University of Graz, Austria					
5	EDGE FINITE ELEMENTS IN SOLVING EDDY CU					
	RENT PROBLEMS					
11.30-12.15	Kay Hameyer					
11.00 12.10	Katholieke Universiteit Leuven, E.E. Dept., Div.					
	ESAT/ELEN, Leuven, Belgium					
5	Computation of quasi-static electromagnetic fields					
12.15-12.45	Michal Křížek, Liping Liu					
12.10 12.40	Mathematical Institute, Academy of Sciences, Czech Re-					
	public Czech ite-					
5	1 -					
l a	Finite element approximation of nonlinear temperature and					
	1					
	magnetic fields in electrical devices					
12.45-13.15	magnetic fields in electrical devices Michael Kuhn					
12.45-13.15	magnetic fields in electrical devices Michael Kuhn Johannes Kepler University Linz, Austria					
	magnetic fields in electrical devices Michael Kuhn					

2 Invited Lectures

EDGE FINITE ELEMENTS IN SOLVING EDDY CURRENT PROBLEMS

Oszkar Biro

IGTE, Technical University of Graz, Austria

The aim of this paper is to review several possible formulations of eddy current problems in terms of scalar and vector potentials with the vector potentials approximated by edge finite elements and the scalar potentials by nodal ones. The formulations are ungauged, leading in most cases to singular finite element equations systems. Special attention is paid to ensuring that the right hand sides of the equations are consistent. If this is the case, the numerical stability of the formulations turns out to be comparable to that of the corresponding Coulomb gauged approaches realized by nodal elements. An eddy current problem arises if a time varying magnetic field is excited within a body made of conducting material. The displacement current density is assumed to be negligible, i.e. the differential equations of quasi-static fields hold. This leads to a static but time varying magnetic field in the nonconducting regions surrounding the eddy current carrying conductors. These constitute the conducting region with an eddy current field present and hence the current density distribution unknown.

The vector potentials are approximated by as many edge basis functions as there are edges in the finite element mesh and the scalar potentials by as many nodal basis functions as there are nodes therein. Both the edge and nodal basis functions are linearly independent, but there are linear interdependencies among the gradients of the nodal basis functions and among the curls of the edge basis functions. The number of linearly independent gradients of the nodal basis functions is one less than the number of nodes, i.e. it equals the number of tree edges in the graph defined by the finite element mesh. The number of linearly independent curls of the edge basis functions is the number of cotree edges in this graph.

There are two ways to describe the static magnetic field in the nonconducting eddy current free region: either by a magnetic scalar potential or by a magnetic vector potential. Two vector potential functions can be used to describe the eddy current field in the conducting region: either a magnetic vector potential or a current vector potential. The magnetic vector potential

can be employed with or without an electric scalar potential, whereas the current vector potential description must be augmented by a magnetic scalar potential.

The various formulations in the conducting and nonconducting regions can be coupled by satisfying the continuity of the tangential component of the magnetic field intensity and of the normal component of the magnetic flux density on the interface between the two domains. Basically all potential pairs in the eddy current region can be used simultaneously either with a magnetic vector or a magnetic scalar potential in the nonconducting domain. Further possibilities arise through the use of the magnetic vector potential in one part of the nonconducting region and of the magnetic scalar potential in another part. This is necessary if the exclusive use of the scalar potential in the nonconducting region is prevented by the multiply connectedness of the eddy current region but it is not desired to use the vector potential everywhere in the nonconducting domain.

All of the above formulations are presented in the paper and they are illustrated by some three-dimensional examples.

Computation of quasi-static electromagnetic fields

Kay Hameyer Katholieke Universiteit Leuven, E.E. Dept., Div. ESAT/ELEN Kardinaal Mercierlaan 94, B-3001 Leuven, Belgium

Abstract— Static electromagnetic fields can be described by partial differential equations of the POISSON type and in the slow time-varying case, the quasi-static field problem, by the diffusion equation. The most common and standard method to solve this type of equations is the finite element method (FEM). Various physical effects, such as ferromagnetic saturation and hysteresis, eddy currents and motional effects can be considered with this method. Looking at the basic equations, typical engineering problems are discussed here, including aspects with respect to coupled quasi-static problems.

INTRODUCTION

Most of the physical issues in electrical energy engineering can be described by quasi-static phenomena. Slow varying and periodic fields up to 10kHz are considered to be quasi-static. Electrical energy devices such as electrical motors and actuators, induction furnaces and high-voltage transmission lines are operated by low frequency. Exceptions are micro wave devices for electro-heat applications, where inherently the displacement current is not negligible.

QUASI STATIC FIELDS

Typical examples of quasi-static electromagnetic fields are the fields excited by coils in rotating electrical machines, in transformers and inductors. Inside these conductors the displacement current is negligible and the magnetic field **H** outside the coil is exclusively excited by the free current current density **J**. For those quasi-static fields, the AMPERE's law is applicable [1].

$$\nabla \times \mathbf{H} = \mathbf{J} \tag{1}$$

To decide whether the displacement current can be neglected or not, is depending on the wave length λ of the problem considered in the frequency domain. If it is large, when compared with physical dimensions of the problem l, the displacement current is negligible. To consider this phenomenon in the time domain, the rise time T_a of a step function must be large inside the problem compared to the run time l/ν . Field problems are quasi-static if eqs.(2) are true.

$$T_a >> l / \nu$$

$$\lambda >> l$$
(2)

Mainly $T_a \approx 5...10l/v$ respectively $\lambda \approx 5...10l$ is sufficient.

For this class of problem, the interesting fields are slow varying and can be of periodic type.

static

- slow varying transient
- time harmonic eddy current problems

In time-harmonic problems sinusoidal varying field quantities are assumed. The numerical solution of such problems may be troublesome with respect to the nonlinear material modelling [2], [3]. A common numerical approach to consider hysteresis effects, is the PREISACH model [4]. The computation of such material properties may raise difficulties considering transient problems. Here, the hysteresis is time dependent and a curve interpolation must exist during the computation for each instant of time [5].

Assuming low frequencies, the formulation of the 2D electromagnetic problem using the arbitrary vector potential \mathbf{A} with the ferromagnetic permeability μ , for the static electromagnetic field is

$$\nabla^2 \mathbf{A} = -\mu \mathbf{J} \tag{3a}$$

respectively for the time domain with the conductivity $\boldsymbol{\sigma}$ is

$$\nabla^2 \mathbf{A} + \mu \sigma \frac{\partial \mathbf{A}}{\partial t} = -\mu \mathbf{J}$$
 (3b)

and in the frequency domain where $\partial \mathbf{A}/dt = j\omega \mathbf{A}$ with the angular frequency ω of the sinusoidal excitation yields

$$\nabla^2 \mathbf{A} + j\boldsymbol{\omega} \cdot \mu \boldsymbol{\sigma} \mathbf{A} = -\mu \mathbf{J} \tag{3c}$$

For the solution of eqs.(3) the finite element method is in common use. The coefficient matrix of these cases is sparse, diagonal dominant. Therefore, special solver schemes can be used to solve the system of algebraic equations. Effective iterative solver, and in common use, are the incomplete CHOLESKY (IC), symmetric successive overrelaxation (SSOR) pre-conditioned conjugate gradient (CG) methods. Taking advantage of the properties of the system matrix, special algorithms, such as algebraic multigrid methods, can be employed to solve large systems very efficiently [6].

The non-linearities can be considered by employing NEWTON-RAPHSON iterations. Material characteristics are given by a list of data samples where cubic interpolating polynoms are used to approximate the data in-between the given samples.

A permanent magnet excitation inside the interesting field domain can be identified as an additional source

term
$$\nabla \times \frac{M_0}{\mu_{PM}}$$
 for the eq.(3a). The magnet material

characteristic is approximated by a straight line $\mathbf{B} = \mu_{PM}\mathbf{H} + \mathbf{M}_0$ determined by the permeability μ_{PM} of the material and its remanence \mathbf{M}_0 . The assumption of a straight line approximation for this type of material is

feasible if modern rare earth materials or ferrites are considered.

To obtain the interesting local field quantities out of the vector potential solution e.g. for the flux density distribution the

$$\nabla \times \mathbf{A} = \mathbf{B} \tag{4}$$

operator can be used.

FIELD QUANTITY EVALUATION AND EXAMPLES

To compute forces and/or the local field quantities of a physical problem to e.g. estimate the function and behaviour of a technical device, the FEM is used to solve the problem on a defined domain. The computed field distribution gives information over the operational conditions of the studied device. Those results can be used to optimise the shape of the device, to localise saturation levels and probably leads to changes of the overall construction. Arbitrary conditions such as dangerous fault situations in large electrical machines, or the behaviour of different materials can be simulated by the computer models without the need of an expensive prototype by monitoring the local field quantities.

To simulate the dynamic behaviour of e.g. rotating electrical machines transient time-stepping methods can be used. Such methods can computationally be very expensive. To avoid long-lasting computations very often equivalent models with concentrated elements of the studied device are chosen. Such lumped parameter models are mathematically not as sophisticated when compared to the FEM and therefore are not that computationally expensive, as well as they are less accurate. To overcome this difficulty, the parameters of such an equivalent model can be computed accurately by using the 2D or respectively 3D FEM. As an example, in fig. 1 the 3D FEM model to compute the leakage inductance of a permanent magnet excited servo motor is shown. This element of the lumped parameter model is linear and not depending on the operational conditions of the studied machine. Because of the

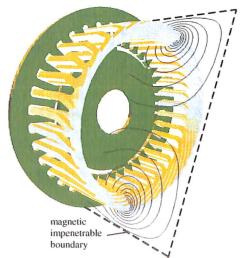


Fig. 1: Field solution on a planar cut in axial direction to compute the end-winding leakage reactance of a permanent magnet servo motor.

dimensions of this machine, other parameter such as main reactances can be computed by 2D FEM models.

Until now, only single field types are considered. In reality, field effects are coupled. As an example a three phase energy cable represents a thermal-electromagnetical-electrostatic problem, where the three static fields are influencing each other by the losses (Fig. 2). Here, an iteration and continued up-date of dependent material properties of the single field computations yields the demanded temperature distribution inside an around the high voltage energy cable. The field solutions are linked by projections of one solution to the other problem definition. Due to the different problem properties, the meshes used differ for each problem formulation.

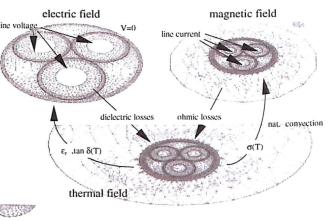


Fig. 2: FEM discretisations used for the coupled approach

ACKNOWLEDGEMENT

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The Finite-Difference Method in Frequency Domain - An Indispensable Tool for the Electromagnetic Analysis of Microwave Integrated Circuits and Multi-Chip Modules

W. Heinrich

Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH), Berlin

Introduction

Mobile communications has stimulated a rapid growth in the microwave field. While until 10 years ago it has been the domain of military and some small-volume special-purpose systems, situation has changed basically. The key word is "wireless". The ever increasing demand for bandwidth and the dense population of the frequency spectrum below 1 GHz has created a whole bunch of new commercial applications in the microwave and lower millimeter-wave range, i.e., for frequencies between 1 GHz and about 80 GHz. This includes the well-known mobile phone as well as wireless short-range broadband links as a substitute for optical fibers and a variety of sensor and radar systems. Briefly speaking, putting the data highway wireless ends up in using microwaves and millimeter-waves.

Most of these applications involve moderate to large volumes and are cost-sensitive. The classical microwave systems do not fulfill these requirements. Therefore, monolithic microwave integrated circuits (MMICs) are to be employed and novel packaging concepts have to be developed, which ease manufacturing and bring down costs. Since the market evolves rapidly, time-to-market is a factor of paramount importance. The main issue is to shorten development cycles and to reduce the number of technology runs towards "first-pass design". Clearly, this strengthens the role of electromagnetic simulation and demands for accurate and effective tools in computer-aided design. Encompassed is circuit design of both the individual chips (MMICs) and the multi-chip and packaging environment.

Why Finite-Difference in the Frequency Domain (FDFD)?

Electromagnetic simulation usually is restricted to the passive parts of the chip or the housing. Active elements are considered in the design process in a second step using measurement-extracted models. Hence, from the electromagnetic simulation point-of-view, the class of structures under investigation can be characterized as follows (Figs. 1...3 provide examples):

- The structures are planar and involve materials of different dielectric constants, most of them with approximately isotropic properties (e.g., semiconductor substrates). Since the shape may vary and parts of complex geometry such as package feed-throughs and so-called air-bridges are included, a 3D description, flexible with regard to geometry, is essential.
- The structures involve thin metalizations with thicknesses in the micrometer range (0.1μm...6μm), patterned with lateral widths from a few μm up to several hundreds of μm. Typical MMIC chip size is 3 x 3 mm², multi-chip modules and packages show maximum dimensions in the centimeter range. Because even the small metalization thicknesses may influence the overall behavior significantly, spatial resolution is a key issue in analysis. This is true in particular for circuits of the coplanar type where the fields concentrate in slots between metallic layers on the wafer surface. Generally, the minimum characteristic dimension is much smaller than the wavelength λ. Total size may be below λ, too, but may extend to a few wavelengths at maximum.
- Commonly, circuits and systems in the microwave frequency range are described in terms of their scattering behavior. This description is based on the wave modes propagating on the transmission-lines forming the input and output terminals. The scattering matrix provides the relationship between these quantities and is formulated in the frequency domain. It is important to note that separation of the modes represents a key issue in this regard. For multi-mode operation in the presence of different dielectrics, as is the case for many of the above-mentioned applications, one must resort to the basic mode-orthogonality criterion which holds only in the frequency domain. Consequently, time-harmonic excitation is mandatory for a large part of the structures of interest.

Although the Finite-Difference method in the time domain (FDTD) is very efficient and widely used among the electromagnetic community, we found that its frequency-domain counterpart is more favorable for many microwave circuit problems, particularly with regard to coplanar MMICs. The reason is as follows: Because of the mode orthogonality problem, one is forced to use time-harmonic excitation in any case. Even then, FDTD is advantageous in some instances due to its fast explicit solution algorithm (leapfrog scheme). The point, however, is the stability limit for the time step, which is determined by the smallest cell dimension, which means about 1 µm for coplanar MMICs. The corresponding time step is of the order of femtoseconds and thus 5 orders of magnitude smaller than the time period at

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10 GHz. This results in an excessive number of time steps to be calculated until transients have vanished. As a consequence, solution time is much higher than for the corresponding frequency domain formulation, though the latter requires a large sparse system of equations to be solved.

One should note that, strictly speaking, our approach is of the Finite-Integration type because it relies on the integral formulation of Maxwell's equations over the elementary cells. In the literature, however, at least in the microwave field, the term Finite-Difference is used for this approach as well as for the differential form. Therefore, we refer to the method as a Finite-Difference method throughout this paper.

Method of Analysis

The principal procedure comprises two steps. First, the propagation constants and the transversal electromagnetic fields of the wave modes on the transmission lines at the ports are calculated. Numerically, this results in a standard eigenvalue problem for a large sparse unsymmetrical system matrix. Only a few eigenvalues are needed. Thus, an implicitly restarted Arnoldi iteration is employed for solution, which preserves sparsity to a large extent. In the second step, the fields within the 3D volume are treated. The fields are excited by the mode fields at the ports with certain amplitudes. Repeating this for linearly independent amplitude constellations, the resulting scattering matrix can be determined. The approach requires solution of system of equations with a large sparse symmetric matrix. One special feature of this procedure is that for a lossless structure it results in a real matrix and not a complex one.

Typical CPU time and storage efforts for a structure with 300,000 elementary cells and a 2 x 2 scattering matrix are ca. 5000 s per frequency point and 450 MB RAM, respectively (data refer to a DEC personal workstation 433au, 212 MFLOPs). So far, meshes with a maximum of about 600,000 cells can be handled.

Special Extensions for Planar Microwave Structures

Due to the great differences in characteristic dimensions, spatial resolution puts a severe limitation on simulation capabilities. On the one hand, metal thicknesses of 1 µm are to be accounted for, on the other hand, the total chip dimension amounts to several millimeters. This leads to excessively large grids. Mesh grading is a prerequisite in that situation but alleviates the problem only slightly. In practice, only parts of a chip or simplified structures can be treated while it would be desirable to analyze the entire chip or even the complete package in a single run. Therefore, modified FDFD formulations are under development exploiting the fact that in regions with strong local variation on the micrometer scale the electromagnetic field is quasi-static in nature for the frequencies of interest. Two schemes are followed, both aiming at the special requirements associated with coplanar microwave structures:

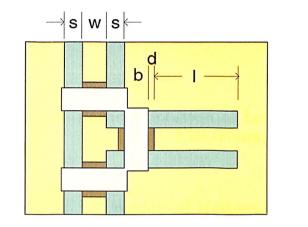
- Incorporating the known singularity behavior at metallic edges and corners into the FD elementary integrals.
- Using a-priori information on the field, e.g., from a static analysis on a fine grid, in order to improve accuracy for a coarse grid in the dynamic case. In this way, a hybrid dynamic-static approach is created.

Results and Conclusions

The FDFD method has proven its usefulness and effectiveness in the simulation of numerous MMIC elements, multi-chip and packaging structures - see Figs. 1...3. Examples will be treated in more detail at the workshop. In general, the FDFD simulation results are used to understand the electromagnetic behavior of a given structure, to optimize geometry and material choice, to develop simplified models, and to set-up design rules.

Acknowledgments

The work presented is the result of a common effort of the simulation group at the FBH and a collaboration with the Weierstraß-Institut (WIAS), which developed optimized numerical solvers. Therefore, the author gratefully acknowledges the contributions by H. Zscheile, S. Lindenmeier, W. Bruns, and M. Kunze as well as G. Hebermehl and R. Schlundt from WIAS.



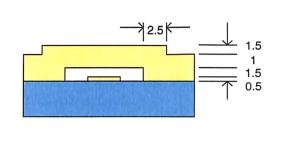
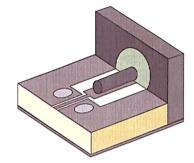
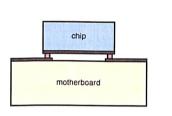


Fig. 1 Coplanar T-junction - top view (left hand) and cross section (right hand); all dimensions in micrometer ($w = 20 \mu m$, $s = 15 \mu m$).





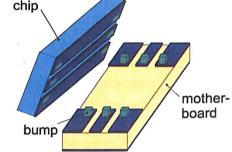


Fig. 2 Feedthrough: transition between coplanar waveguide and coaxial connector in housing.

Fig. 3 Multi-chip module in flip-chip technique (chip is connected to motherboard by bumps, for test purposes both substrates contain a coplanar transmission line).

Numerical Solution of Interior and Exterior Domain Problems in Electromagnetic Field Computation

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We consider the computation of electromagnetic fields for interior and exterior domain problems related to Maxwell's equations.

In case of interior domain problems the emphasis is on adaptive multilevel methods based on a discretization by Nédélec's curl-conforming edge elements with respect to an adaptively generated hierarchy of simplicial or hexahedral triangulations of the 3D computational domain. Local grid adaptation can be realized by means of efficient and reliable residual based on hierarchical type a posteriori error estimators. The basic tools both for the multilevel solver and the a posteriori error estimators are Helmholtz decompositions of the underlying function spaces into subspaces of irrotational and weakly solenoidal vector fields.

For exterior domain problems we focus on a boundary element approach based on a splitting of the associated Steklov-Poincaré operator. This splitting essentially relies on a Helmholtz decomposition of a related tangential trace space and allows to construct appropriate preconditioners.

Transversal modelling of semiconductor lasers with ToSCA

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Semiconductor lasers are, due to their miniature shape and their efficiency, a potentially attractive and already widely used source of coherent optical radiation. Applications range from fiber optical communication systems and inter satellite links to smart tools in medicine and ordinary CD-players. One of the main objectives in the development of new lasers is the increase in output power up to 100 Watt, which requires besides longitudinal simulation increasingly sophisticated transversal simulation of the device.

The transversal modelling of semiconductor lasers has to cope with the electronic behaviour of the semiconductor, the optical field, mechanical stress in the composite material, and the warming up of the device. The question is, how all these influences intertwine. That leads to coupled systems of partial differential equations on the device domain including Poisson's equation for the electrostatic potential, current continuity equations for electrons and holes, Helmholtz' equation for the optical field, and eventually an energy balance equation.

Quantum effects are an important feature of the semiconductor laser, the active zone of which is a nanostructure — one or more in general strained quantum wells, quantum wires or quantum dots. While Van Roosbroeck's equations provide a good landscape view on an electronic device, Schrödinger-Poisson systems portrait the individual features of such a nanostructure within the device. The problem is to draw a picture where both points of view come to bear. This leads to hybrid models for the electronic characteristics of the device and the serious question how to connect the different models.

In semiconductor device modelling one has to cope in general with rather complex, mixed boundary conditions which account for the coupling of the device to its environment. As for the embedding of a nanostructure into the device, apart from the boundary conditions the charge import/export relations of the nanostructure play a crucial role.

Our Two dimensional Semi-Conductor Analysis package ToSCA serves the solution of the stationary or transient Van Roosbroeck equations with Boltzmann or Fermi-Dirac statistics in arbitrarily shaped two dimensional domains, including optionally Helmholtz' equation for optical modes, an energy balance equation, and Schrödinger-Poisson systems on sub domains. Thus ToSCA provides a tool for the development of electronic devices including nanostructures such as quantum well and quantum wire semiconductor lasers.

Electromagnetic Field Computation for Linear and Nonlinear Shielding by Thin Magnetic Layers in EMC

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The influence of field-guided disturbances on sensitive measurement and control equipment is one of the central problems in electromagnetic compatibility. Thin shielding sheets of conductive and magnetic material can achieve a removal or reduction of such disturbances. To design the optimal shape of the sheets (geometry, open or closed, material, number of sheets) a powerful method for the electromagnetic field calculation of such configurations is needed.

The paper at first describes briefly the hybrid BEM/FEM method, which analyzes a 3D distribution of the fields numerically in the interior of the shielding sheet as well as in its surroundings.

Then in the case of linear shielding material a special Boundary Element Method (BEM) in conjunction with the Impedance Boundary Conditions (IBC) on both sides of the layer is presented. Its formulation by the magnetic vector potential turned out to be the most appropriate one for 2D as well as 3D problems. Concerning the spatial discretization only the surface of the sheet has to be discretized.

In the case of strong disturbing fields (high voltage and high current cables, overload-, short circuit-cases) the nonlinear behaviour of magnetic shielding material has to be taken into account. To deal with these cases the paper shows the introduction of a complex effective reluctivity or a modified Impedance Boundary Condition.

Finally some EMC applications and their results illustrate the use of the methods.

Design and Modeling for Integrated Optics

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The term "integrated optics" was introduced in 1969 when Miller presented the concept of integrated optical circuits that should be integrated on a single substrate. In parallel to the evolution of technology the theoretical background of integrated optics was successively established. Today, crafty design strategies and robust and flexible modeling tools are increasingly available [1,2]. A variety of software packages for the computer aided design [3] and modeling of integrated optical waveguide structures were going into the market. The design and modeling for integrated optics concentrates on the following tasks:

Eigenmode Analysis: The eigenmodes of a waveguide structure, i.e. the propagating or evanescent modes

$$\Psi^{(m)}(\mathbf{r}_t, z) = \psi^{(m)}(\mathbf{r}_t) \exp(ik_0\sqrt{\epsilon_m}z)$$
 (1)

that maintain their shape during propagation at a wave number k_0 , form the basis of many theories applied in integrated optical device modeling. The eigenmodes $\psi^{(m)}$ and their effective dielectric constants ϵ_m are calculated by solving standard eigenvalue problems $\mathcal{H}\psi^{(m)} = \epsilon_m\psi^{(m)}$ in which the operator \mathcal{H} may be regarded as the Hamiltonian of integrated optics.

The vector H-field formulation for the transverse field components of the magnetic field

$$\mathcal{H}_{\mathbf{h}} = \frac{1}{k_0^2} \left(\triangle_t + k_0^2 \epsilon + \nabla_t (\ln \epsilon) \times \nabla_t \times \right)$$
 (2)

 $-\epsilon = \epsilon(\mathbf{r})$ stands for the dielectric profile – represent a common formulation for the integrated optical eigenvalue problem. For weakly guiding waveguides, the coupling of the vector components via $\nabla_t(\ln \epsilon)$ can be treated as a perturbation. The eigenmodes are then described by the eigenvalue problem of the scalar Helmholtz equation $\mathcal{H}_s = \frac{1}{k_0^2} \left(\nabla_t^2 + k_0^2 \epsilon \right)$ which is diffeomorph to the time-independent Schrödinger equation of quantum mechanics.

Beam Propagation: In contrast to the eigenmode analysis, the beam propagation method (BPM) is not a constructive design tool, but a computer

simulation. As in the experiment, the BPM delivers the response of a device to an external optical stimulus.

Any Helmholtz equation can be formulated as $\frac{\partial^2}{\partial z^2}\Psi = -k_0^2\mathcal{H}\Psi$ in which the Hamiltonian \mathcal{H} acts only on the transverse coordinates as shown above. The forward and backward Helmholtz equations governing the propagation of beams are derived by taking the square root of the corresponding Helmholtz equation, i.e. $\frac{\partial}{\partial z}\Psi_{\pm} = \pm ik_0\sqrt{\mathcal{H}}\Psi_{\pm}$. These initial value problems possess the formal solutions

$$\Psi_{\pm}(z + \Delta z) = \exp\left(\pm ik_0\sqrt{\mathcal{H}} \Delta z\right)\Psi_{\pm}(z).$$
 (3)

The beam propagation method can handle perturbed plane waves propagating close to the z-axis through a medium with small inhomogeneities.

Coupled Mode Theory: The coupled mode theory (CMT) corresponds to the time-dependent perturbation theory of quantum mechanics. It is used to analyze coupled waveguide structures such as directional couplers, Bragg gratings and Mach-Zehnder devices. In the framework of the CMT, the evolution of the guided modes is governed by a dynamic system $\frac{\partial \mathbf{a}}{\partial z} = i\mathcal{K}\mathbf{a}$ where \mathbf{a} designates the vector of the expansion coefficients and \mathcal{K} the coupling matrix. Lossless waveguide structures are described by Hermitian coupling matrices, i.e. by unitary propagators $\exp(i\mathcal{K}\Delta z)$.

The coupled mode theory form the basis of the transfer matrix theory which is used to describe compound and more complex networks by stacking up the transfer matrices of the constituent parts.

Further Tasks: Multimode structures are often investigated by ray tracing, i.e. on the basis of the eikonal equation. The modeling of focusing gratings and optical phased arrays is tackled by the analysis of the light-path function [4], which represents a generalization if Huygen's principle. The electromagnetic theory of gratings, i.e. the efficiency analysis of reflection gratings taking the boundary conditions at the corrugated surface into account forms another important modeling task.

Algorithms: Many algorithms including finite difference (FD) and finite element (FE) methods, mode matching (MM), the method of lines (MoL), Green's functions and many more have been applied to tackle the eigenvalue and beam propagation problems. A great variety of these algorithms were tested within two benchmark activities [5,6]. The results stimulated a development towards algorithms which will remain stable for step index structures, high refractive index contrasts and and wide angle propagation.

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Differential-Algebraic Equations in Electric Circuit Simulation

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Circuit analysis programs are standard tools in industry for the design of electric circuits. The automatic modelling process creates differential-algebraic network equations (DAE) which differ from ordinary differential equations (ODE) both in analytical and numerical respects. We introduce the DAE index as a measure for the numerical problems to be expected when solving DAEs numerically. Using circuit examples as a motivating starting point, we deriver the basics of the index concept by linear circuits. The consequences for numerical integrations schemes are discussed in the high index case, which focus on alternatives to the standard backward difference (BDE) approach.

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Transparent Boundary Conditions for the Numerical Solution of Scattering Problems in Integrated Optics

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In general, the phenomena of optical field propagation are described by time-harmonic Maxwell's equations. The special structure of fiber optics and integrated optics components, however, often allows the use of simplified model equations [1]. Especially, vectorial and scalar Helmholtz approximations and the paraxial or Fresnel approximation of Maxwell's equations play an important role in integrated optics simulations. Helmholtz approximations supply suitable models to describe resonance and scattering phenomena, whereas Fresnel-type approximations model the propagation of optical beams in weakly disturbed homogeneous media.

The computation of the field behavior in the vicinity of scattering, reflecting, or waveguiding objects, modeled by the scalar Helmholtz or by Fresnel's equation, requires the knowledge of proper boundary conditions. We present a general technique for constructing such boundary conditions for both types of equations.

First, transparent boundary conditions for Fresnel's equation in two space dimensions are discussed [2]. The interior domain, which surrounds some given waveguiding structure, is discretized in the standard way, i. e. an implicit one-step discretization scheme is applied in the direction of propagation, and a finite element or finite difference method is used in the transverse direction. Now, the main idea is to discretize the exterior domain, but only in the direction of propagation, with the same scheme as applied for the interior domain.

This type of semi-discretization of the exterior domain is called a Rothe-typ discretization. This way, we end up with a discrete scheme describing the interior domain, and a system of ordinary differential equations (ODE's) with constant coefficients describing the exterior problem. The system of ODE's is solved by means of the Laplace transformation, which converts the whole semi-discretized exterior problem into an algebraic one. The solution of the transformed exterior problem depends directly on the initial conditions of the system of ODE's, which are at the same time the boundary conditions of the interior problem. A study of the algebraic structure of the exterior space solution shows that these boundary conditions can be fixed in such a way that only outgoing modes exist.

Second, we discuss the application of the same strategy to the scalar Helmholtz equation in two space dimensions. Regardless of the fact that Fresnel's equation and the Helmholtz equation represent different types of partial differential equations - the first is an initial boundary problem whereas the latter poses a boundary value problem - we can repeat the same steps in a similar way. The interior domain, a bounded, convex, polygonal shaped sub-domain of R2 is discretized in the usual finite element style. The semidiscretization of the exterior domain is performed by means of straight rays, which connect each of the boundary nodes with infinity. Along these rays a radial distance variable r is defined. In analogy to the previous case, the semi-discretization yields a system of ODE's, however, with non-constant coefficients. This time, the Laplace transformation of the system of ODE's results again in a system of ODE's, defined on the dual domain with respect to the distance variable. The general solution of the problem in the dual domain can be given in form of a path-integral representation. An analysis of the structure of the derived solution of the exterior problem enables us to fix the initial conditions of the system of ODE's again such that only outgoing modes exist. In contrast to the case of Fresnel's equation, where the derived transparent boundary conditions appeared in an algebraic form, the boundary conditions for the Helmholtz equation involve path-integral terms. In both cases - Fresnel equation and Helmholtz equation - the proposed technique supplies discrete transparent boundary conditions which fits, by construction, the structure of the discretized interior problem. This means that adaptive discretizations of the interior domains are taken into account in a natural way. Further, typical inhomogeneities of the exterior domains can be considered, e. g. waveguide-type inhomogeneities of the exterior domain in conjunction with the Helmholtz equation. Due to the nature of the

underlying partial differential equations, the derived discrete boundary conditions are nonlocal. Local approximations are obtained by a restriction of the recursive construction procedure to a fixed number of steps.

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Numerical Analysis of Distributed Inductive Parasitics in High Power Bus Bars

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In the recent years power electronics has made rapid progress in the development of applications which are based on the pulse width modulation method. A widely encountered example are pulsed DC-AC converters, which are operated at progressively higher pulse frequencies to achieve enhanced efficiency and higher flexibility in the operating conditions. Using modern high power semiconductor devices, switching times of about 100 nanoseconds or shorter and switched currents in the range of one kiloampere have been demonstrated.

As a consequence of the steep current ramping, distributed electromagnetic parasitic effects become an increasingly serious problem which governs the design of the bus bars interconnecting the individual devices in a high power module. According to the basic laws of electrodynamics, these effects are basically inevitable but have to be reduced to a minimum by design optimization. So, for instance, undesired eddy currents are induced inside the

bus bars which contribute to the quasi-static current flow in such a way that the resulting transient current distribution is forced to a thin region underneath the conductor surfaces (skin effect). The local crowding of the current density leads to considerable electro-thermal heating on certain locations within the bus bars. Furthermore, the distributed parasitic self- and crossinductances of the interconnects produce overvoltage peaks which endanger the safe operation of the attached devices and other circuit elements. Moreover, parasitic inductances cause a significant delay in the time the current can be switched on.

As a first step on the way to shape-optimized solutions to the above-mentioned problems, we present a practical methodology for the numerical analysis of distributed electromagnetic parasitics in interconnects and other related quantities. We apply this method to demonstrate that, due to the short switching times, only a full three-dimensional transient simulation of the entire module under realistic switching conditions can give us the necessary insight in the time-dependent electromagnetic behavior. The intuitive visualization of the electromagnetic fields inside and outside the bus bars allows us to study the details of the resulting current distributions and, thereby, to minimize the distributed parasitics.

Maxwell's Grid Equations as Basis for **EMC Computations in Time and Frequency Domain**

T.Weiland¹

INTRODUCTION

Maxwell's Grid Equations (MGE) are a universal basis for the computation of electromagnetic fields in realistic applications. Starting from Maxwell's equations in Integral form

$$\oint_{\partial A} \vec{E} \cdot d\vec{s} = -\frac{\partial}{\partial t} \iint_{A} \vec{B} \cdot d\vec{A} \qquad , \qquad (1)$$

$$\oint_{\partial A} \vec{H} \cdot d\vec{s} = \iint_{A} \left(\frac{\partial \vec{D}}{\partial t} + \vec{J} \right) \cdot d\vec{A} , \qquad (2)$$

$$\oint_{\partial V} \vec{D} \cdot d\vec{A} = \rho , \qquad (3)$$

$$\oint_{\partial V} \vec{B} \cdot d\vec{A} = 0 , \qquad (4)$$

$$\oint \vec{D} \cdot d\vec{A} = \rho \qquad , \qquad (3)$$

$$\oint_{\partial V} \vec{B} \cdot d\vec{A} = 0$$
, (4)

each of these four equations is solved on a two- or three dimensional Yee-grid[1] and thereby transformed into a set of matrix equations using the Finite Integration Technique (FIT)[2][3][4]. However, the base grid within this theory is not restricted to Cartesian nor coordinate grids but is applicable to very general classes of grid doublets, such as triangular meshes or non regular cubic meshes (as commonly used in Finite Element methods)[5][6]. As a result of this discretization there exists a set of matrix equations, that is as generally applicable as are Maxwell's equations itself. Specific solutions are obtained by deriving linear or non-linear systems of equations, time step recursions or eigenvalue problems from the original matrix equations.

THE METHOD

For simplicity we consider here only Cartesian meshes and briefly review the basic steps in deriving MGE. Starting with a grid

$$G = \{(x_i, y_i, z_k); i = 1, ..., I; j = 1, ..., J; k = 1, ..., K\}$$
 (5)

we first define electric voltages along the edges of a surface of an elementary cube as well as magnetic fluxes through theses

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surfaces. Maxwell's equation (1) can be rewritten for these integral quantities in a nonapproximative form as

$$\hat{e}_i + \hat{e}_j - \hat{e}_k - \hat{e}_l = -\frac{\partial}{\partial t} \hat{\hat{b}}_n. \tag{6}$$

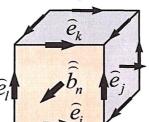


Fig. 1: Elementary cube of the three dimensional Grid Gand the electric voltages and magnetic flux for on elementary surface

By collecting all electric voltages and magnetic fluxes defined in the grid into vectors one can write the equations of type (6) for all grid cell surfaces as

$$C\,\hat{e} = -\frac{\partial}{\partial t}\hat{\hat{b}} \ . \tag{7}$$

Introducing a second dual grid \widetilde{G} such that all edges of one grid penetrate exactly one surface of the other and vice versa, one can rewrite Equ. (2) for magnetic voltages and electric fluxes respectively as:

$$\widetilde{C}\,\widehat{h} = \frac{\partial}{\partial t}\widehat{d} + \widehat{j}\,. \tag{8}$$

Finally, the remaining two equations (3) and (4) are similarly discretized to:

$$\widetilde{S} \hat{d} = q$$
 (9) , $S \hat{b} = 0$ (10)

This discrete representation of Eqs. (1-4) is so far exact and introduces no discretization error. The actual discretization occurs only when in addition to Equs. (7-10) the material relations are replaced by matrix relations.

$$\vec{D} = \varepsilon \vec{E} \implies \hat{\vec{d}} = D_c \hat{e} , \qquad (11)$$

$$\vec{B} = \mu \ \vec{H} \Rightarrow \hat{\hat{b}} = D_{\mu} \hat{h} \ . \tag{12}$$

The combination of Eqs. (7-12) now represents a fully general discrete replacement of the analytical Maxwell equations.

PROPERIES OF MAXWELL'S GRID EQUATIONS One of the main advantages of MGE is the fact that analytical properties of electromagnetic fields can be found as algebraic properties in the MGE. Thus, many basic laws, such as energy conservation, Poyntings law, equality of electric and magnetic energy in time harmonic fields and many more are easily proven using matrix theorems. The practical importance of this fact is that these discrete conservation laws allow effective control of numerical accuracy and correctness of the

software implementations. In three dimensional frequency domain problems, these properties furthermore guarantee unique solutions free of spurious contents.

EMC APPLICATIONS

Recently, EMC problems have attained wide scientific and public interest. One of the most discussed electromagnetic problems is the radiation of mobile phones. With the above shortly described method, one can perform rather complex computations due to the linear dependence of the necessary core space on the number of mesh cells. Thus it was possible to simulate a human head with many detailed interior material distribution on a desk-top workstation[7]. From such computations one may obtain the amount of power radiated into a human head as well as detailed local distribution thereof.



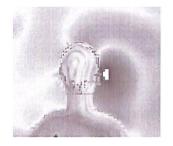


Figure 2: A three dimensional model of a human head exposed to the radiation of a mobile phone. The left plot shows the three dimensional set up with a mobile phone and antenna. The right hand side plot shows the absolute value of the electric field at one position in time showing the radiation towards the inside of the head.

A more technical aspect is the effect of a human head on the radiation pattern of a mobile phone influenced by the human head can as well be investigated as shown in Fig. 3.

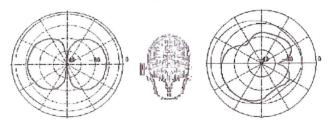
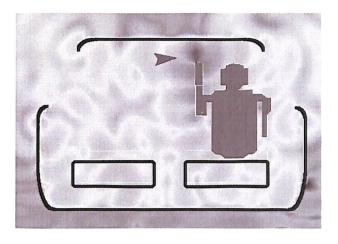


Figure 3: The radiation pattern of a mobile phone in free space (left) and close to a human head (right). The patterns clearly show the strong influence of the head on the radiation pattern.

An even more complex situation is shown in Fig. 4: A complete automobile is simulated

including a driver using a mobile phone inside the car without being connected to an outside antenna.





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3 Contributed Presentations

Energy Calculations for Localized Multiparticle States in Quantum Wells

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Current short-wavelength laser diodes are based on (Zn,Cd)Se/ZnSe and (In,Ga)N/GaN quantum well (QW) structures. Alloy disorder and localization is an inherent feature of the present structures, characterized by a ternary QW as the active layer. In this case, lasing may once arise from localized excitons (X). Moreover, localized biexcitons (XX) have been observed in (Zn,Cd)Se QWs and demonstrated to cause low-threshold gain. In (In,Ga)N/GaN QWs, extremely broad photo luminescence and gain spectra are found indicating much stronger exciton localization.

We present a theoretical study of localized multi-particle states for the entire range between weak and strong localization. Besides single excitons, also multi-exciton states are considered. The energy of a multi-exciton state can be derived from the solution of a Schrödinger-Poisson system. The effective mass electron-hole Hamiltonian is treated within the local density approximation (LDA) in the framework of a multicomponent density functional theory (DFT). Within this approach, multi-particle effects are incorporated via a density-dependent exchange-correlation potential in the Hamiltonian. For computing the multi-exciton energy our 2D FV Schrödinger-Poisson solver has been used which operates within the framework of the Two dimensional Semiconductor Analysis package ToSCA of the WIAS.

As a first step towards a better understanding of (In,Ga)N/GaN QWs the experimentally reported nanometer-scale regions of phase segregated In are simulated as cylindrical quantum boxes (QB) within the quantum well. Indeed, stable exciton and biexciton states are found in a physically reasonable range of QB depth and radius. In small QBs, the biexciton binding energy quite surprisingly decreases with increasing QB depth. This anomalous behaviour occurs when the hole of a single exciton is much more localized than the electron, while the Coulomb repulsion in a biexciton still prevents an effective localization of a second hole. For wider QBs, the biexciton binding energy rises with the QB depth but does not exceed 20 meV.

Our calculations show, that a single quantum box cannot bind more than two excitons, unless the exciton localization energy exceeds 300 meV. This value is larger than the usual subband splitting. Hence more sophisticated multi-exciton energy calculations require the incorporation of multi-band matrix Hamiltonians into the model.

Revisiting Spurious Modes

Alain Bossavit

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Whitney has bequeathed us a wonderful tool: a discretization of the de Rham complex, with an amazing wealth of functorial properties. One among these, which in simple topologies can be written

(1)
$$\ker(\operatorname{rot}; W^1) = \operatorname{grad} W^0,$$

where W^0 and W^1 are the spans of edge elements and scalar nodal elements respectively, is especially useful: It's the reason why edge-element computations of resonant cavities never produce "spurious modes". Such eigenmodes, that largely fail to be divergence-free and therefore, would have to be spotted and rejected as unphysical, did occur when standard node-based elements (with vectorial DoFs at nodes) were used.

This nuisance has disappeared with edge elements, but the centrality of relation (1) in this respect continues, I think, to be overlooked, while attention is called on issues such as "lack of compactness", which I purport to show are secondary (though of course, quite real).

To this effect, the basic theory is reviewed, with a new twist: it's not vector fields we are after, but CLASSES of cohomologous vector fields (that is, equal up to a gradient in our case). By passing to the quotient with respect to this equivalence relation, one finds a standard eigenvalue problem, with all the compactness needed to apply Fredholm's theory. (An easy compactness lemma, addressing classes, and not individual fields, establishes this once and for all.) Discretization then requires a convergent approximation scheme for

CLASSES, too, and this is where (1) comes to front stage, allowing one to prove that discrete eigenmode number k does converge to continuous eigenmode number k. In contrast, standard (node-based vectorial) elements fail at this precise juncture, and one can then see what goes wrong with them. (In particular, though true modes are indeed accumulation points of discrete ones, discrete eigenvalue number k always converges to 0, which explains "spectral pollution".)

I feel concerned that efforts of the applied mathematics community to clarify this question may risk taking a wrong turn, if one indulged in the overzealous desire to tackle all difficulties at once, including the "open guide" situations, where the presence of a continuous spectrum does complicate matters, indeed. We should emphasize the central feature, which I maintain is relation (1), and properly frame it within the broader picture of the de Rham complex and its discretization via Whitney forms. Making all efforts to simplify all the rest should bring pedagogical benefits, and hopefully promote in electrical engineering curricula what appears to be the hard-core vademecum: compact self-adjoint operators, Fredhom's theory, Galerkin-like approximation of modes.

Numerical Calculation of Slowly Varying Electromagnetic Fields Using the Finite Integration Technique

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For the numerical simulation of slowly varying electromagnetic fields we use the Finite Integration Technique (FIT), a proven consistent discretization scheme mapping Maxwell's equations in integral form on a dual-orthogonal grid which does not necessarily have to be Cartesian. This results in a set of matrix-equations, the so-called Maxwell-Grid-Equations (MGE). The most flexible approach considers general transient electromagnetic processes by time integration of the electric wave equation. For this implicit Newmark-type timemarching schemes can be applied. For slowly varying electromagnetic fields however the displacement currents are small when compared to

sistatic formulations. The arising differential-algebraic systems of equations of Index 1 can be solved by standard implicit time-stepping methods [1]. For general timeharmonic problems the electric wave equation is transferred into the frequency-domain and yields a complex symmetric Helmholtz equation. For timeharmonic problems occuring with the simulation contaminated high voltage insulators the specialized approach of electroquasistatics is used which yields a complex-valued potential problem. In both cases the solution of the FIT-discretized large sparse complex symmetric linear algebraic systems is performed using especially suited preconditioned conjugate-gradient-type methods [2].

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Discrete Transparent Boundary Conditions for General Schrödinger-Type Equations

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Transparent boundary conditions (TBCs) for Schrödinger-type equations on a bounded domain can be derived explicitly under the assumption that the given potential V is constant or linear on the exterior of that domain. In 1D these boundary conditions are non-local in time (of memory type).

Existing discretizations of these TBCs introduce slight numerical reflections at this artificial boundary and also render the overall Crank-Nicolson finite difference method only conditionally stable. Here, a novel discrete TBC is derived directly from the fully discretized whole-space problem that is reflection-free and yields an unconditionally stable scheme.

While we shall assume a uniform discretization in time, the interior space discretization may be nonuniform, and we shall discuss strategies for the 'best exterior discretization'. Moreover, we sketch how the construction of discrete TBCs could be generalized to 2D transient Schrödinger-type equations. Numerical examples illustrate the superiority of the discrete TBC over other existing consistent discretizations of the differential TBCs.

As an application of these boundary conditions to radiowave propagation problems in the troposphere or soundwave propagation in underwater acoustics (assuming cylindrical symmetry) results for the so-called standard and wide angle "parabolic" equation (SPE, WAPE) models are presented. Furthermore, we analyze under which conditions the coupling of different WAPEs (or WAPE and the SPE) yields a conservative hybrid model.

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THE TOLERANCE OF ADHERENTLY GROWING CELLS TO PERMANENT HIGH FREQUENCY ELECTRICAL FIELDS

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We investigated the influence of high frequency electrical fields on biological cells. Cells and cell cultures of adherently growing mouse-fibroblasts (L929) were cultivated in micro electrode structures under physiological conditions with permanent field application. The field strength was in the range 10 kV/m up to 80 kV/m and the frequency between 500 $k\rm{Hz}$ and 30 MHz. Using micro electrodes systems makes it possible to investigate cell cultures over long times under defined conditions. The field exposure times ranged from several minutes up to more than 3 days. To evaluate electrically induced effects, typical cell parameters (cell division time, survival rate, mobility) were used. Only single cells were investigated. To distinguish electrically induced thermal effects from purely electrical ones, the temperature of the solution was recorded during field application and its influence on the biological parameters was investigated. Application of a.c. and/or d.c. fields to cells, superimposes a frequency dependent component on the natural membrane potential. The size of an additional potential can be estimated from the numerically determined electric field distribution around the cell and it is this value that mainly determines survival time or changes the other parameters. The newly developed measurement system shows that cells can tolerate an additional membrane potential in the range of the natural value with little change. But if a field with an induced potential slightly higher than the natural membrane potential is applied, survival rate and survival time are markedly reduced

Computation of axisymmetric Eigenmodes of Maxwell's Equation

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The poster will treat the computation of axisymmetric non-trivial eigenmodes of Maxwell's equation in an axisymmetric domain using a singular multigrid method.

Computation of Eigen Modes for Transmission Lines

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Microwave circuits are characterized by the scattering matrix. It describes the structure in terms of incoming and outgoing wave modes on transmission lines forming the ports of the structure. The scattering matrix can be computed from the electromagnetic field of the entire three-dimensional structure using a finite-volume method for the integral form of the Maxwellian equations in the frequency domain. As a first step one has to calculate the field distribution in the transmission lines. Because the transmission lines are longitudinally homogeneous, the electromagnetic field can be expanded into wave modes with each of them varying exponentially in the longitudinal direction z. Introducing the ansatz $\vec{E}(x,y,z) = \underline{\vec{E}}(x,y)e^{jk_zz}$ results in an eigenvalue problem with a sparse non-symmetric or non-Hermitian (lossy case) matrix: $Cx = \gamma(h)x$, type(C) = (n, n), $\gamma(h) = -4\sin^2(k_z h)$. The propagation constants k_z can be computed from γ after the solution of the eigenvalue problem. The corresponding eigenfunctions represent the fields of the wave modes and forces the boundary values for the calculation of the fields in the three-dimensional structure. In technical applications only a small number m of modes are of interest:

Criterion: The complex propagation constants $k_{z_i} = \beta_i - j\alpha_i$, i = 1(1)n, are

sorted in ascending order of $|\alpha_i|$. In the case that some $|\alpha_i|$ have the same value the constants k_{z_i} are sorted in descending order of $|\beta_i|$.

We avoid the time and memory consuming computation of all eigenvalues to find the few required propagation constants by using the implicitly restarted Arnoldi iteration that is carried out for the original and for an extended matrix. Because the Arnoldi method only converges in inverse mode for our problem we have to solve systems of linear algebraic equations. The number of non-zero elements of the sparse matrix is reduced neglecting small elements while preserving the symmetric structure of C. The system of linear algebraic equations is split into a diagonal and a sparse system using a similarity transformation of the eigenvalue problem. The similarity transformation is performed by independent set orderings using an inexpensive greedy heuristics for the matrix C. We use a combined unifrontal/multifrontal method for the solution of large sparse sets of ill-conditioned linear equations.

Multigrid Method for Eddy Current Problems

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Quasistatic models for the behavior of electromagnetic fields have proved highly successful for the description of eddy current phenomena. Several different approaches are feasible. They invariably lead to a parabolic problem involving the double-curl-operator in combination with a gauge condition. We employ a finite volume scheme (FIT) to discretize the equations in space in conjunction with implicit timestepping. Thus a large sparse system of equations has to be solved in each timestep, which has to be done by an iterative method.

However, standard multigrid fails since the discrete problem lacks uniform ellipticity. At second glance we realize that the discrete problem has an elliptic character, when restricted to the orthogonal complement of the kernel of the curl-operator. Thus an effective Gauß-Seidel smoothing of error components in this subspace is possible.

The treatment of the remaining irrotational error components exploits the close relationship between the finite volume scheme and so-called edge elements. It reveals that irrotational vectorfields are accessible through discrete potentials. Hence smoothing in the space of discrete potentials can deal with the error in the kernel of the **curl**-operator.

Under certain assumptions on the computational domain and material functions, a rigorous proof of asymptotic optimality of the multigrid method can be given; it shows that convergence does not deteriorate on very fine grids. The results of numerical experiments confirm the efficiency of the method.

Finite element approximation of nonlinear temperature and magnetic fields in electrical devices

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We present a survey of results which we have obtained in solving stationary nonlinear physical fields in large transformers and rotary machines by the finite element method. In particular, we present uniqueness theorems for the classical and weak solutions, a comparison theorem, existence theorems for the weak and finite element solutions, approximation of a curved boundary and numerical integration, a discrete maximum principle, convergence without any regularity assumptions, a priori error estimates, nonlinear boundary conditions and numerical algorithms.

Several years ago the first author used the finite element method to compute a temperature distribution in the magnetic circuit of large oil-immersed transformers. The heat sources are due to the alternating electromagnetic field. The biggest computed transformers (5 m high) were designated for the atomic power station in Temelín in the south of Bohemia. Each of its reactors has the power output 1000 MW and the whole produced energy passes through these transformers, the efficiency of which is about 97 %. That is why 3 % of the total energy changes to heat. This means that every second 33.3 MJ of heat have to be extracted, otherwise the temperature of cooling oil exceeds certain prescribed limits and the oil starts to boil which may cause a destruction of the whole transformer.

Note that the magnetic circuit of the transformer represents an orthotropic material, which consists of iron sheets. Their heat conductivities across and along sheets substantially differ and depend nonlinearly on temperature. We also present another real-life example of calculation temperature in rotary machines. Their body again represents a nonlinear anisotropic material which is highly nonhomogeneous. This causes big jumps in coefficients of the appropriate heat equation and is the main source of numerical difficulties in practical calculations. If the difference between temperatures in one millimetre of wire insulation is greater than some prescribed limit (e.g., 30 K) then the heat flux becomes so large that the insulation starts to burn up. That is why a detailed knowledge of temperature and magnetic fields is very important when designing electrical machines.

Concepts for the Formulation of 3D Magnetic Field Problems

Michael Kuhn

Johannes Kepler University Linz, Austria

We consider magnetic field problems which can be described by Maxwell's equations. Although these (physical) equations are fixed, there exist a variety of different correct mathematical formulations representing the original magnetic field problem. Those formulations are primal as well as mixed variational formulations in different Sobolev spaces. We restrict our considerations to problems which have a unique solution. Then we can select any of those formulations for further treatment. Hereby our choice depends on the analytical properties of the formulation. In particular it should be well suited for discretization and numerical solution. A careful analysis is required since incorrect discretizations may have the same effect as incorrect gauging conditions imposed on the vector potential. Finally we design the discrete problem such that the system matrix becomes symmetric and positive definite and such that preconditioners can be constructed. Then the resulting system can be solved by the preconditioned conjugate gradient algorithm. In the talk we discuss and analyze several formulations and propose algorithms for the efficient numerical solution. As a generalization to Finite Element discretizations based on the introduction of a vector potential we consider coupled Finite Element – Boundary Element formulations where a scalar potential is used in the case of boundary elements.

Simulation of the electromagnetic field of an induction hardening set-up

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The advantage of a process model compared with a general model will be discussed at an example for the calculation of the electromagnetic fields at the heating for the inductive surface hardening. It turns out that by introducing a new boundary condition a process model can be designed which allows a fast or efficient determination of the relevant parameters of the process. For a general model in all examined spaces the MAXWELL equations and the respective boundary conditions have to be fulfilled. The process model, however, is contructed out of physical considerations. Only in the non-conducting space the MAXWELL equations have to be fulfilled, with a boundary condition at the surface which results from the analysis of a planar eddy cuurrent problem. The use of this boundary condition is the main issue of the process model. With the knowledge of the tangential component of the magnetic field strength on the boundary surface the current density should be calculated. The boundary condition which is discussed for an analytical example is also advantageous for simulations in numerical methods with low penetration depth in consideration of the dimensions of the examined area. Usual methods such as the difference method or the finite element method need small elements in the conducting space. With these small elements and the large dimensions of the examined area the number of elements is very large. The new boundary condition is able to reduce the number of elements for simulation and so the required time is also reduced.

Multigrid Methods for Coupled Nonlinear Magneto-Mechanical Problems

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Current techniques for calculating nonlinear magnetic field problems are based on iterative approaches which are either poor or only local convergent. Especially for coupled, transient problems such formulations are too slow.

In this paper a global convergent multigrid method for the nonlinear magnetic field problem is used. By solving the problem at the coarser grids, a very good start approximation for the time consuming iterations at the finer grids can be obtained. Strong non-linearities, caused by saturation effects in ferromagnetic materials, are considered at the coarser grids and don't increase the number of iterations at the finer grids.

For a given deformation at the current time step the nonlinear magnetic field as well as the magnetic force density are calculated. Thereafter the magnetic force is considered in the mechanical equation to calculate the displacement field. The mechanical problem is solved by applying a conjugate gradient method with multigrid preconditioning. With the predicted deformation the geometry of the problem is updated to carry out the next magnetic field computation. If attaining convergence of the solution the calculation of the next time step is performed. The magnetic force density is computed by local application of the Maxwell stress tensor.

As example the transient behavior of a coupled electromagnetic - acoustic transducer (EMAT) is calculated. Thereby the proposed method is compared to standard iterative methods and it's advantages are verified.

On the Computation of Systems of Linear Algebraic Equations for Monolithic Microwave Integrated Circuits

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The scattering matrix describes monolithic integrated circuits that are connected to transmission lines in terms of their wave modes. Using a finite-volume method a three-dimensional boundary value problem for the Maxwell's equations in the frequency domain can be solved. This results in the solution of a large-scale system of linear equations with indefinite symmetric matrices. The high-dimensional system of linear algebraic equations is solved using iterative methods. A commonly used approach for solving large sparse linear systems is to find sets of unknowns which are independent.

Generalized FEM for Helmholtz equations

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Standard domain based FE or FD methods for solving boundary value problems governed by the Helmholtz equation provide solutions which differ significantly from the best approximation with increasing wave number. Various modifications of FEM have been proposed to avoid this pollution effect. We consider the construction of discretizations of the Helmholtz operator leading to generalized FEM with minimal pollution.

High frequency electric fields in microstructures - simulation and biological applications

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In an inhomogeneous electric field, polarisable particles experience a force that moves them to regions of higher or lower field strength (positive and negative dielectrophoresis). Dielectric forces can be utilised to transport, trap, separate and charactrise suspended biological cells, viruses, artificial particles and liquid droplets. Closed field cages, traps, particle filters, particle transport systems, liquid and Brownian pumps can all be made with appropriately designed and driven micro electrodes. We show how particle behaviour is influenced by heating, liquid streaming and particle-particle interaction. Due to the complex electrode geometry, numerical treatment for electric field calculation is required. In addition, application of electric fields to conducting liquids (cell culture media at about 1.5 S/m) causes inhomogeneities due to Ohmic heating. This changes the electric gradients that determine the dielectrophoretic forces and can give rise to electrohydro-dynamic liquid streaming. Numerical calculation is done with a finite difference method and is compared with analytical and experimental results of idealised electrode geometry. For submicron particles, Brownian motion becomes important. This and particle-particle interaction are evaluated by numerical integration of the corresponding Langevin equation. Single particles down to a size of 50 nm can savely be trapped by negative dielectrophoresis. Smaller particles (down to 14 nm) have been successfully enriched from suspensions and trapped as aggregates.

Numerical Simulation of Self Pulsating Semiconductor Lasers

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We consider a simple mathematical model of a multi-section distributed feedback (DFB) semiconductor laser. This model reproduces the phenomenon of fast oscillating (5-40 GHz) quasi-periodic solutions (Self Pulsations, or SP) and is represented by a system of Travelling Wave Equations (TWEs). The SP of similar kind were also demonstrated experimentally. An important industrial application of SP is the all-optical clock recovery (at 18 Gbit/s) mentioned in [1].

The TWE system contains two dynamic PDEs of hyperbolic type with one spatial dimension describing coupled forward and backward travelling optical waves inside the laser device. It is linear with coefficients depending on the carrier density in the laser. The third equation is an ODE, which depends on the spatial variable parametrically and models the evolution of the carrier density inside the device.

We want to present two approaches to the investigation of parameter regions with stable SP.

The first approach is the direct dynamic simulation using time-domain algorithm. Such model and algorithm was discussed in [2]. Spatial and time discretization steps were connected via group velocity, each time step of the algorithm was resolved using transfer matrix method.

During calculations we have observed some hysteresis of the solution increasing or decreasing the values of different parameters of the TWEs. For example, sometimes it was possible to find two different types of SP solutions with different frequencies (5-15 GHz and 25-40 GHz) while the values of the parameters were the same.

Some cases of this hysterical behaviour were noticed during the experiments with DFB devices, but some of them, as we know, were not.

Alternatively, the TWE system is considered as an evolution equation. A reduction to the eigenspaces of the evolution operator with the largest real part of the corresponding eigenvalue leads to a "mode approximation" by a ODE. It has been shown in [3] that SPs calculated by a single-mode approximation of the TWE is in excellent agreement with the full PDE as well as with experiments.

A detailed investigation of hysteresis of the solution as well as comparison between two models mentioned above is presented.

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Model Reduction By the Rational Krylov Method

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In model reduction for a linear network we want to create a reduced order model \hat{d} , \hat{G} , \hat{C} and \hat{b} of the exact model d, G, C and b in a such a way that the approximate transfer function $\hat{H}(s) = \hat{d}^t(\hat{G} + s\hat{C})^{-1}\hat{b}$ matches as many moments $(-1)^j d^t((G + s_iC)^{-1}C)^j (G + s_iC)^{-1}b$ around the interpolation points s_i , $i = 1, \ldots, \bar{i}$ of the exact transfer function $H(s) = d^t(G + sC)^{-1}b$ as possible.

Direct moment matching methods like AWE (asymptotic waveform evaluation) shows numerical instabilities. Recent work has been on model reduction by Krylov subspace methods. Krylov subspace methods shows much better numerical stability properties than direct moment matching methods.

Two sided Krylov subspace methods for model reduction like PVL (Pade' via Lanczos) and rational Lanczos, builds up a biorthogonal basis.

The rational Krylov method for model reduction is a one sided subspace and a multipoint approximation method. First it builds up an orthogonal basis $v_1, \ldots, v_{\bar{k}}$ for a union of Krylov spaces by operating with the matrices $(G + s_i C)^{-1} C$, $i = 1, \ldots, \bar{i}$ on a linear combination of the basis vectors

and expand the basis with the orthogonalised result. Then an approximation $\tilde{x}(s)$ to the equation system (G + sC)x(s) = b is found and H(s) is approximated by $d^t\tilde{x}(s)$. The reduced order model matches moments up to the power $\bar{j}_i - 1$ around the interpolation points s_i , $i = 1, \ldots, \bar{i}$, where \bar{j}_i is the number of times the matrix $(G + s_iC)^{-1}C$ was used in building the basis. One sided methods are expected to have good numerical properties since the orthogonalisation is more stable than biorthogonalisation. Furthermore the total number of matrix vector products is expected to be smaller than for the biorthogonal methods. The eigenvalues and corresponding right eigenvectors converge around the interpolation points. By getting an estimate of the left eigenvectors by using the basis it is possible to get an error estimate of $\tilde{x}(s)$ and thus of the approximate transfer function $\hat{H}(s)$.

OVERLAPPING SCHWARZ METHODS FOR MAXWELL'S EQUATIONS IN CONDUCTIVE MEDIA

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The use and the analysis of Domain Decomposition Schwarz preconditioners for Finite Element approximations of Maxwell's equations, is considered in this presentation. One- and two-level overlapping methods are considered for 3D Maxwell's equations in conductive media. Nédélec finite elements and implicit time—stepping are employed. We show that the condition number of a two-level additive algorithm is bounded independently of the diameter of the triangulation, the number of subregions and the time step, and improves when the overlap is increased. A similar result is obtained for a two-level multiplicative method. We also show that in certain cases, a one-level methods can be preferable to a two-level one, since the condition number of the former method decreases with the time step. Numerical results, obtained with the PETSC 2.0 library, are presented to validate our analysis.

Numerical simulation of induction hardening of steel

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We discuss a model that is capable of describing the process of induction hardening of steel: Induction heating - heat transfer - solid-solid phase transitions in steel [1]. It consists of a reduced system of the Maxwell equations, the heat transfer equation and a system of ordinary differential equations for the volume fractions of the occurring phases [2].

The model is applied to simulate surface heat treatments, which play an important role in the manufacturing of steel. Our aim is to develop a simulation tool for optimal shape design of inductor coils for surface hardening.

The numerical methods are implemented with tools from PDELIB, a collection of modular algorithms [3]. We would present numerical simulations of surface hardening applied to the steel 42 CrMo 4.

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Numerical simulation of optical transmitters and optoelectronic transponders in optical networks

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Optical transmitters are the sources for optical fiber communication systems and consist of lasers and modulators. Optoelectronic transponders amplify and reshape the optical signal after a certain distance. They consist of an optical receiver converting the optical signal into an electronic signal which is used to modulate a laser, thus creating a regenerated output signal. Optoelectronic transponders are of great interest for the installation of wavelength division multiplex (WDM) transmission networks.

For optical network simulation it is essential to know to what degree the optical signal is influenced by the properties of transmitters and transponders. Since numerical simulation of the complete laser and modulator physics is too cumbersome simplified numerical models have to be found which are able to describe the system aspects of optical transmitters and optoelectronic transponders. In close connection with experimental work, the salient parameters of optical transmitters and optoelectronic transponders are extracted and simple computation models are set up which are able to describe signal degradation in terms of these parameters. In addition, measurement techniques are discussed which allow to extract the important parameters from fabricated components for which the relevant system parameters are in general not known. This allows a black-box modelling of devices. The main parameters for modelling the devices are:

- chirp of laser and modulator
- extinction ratio of modulation
- pulse rise time
- laser linewidth as a measure of laser phase noise

For the optoelectronic transponder additional knowledge is needed about the time jitter caused by the transponder electronics.

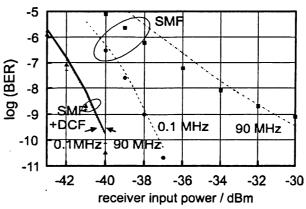


Fig. 1 BER measurement (symbols) and simulation (lines) for transmission over SMF and SMF+DCF. Parameter: laser linewidth.

Numerical models for the laser-modulator and for the optoelectronic transponder will be discussed and the relevant system parameters will be given. The experimental verification of the simulation work is performed by measuring the bit error rate (BER) of optical transmission along standard single mode fibers and dispersion compensated fiber trunks. An example for

simulation and measurement of the effect of laser linewidth on the BER for transmission over SMF fiber and dispersion compensated fibe trunks (SMF+DCF) is depicted in Fig. 1.

This work was performed under research contract with Deutsche Telekom AG

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