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Three Dimensional Algorithms for a Robust and Efficient Semiconductor Simulator with Parameter Extraction: The EVEREST Final Report

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Editor: Dr C. Greenough (RAL)

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Abstract

EVEREST was a four-year project supported by the European Community under the European Strategic Program for Research in Information Technology (ESPRIT). The main aim of the project was to provide general methods for the analysis of silicon semiconductor devices which would be especially applicable at sub-micron geometries. It was clear that this goal would exploit the full capability of numerical modelling techniques in generating an approximation to the complex three-dimensional geometries found in modern devices.
The partners in the project were:

Analog Devices (IR)
Philips (NL)
SGS-Thomson (I)
STC Technology (from April 1989) (UK)
GEC (until March 1989) (UK)
IMEC (B)
NMRC (IR)
Rutherford Appleton Laboratory† (UK)
Trinity College Dublin (IR)
University of Bologna (I)
University College of Walse, Swansea (UK)

† Prime Contractor

This report reviews the activities and achievements of the project and provides a complete biliography of the reports and papers produced by the project.

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1 Introduction

1.1 Overview of the Project

The numerical simulation of semiconductor devices in two dimensions is well-established for the design of advanced electronic components and processes. As device miniaturization approaches submicron feature sizes, three-dimensional effects are becoming important even for nominally standard planar devices. In many devices key physical effects occur at corners where three-dimensional models are the only way to obtain an accurate solution. The need to simulate the essentially three-dimensional effects of threshold shift for small channel devices, channel narrowing and the accumulation of carriers at the channel edge is growing. These effects make two-dimensional simulation codes inadequate for device-performance prediction.

EVEREST is a four-year project supported by the European Community under the European Strategic Program for Research in Information Technology (ESPRIT). It is investigating suitable algorithms for the analysis of semiconductor devices in three dimensions, and developing software implementing the most effective of those algorithms. Companies in both Japanese and USA have already been very active in this area of three-dimensional modelling and it is appropriate that a joint European effort be focused on the solution of such problems.

The code under development within the project provides Europe with an important set of analysis tools which ensure that the European semiconductor industry is well placed in the race to develop new device structures.

1.2 Structure of the Project

The partners in this project are drawn from some of the major industrial and academic research and development teams in Europe. They are listed below.

- Analog Devices (Ireland)
- Philips (The Netherlands)
- SGS-Thompson (Italy)
- STC Technology Ltd (UK)
- Rutherford Appleton Laboratory (UK – Project Leader)
- NMRC (Ireland)
- IMEC (Belgium)
- University College Swansea (UK)
- University of Bologna (Italy)
- Trinity College Dublin (Ireland)

The list comprise four industrial partners, three national research laboratories and three universities. The Rutherford Appleton Laboratory is the overall project leader and prime contractor of the project.

Five main areas of activity have been identified and the project is divided into five workpackages, each with its own Workpackage Director. These five workpackages, with the Workpackage Director shown in parentheses, are:

- Physical Models and Validation (SGS)
- Discrete Problem Formulation (Philips)
- Mesh Generation and Refinement (UCS)
- Solution Procedures (Philips)
- Project Software Suite (RAL)

The first four of these workpackages each address one aspect of device modelling and the results produced are represented in the project code. The project directs some one hundred man-years towards developing solutions to the problems in simulating semiconductor devices.

1.3 Physical Models and Validation

Correct and reliable physical models are the key to establishing the validity and accuracy of numerical device simulation in two or three dimensions so as to account for physical effects such as mobility and heavy doping. This workpackage is investigating the validity of the physical models being used within the project. This has lead to the development of new physical and analytical models which have been assessed against the results of parameter extraction and measurement on fabricated benchmarks devices.

1.4 Discrete Problem Formulation

The objective of this workpackage is to investigate different approaches to the discretisation of the conventional continuum device modelling equations. The extension of the standard Scharfetter-Gummel scheme into two and three dimensions is being considered as well as the use of fitted and mixed finite element methods. A second strand to this workpackage is the development of error estimates to be used to control the propogation of errors in the solution when adaptive mesh techniques are used.

1.5 Mesh Generation and Refinement

As three-dimensional simulations are very complex in nature it is important to develop effective techniques to generate the discrete model mesh automatically. There is considerable activity in developing strategies to produce meshes in three-dimensions with the potential to be used adaptively. These techniques are then coupled with the element selection algorithms to perform mesh refinement.

1.6 Solution Procedures

The most computationally intensive part of the majority of numerical simulations is the solution of large systems of linear equations. Within the project there is a continual effort in improving the solution procedures being used. Currently the two most successful methods being used within the project are Incomplete Choleski Conjugate Gradients (ICCG) and the Preconditioned Conjugate Gradient Squared (PCGS) algorithm . Research is continuing to improve these solution techqniues.

1.7 Project Software Suite

An important part of the project is the design and implementation of a complete simlutation system using the best consistent set of the algorithms developed by the project. This part of the project will be described in detail on a separate information sheet.

The main aim of the project was to provide general methods for the analysis of silicon semiconductor devices which would be especially applicable at sub-micron geometries. It was clear that this goal would exploit the full capability of numerical modelling techniques in generating an approximation to the complex three-dimensional geometries found in modern devices.

The starting point for the project was the experience gained in a similar project investigating two-dimensional algorithms. With this common background extensions into three dimensions were sought. The initial work concentrated on steady state solutions but it was recognised that transient solutions were of great importance. A major output of the project was intended to be a three-dimensional simulator capable of both steady state and transient simulations.

The project was organised into five workpackages: physical models, discretisation schemes, mesh generation, linear algebra and software development. The activities and achievements of these strands of the project are described in the following sections.

A special section devoted to a description of the final project research program, EVEREST, which give some detailed on its capabilities and limitations. This section also includes the results of examples from the benchmark suite and the industrial problems used in the validation of the suite.

Although in general the project progressed well, there were two occasions when the Technical Annexe of the project required modification. The first of these was after Workpackage 5 had made an assessment of the requirements of the project code and the resources required to perform the task. This assessment required the project to re-allocated effort, taking it from Workpackages 2, 3 and 4 and placing it in Workpackage 5. The goal of this re-distribution was to ensure that the deliverable of the project code would be made.

A second event that required a major restructuring of the project was the withdrawal of GEC. GEC were major contributors to the project and their withdrawal had a significant impact. As a result of GEC's action, STC Technology joined the project and was able to take up some of the work proposed by GEC. Those activities proposed by GEC that STC could not take responsibility for were taken up by the other partners. This re-distribution required a second revision of the Technical Annexe.

Although some difficulties were encountered by most partners, over the four years, in securing the necessary technical staff to work on the project, in general there were few delays in the work plan. The only major problem that delayed work was in Workpackage 5 during the phase on implementing adaptive mesh generation and refinement. This led to a second review of these results.

1.8 Achievements

Although the major goals of any project are laid down in the project plan, and that the main achievements of the project are to meet these, each partner of such a large project as EVEREST will be able to identify achievements relating specifically to themselves. EVEREST as a whole succeeded in achieving its primary goal: the development of general numerical techniques to provide simulation of sub-micron silicon based devices in three dimensions and time. A major achievement for the community is the availability of these techniques in a number of simulators: CURRY, HFIELDS-3D and EVEREST.

The project has published its results through conferences, journals and a special workshop at the ESPRIT week. In total over 150 reports and papers have been produced. These are in general available to the community through their authors and the European Commission.

Below is detailed some of the achievements each partner wished to highlight as results produced within the project.

1.8.1 STC Technology Ltd

Within Workpackage 1, STC have been involved in the development of accurate physical models for the simulation of silicon bipolar transistors. In particular this has resulted in the definition of a self-consistent set of models for minority carrier mobility, lifetime and also doping dependent intrinsic carrier concentration. These models have proved successful in existing two-dimensional simulation and have also been satisfactorily installed in the project three-dimensional simulator. STC have also successfully achieved establishing three benchmarks problems based on real devices to validate the accuracy of the physical modelling.

As part of the exercise in modelling an advanced STC bipolar device an improved analysis of the base doping was developed. Confidence in the model was justified by calculating the base profile to be estimated by correlating SIMS, spreading resistance, pinched base resistance, capacitance-voltage and Early voltage data. The benchmarks were successfully simulated with two-dimensional simulators, thereby proving the suitability of the physical models. They were also simulated with the project simulator, thereby demonstrating the accuracy of the project code. STC were also successful, through their role in testing and specifying the project code, in ensuring that the code could practically handle devices of interest.

For example, the means of specifying doping profiles based on 'mask' window areas and profiles that can be taken from SIMS profiles suitably spread around the window edges, allows realistic quasi-three-dimensional doping profiles to be generated from information that is readily available to the device engineer.

1.8.2 Philips

Philips has been mainly involved in algorithmic development of discretisation techniques, meshing and solution techniques. In these areas, several methods were developed successfully.

The main achievement has been the adaptive solution of semiconductor problems. This is of the great importance, since it is clear that the manual meshing of three-dimensional problems is a formidable task. Also, one can question the accuracy of results obtained for manually meshed problems. In the context of adaptive solving, several new techniques have been developed and existing techniques improved.

The Scharfetter-Gummel scheme has been extended to include the case of avalanche generation, thus enabling a robust solution of this important class of problems. For example, using this technique the electrostatic discharge of MOS transistors has been simulated.

Existing iterative solution techniques for the linear systems involved have been used and improved where necessary for the specific application to semiconductor problems. Also, the technique of correction transformation for the solution of nonlinear problems was developed and successfully used for simulating state-of-the-art devices. A two-stage procedure for the solution of adaptively meshed problems was developed. A similar technique was developed by UB, which strengthened our belief in the method. Finally, Gear's method was adapted to handle semiconductor problems.

1.8.3 Rutherford Appleton Laboratory

As the leading contractor in the EVEREST Project, RAL would claim that the successful completion of the project is a major achievement. The organisation and co-operation between so many partners had the potential to create many difficulties. The good working relationships and the large output of the project can to attributed to the Project's very able partners but also to the overall direction and management of the Rutherford Appleton Laboratory. In an age when funding is difficult to secure, the ability to plan and manage research projects effectively is essential.

Although the leading contractor RAL was also coordinator of two workpackages within the project: Workpackage 3, mesh generation and refinement and Workpackage 5, project software development. Responsibility of Workpackage 3 was taken up by UCS when the scope of Workpackage 5 had been defined. RAL also contributed the Workpackages 2 and 4. The main technical achievements were:

- The development of a full three-dimensional device simulator which has been tested on wide range of devices.
- The development of mesh generation and adaption methods for three-dimensional problems.
- Development and implementation of mesh generation algorithms that exhibit a large measure of parallelism.
- Implementation of semiconductor simulation software on share-memory multi-processor systems exploiting task level parallelism.

1.8.4 SGS-Thomson

The main achievements by SGS-THOMSON were:

- To develop and verify a new mobility model suitable for two and three-dimensional simulations of planar and non-planar transistors.
- To determine the ionization energy of boron in silicon as function of impurity concentration.
- To establish a suitable methodology for the statistical analysis of semiconductor devices by using process and device simulation. To this purpose both sensitivity analysis and Response Surface Method (RSM) methodologies have been analyzed, tested and compared by using both the approaches on real examples.

1.8.5 Trinity College Dublin

Trinity College made major advances in the discretisation techniques. In addition it was one of the three main contributors to the Project Code EVEREST (Workpackage 5).

1.8.6 University College Swansea

The three main achievements of University College Swansea are:

- The successful participation in Work Package 3 (Mesh Generation Algorithms) for which we also took the coordinator role.
- Our involvement in the EVEREST Project software itself was a major one.
- Also of note was the production of the Post-Processor section of EVEREST.

1.8.7 University of Bologna

A summary of the achievements of the University are given below:

- Error Analysis and Adaption, aimed at developing an automatic grid-refinement technique to be used in the two-dimensional device simulations.
- Discretisation with Hot-Electron Effects, has dealt with the development of an impact-ionization model based on the mean energy of the carriers, to be used in the frame of the so-called "hydrodynamic" model of semiconductor devices.
- Mesh Generation and Refinement, was concentrated toward the development of a three-dimensional mesh generator based on prismatic elements, ATMOS-3D.
- Linear Solvers, aimed at the development of a vector version of the three-dimensional device analysis code HFIELDS-3D, suitable for a CRAY-XMP machine available in Bologna. In order to achieve this goal, a rather deep restructuring work of the data structures within the program was carried out. At the same time, the vector version of the linear solver based on the ICCG method (see also below), was incorporated in the vector version of the code.
- Non-Linear Solvers, aimed at implementing and improving the performance of, the scalar version of HFIELDS-3D. This goal has been pursued by a rather deep restructuring work of the data structures within the program, which has been carried out with the aim of making compatible with the iterative algebraic solvers, namely those based on the ICCG and GCS methods, provided to UB by STC.

1.8.8 IMEC

It has been demonstrated that in all device simulators the effect of the drain and source series resistance has to be included.

A new analytical MOS model has been developed with improved bulk effect for non-uniform doping. Improved models for threshold voltage and mobility degradation have been developed. These are based on a local potential approach and the approach has been validated down to a 0.7 μm channel length.

A new algorithm for incorporating an avalanche model in a device simulator, taking secondary ionization into account and independent on grid-size has been developed. The validity of the ionization coefficients of Van Overstraeten and De Man for low electric fields has been proven.

For extracting the ionization coefficients a special test structure was designed. SIMPAR and EXPER have been proven to be reliable tools for parameter extraction for circuit simulation as well as for any physical model fitting. The program includes slope fitting and sensitivity analysis.

1.8.9 NMRC

A parameter extraction program which reliably fits measured MOSFETs to SPICE models has been developed. Also developed have been improved MOSFET models, particularly NMOD which predicts analog circuit behaviour well. Parameter extraction procedures from device to circuit models for MOSFETs and JFETs have been devised which greatly improve overall device simulation speed.

2 Task Summaries

2.1 Workpackage 1 – Physical Models and Validation

Coordinator: SGS
Members: ADBV, IMEC, NMRC, SGS, STC

2.1.1 Introduction

Correct and reliable physical models are the key to establishing the validity and accuracy of a numerical device simulation. The four main strands of this workpackage were to provide the necessary information and insight to three-dimensional modelling to develop effective physical models. The four tasks defined were:

- Task 1.1 Validation
- Task 1.2 Physical and Analytical Models
- Task 1.3 Parameter Extraction
- Task 1.4 Fabrication & Measurement of Test Structures

2.1.2 Summary of Activities

The activities of Workpackage 1 cover a very broad spectrum ranging from the manufacture of test devices to the assessment of the current device and circuit simulators. The workpackage completed many tasks during the project and it is not possible to review all of them in any detail. A brief view of some of the activities will be given although full details can be found in the project reports and publications.

Within the workpackage each partner had a well laid plans. The first year saw activity in most of the workpackage areas. In particular, the design, fabrication and measurement of test structures was started very early in the project and continued throughout its duration. Special devices such as a resistive gate IGFET were designed and fabricated.

As the performance of all simulators is based on the quality of the physical processes represented in the model considerable effort in the project was given over to the assessment and development of physical models. The first period of the project saw a major assessment of the current models. Consideration was given to all the basic physical processes. For example the effects of the saturation drift velocity and those of short and long channels in MOS design were the first to be considered. In each case the requirements of three-dimensional modelling were investigated. Clearly in some cases the dimensionality of the simulation had no significant effect on the modelling.

As a major goal of the project was to develop a full three-dimensional device simulator, Workpackage 1 started a task on the evaluation of existing simulators. Programs such as BAMBI, MINIMOS, PISCES and PRISM were assessed against a variety of devices and the results compared with measurements. The conclusions of this evaluation would help in specifying the requirements for the project simulator.

Two complementary activities were also started: the development of analytic models and parameter extraction. Investigations into analytic models were started to gain more insight into local phenomena and to compare the results from the numerical simulations. As the results from device simulator would finally be used as input to circuit simulation, methods of extracting the circuit model parameters were to be investigated. As an initial step a number of different circuit simulators, such as SPICE were compared and proposals for their improvement developed.

During the second year the project started to use the results, from the devices designed and fabricated during the first year, in the validation process. This work continued in parallel with the program of software assessment as the scope and complexity of the device structures was increased. Studies on the calculation of more basic parameters such as threshold voltage and MOS capacitance were started. Improvements to SPICE models were made to fit the drain conductance in MOS devices. In the realm of circuit simulation efforts were made to reduce the amount of data required to produce reliable circuit parameters. Many of these activities centred around programs such as POPS, SIMPAR and ADEPT.

The general physical models required by device simulators were improved reflecting the comparisons with measured results. One such improvement was a new mobility model taking into account more effectively of the difference natures of holes and electrons in the silicon lattice. Avalanche multiplication was addressed and the various models assessed.

In all these activities the sensitivity of the results to changes in the data and model parameters was under consideration. In particular the input of changes in process parameters on the final profiles was investigated in both TITAN and IMPACT simulators, as these modifications in profile would greatly effect the final electrical behaviour of the devices.

Work on physical model assessment and development continued in the following years. For example the requirements for accurate saturation velocity in MOS devices, realistic channel mobility and an understanding of heavy doping effects provided the driving force for this task. A set of benchmark problems to investigate such effects were designed and fabricated. Models including temperature dependence of carrier mobility and avalanche phenomenon were developed, as were representations for the effects of non-uniformity in channel doping in MOS devices. Measurements were made on NMOS LDD structures and a variety of bipolar devices to compared against the new models.

In the activity on parameter extraction for circuit simulators large quantities of data were transferred between partners. Each then used the data to extract parameters for the MOS Level 3 model in SPICE. A detailed comparison of the results was made. Similar data collection activities were performed on n-channel MOS devices for the sensitivity analysis.

During each period, results from Workpackage 1 that had an impact on other activities within the project were fed back. In the final year efforts were concentrated on a number of specific objectives. These were: modelling and validation of impact ionization, modelling and validation of bipolar devices, links between device and circuit simulators and the analysis and measurement of the statistical distribution of device parameters. Among techniques developed and assessed was the Response Surface Method (RSM). This method attempted to characterise the relationship between process variables and electrical response by a simple analytic function. If successful this technique would of great advantage to designers trying to improve device performance. As part of the circuit simulation activity the package CODECS was assessed. This was one of the first simulators that attempted to combine device and circuit simulation in a single piece of software.

2.1.3 Major Achievements

Workpackage 1 had set out to progress the state-of-the-art in four major areas of device technology. The first, physical models, which are the heart of any device simulator, have been reviewed, assessed and developed. The developments have been implemented in both in-house software and the project research code. Their impact on the design process has been considered and recommendations have been made on how best to used such models.

Methods for extracting SPICE and other circuit simulator parameters have been developed and the sensitivity of these to the fabrication process investigated. The links between device and circuit simulators have been improved and an assessment made of the coupling process.

Throughout the project, Workpackage 1 has designed, fabricated and measured many test structures the results of which have been distributed to the partners and reported in the project reports. These experiments have provided essential data in the development and validation of the physical models and have improved the basic understanding of the physical behaviour of device structures.

2.2 Workpackage 2 – Problem Discretisation

Coordinator: Philips
Members: IMEC, Philips, RAL, TCD, UB, UCS

2.2.1 Introduction

The main aim of Workpackage 2 was to provide robust and efficient algorithms for the discretisation of the equations modelling the behaviour of semiconductor devices in three space dimensions. Since there are several ways to achieve this, the work was subdivided into the following tasks:

- Task 2.1 General discretisations
- Task 2.2 Fitted discretisations
- Task 2.3 Error analysis and adaption
- Task 2.4 Discretisation under parallel hardware
- Task 2.5 Discretisation with hot electron effects

Within each of these tasks, a plan of work was agreed which consisted of a gradual development from relatively simple discretisation techniques on fixed grids for the stationary problem towards adaptive techniques for the time dependent problem.

2.2.2 Summary of Activities

In the first year of the project focus has been mainly on techniques for discretising the stationary equations on a fixed mesh. First of all, the discretisation of Poisson's equation in three-dimensional problems was investigated using several different element types (tetrahedra, hexahedra, prismatic elements) and discretisation methods (box method, finite element method, finite differences). Using these techniques, several partners solved the three-dimensional off-state problem, and results were compared for a number of benchmark problems. Also, work started on extensions of the Scharfetter-Gummel scheme for the continuity equations, again for several element types.

In the second year a change of emphasis was given in the direction of error analysis and adaption and discretisations for the transient problem. Close cooperation with the partners working in Workpackage 3 was set up since it became clear that it is not possible to design a discretisation on arbitrary elements that will guarantee positive carrier concentrations. In other words, meshing must pay particular attention to the characteristics of the mesh in order that a stable and accurate discretisation be possible. During the second year of the project, research was initiated on a promising new technique for discretising the semiconductor equations: the mixed finite element method. Although this method had been in existence for many years, its application to the device problem was relatively new. Both Philips and TCD made much progress in understanding the advantages and disadvantages of the method, and several remedies to overcome the latter were developed successfully. Finally, work started on hot electrons, the aim being improved mobility and avalanche modelling.

During the third year of the project, work on strategies for adaptive meshing was intensified since Workpackage 5 needed such strategies in the final year of the project. To this end, error estimates based on changes in the components of flux across element boundaries were developed. For the Poisson equation the flux change corresponds to a change in electric displacement and for the continuity equations a change in current density. Both UB and Philips produced an adaptive version of their in-house codes in order to demonstrate the practical value of the techniques developed. Also, in the third year, work on the mixed finite element method and on the discretisation with hot carrier effects continued. TCD worked on an extension of their mixed finite element method to three-dimensional, and showed that the method is conservative and convergent when a Delaunay triangulation is used. Philips introduced the so-called Q-trick which stabilised the mixed finite element method and thus made it applicable to semiconductor device problems. Concerning hot electron effects, UB studied a physical model for impact ionization based on carrier energy. This model overcomes the difficulties related to an expression based on the local value of the electric field, which is the technique used so far. Finally, work was performed on discretising the time dependent semiconductor equations. Several schemes were compared with respect to efficiency, robustness and stability. Also, time stepping strategies were investigated for all of these methods.

In the fourth and final year of the project, focus remained on error indicators for use in an adaptive refinement, and discretisation techniques for the time dependent problem. Results of these activities were urgently needed for use in the Project Research Code being developed in Workpackage 5. Furthermore, Philips worked out a variety of ideas for developing stable mixed finite elements; this activity was closely related to the work on multigrid methods. Philips extended the Scharfetter-Gummel scheme for the case where avalanche generation is included in the equations. The latter is one of the most challenging problems; it was shown that the method developed enables a stable solution of this problem. The activity carried out by UB during the fourth year dealt with the final merge of the recently developed impact ionization model into the hydrodynamic version of their programme HFIELDS, and with testing the model against a specific device structure. Furthermore, RAL investigated the implications of parallel architecture on the discretisation, and Philips also concentrated on error criteria for adaptive AC and transient calculations.

2.2.3 Major Achievements

In the following a summary of the main achievements is given. For the discretisation of the steady-state, fixed mesh problem, a number of algorithms have been investigated and developed. The main conclusion is that the box method using the extended Scharfetter-Gummel scheme should be used for the discretisation. When used on a Delaunay mesh, this method is stable, convergent and conservative, which are exactly the requirements formulated at the beginning of the project. A negative result has been obtained for the mixed finite element method: this method (in its present form) does not comply with all requirements formulated. However, the method has been considerably improved by the partners in this project and, as a result of this, future developments may lead to a method which is applicable to the device problem. The major achievement has been the development of discretisation techniques and error estimators for use in an adaptive environment. The need for such techniques is high, since it is clear that the meshing of three-dimensional problems is a formidable, and sometimes impossible, task. The techniques developed for adaptive meshing in this project have been at the forefront of research. For the first time, truly adaptive device modelling tools have been produced. Both Philips and UB have demonstrated the effectiveness of the algorithms developed, especially for new device structures where the knowledge about mesh placement is not available a priori. The implementation of these techniques into the project research code and the subsequent application to the adaptive solution of three-dimensional problems is unique in the world. Several scattered results have been obtained, some of which are also unique. For example, the activity on the modelling of hot carrier effects has been successful in designing discretisation methods for this type of problem, and new approaches to the modelling of avalanche generation. Also, an extension of the Scharfetter-Gummel scheme for the case of avalanche generation has been developed, which is much more stable than the ordinary Scharfetter-Gummel scheme. Several very advanced problems have been solved using this new technique, which failed using existing techniques.

2.3 Workpackage 3 – Mesh Generation and Refinement

Coordinators: RAL, UCS
Members: Philips, RAL, TCD, UCS, UB

2.3.1 Introduction

This workpackage aimed to generate automatically finite element and finite difference base meshes and grids which were optimised for the semiconductor simulation problem. The automatic nature of such techniques was thought of great importance in the realm of three-dimensional simulation since there was little likelihood of the user being able to direct the development of a mesh for complex multi-layered structures. The three major tasks identified were:

- Task 3.1 Manual and Automatic Schemes
- Task 3.2 Adaptive Refinement
- Task 3.3 Exploitation of Advanced Hardware

2.3.2 Summary of Activities

The area of mesh generation in two dimensions was a well developed field at the start of the project. Many partners had had experience with two-dimensional generator schemes. The extension of these techniques to form three-dimensional generators was not so well advanced. In the fields of stress analysis, computational fluid dynamics and electromagnetics geometric modelling and mesh generation had advanced in three dimensions. However in general these techniques had been developed for specific problems and applications.

Workpackage 3 intended to provide general three-dimensional mesh generation and adaption methods. Work in the first year of the task centred around existing techniques being used in two-dimensional software and investigating methods by which these could be applied to three-dimensional problems. The main methods under consideration were: Delaunay triangularisation using tetrahedra, generation of prismatic extensions to a two-dimensional triangular mesh, simple mapping and generation methods in cartesian systems using hexahedra and multigrid methods. The two-dimensional Delaunay techniques were review and enhanced to modelling and mesh more complex geometries. These were then extended into three dimensions.

The other main strand of the workpackage during the first year was on mesh adaption. A review of error estimators and adaption strategies was completed and methods suitable for three-dimensional implementation identified. The selected estimators and refinement strategies were first implemented in two-dimensional programs to investigate there properties.

The second year of the project saw the successful implementation of a number of three-dimensional geometric modellers and mesh generators based on the techniques identified. These were applied to many different types of device structure. Many problems were uncovered during this period in the modelling and meshing of the complex multi-layered structure of modern devices. All the methods developed had their problems. From the difficulty of node placement in the Delaunay generators to the problems in provide mesh density transition in the z-direction in the prismatic approach. As part of the development and assessment these generators were interfaced to particular device simulators and geometric modellers. The initial version of the Workpackage 5 geometric modeller and mesh generator was developed using the Delaunay base methods. In parallel with these three-dimensional developments work continued on improving the efficiency of the established two-dimensional systems.

Work on error estimators continued and a number of methods tested in simulators. The main problem was found to be choosing estimators that not only detected errors in the solution but were cheap to compute. The refinement strategies continued in the two directions: enrichment by the addition of new nodes and mesh re-distribution.

During the subsequent years of the project attention was centred on mesh adaption and refinement. The error estimates developed and test on two-dimensional problems showed great promise. They were showing that this type of mesh control would provide significant benefits. Robustness and efficiency became the prime research topics. These would be essential in a three-dimensional simulator. Test were generally based on the benchmark set developed in Workpackage 5 and in the on-state. Devices of large complexity were considered: EPROM cells and CMOS structures were meshed statically and adaptively.

The results of this work were collected and discuss with those developing the project code and suitable techniques and strategies implemented.

2.3.3 Major Achievements

Throughout the project Workpackage 3 developed and implemented a variety of two and three-dimensional mesh generators. Three major achievements were: the development of a full three-dimensional generator using prismatic elements, a three-dimensional Delaunay generator using tetrahedral elements and the development of a hybrid generator forming a Delaunay mesh using a mixture of tetrahedra and hexahedra.

The work on error estimates and refinement strategies gave rise to a selection on estimates based on charge, potential, electric fields and current densities and a number of overall refinement and mesh re-distribution strategies.

2.4 Workpackage 4 – Linear and Non–linear Solution Strategies

Coordinator: Philips
Members: IMEC, Philips, RAL, TCD, UB

2.4.1 Introduction

The main aim of Workpackage 4 was to provide robust and efficient algorithms for solving the discretised semiconductor equations in three dimensions. A natural subdivision into tasks was employed:

- Task 4.1 Linear solvers
- Task 4.2 Nonlinear solvers
- Task 4.3 Transient solvers

Within each of these subtasks, workplans were designed which complied with the development of the project research code. Also, strong links with Workpackages 2 and 3 existed. Therefore, the emphasis gradually shifted from solution techniques on fixed grids to solution methods on adaptively generated grids.

2.4.2 Summary of Activities

In the first year of the project focus had been mainly on Tasks 4.1 and 4.2 because techniques for solving the nonlinear and linear systems were required immediately (for obvious reasons). The extensive research in Task 4.1 led to two robust and very efficient methods for solving the linear systems of equations: ICCG for the symmetric systems and incomplete LU preconditioned CGS for the non-symmetric systems. Task 4.2 mainly concentrated on solution techniques for the Poisson equation. Damping and clamping techniques were developed and investigated. Also, a new technique called *correction transformation* was succesfully applied to the solution of Poisson's equation and shown to lead to a considerable decrease of the number of nonlinear iterations.

In the second year of the project, partners in Workpackage 4 concentrated on the solution of the nonlinear and transient problem. Damping techniques were further developed and tested, and time stepping strategies were investigated. Furthermore, several partners solved three-dimensional off-state problems using the algorithms developed, with results showing good agreement. Also, initial tests with on-state solvers were carried out in three-dimensional: UB developed a three-dimensional code based on prismatic elements and demonstrated significant differences with results obtained from two-dimensional simulations. At the end of the second year, a re-allocation of effort was defined because of the withdrawal from the project by GEC. It was decided that the new partner, STC, was not going to take over GEC's tasks in the Workpackages 2, 3 and 4, and therefore several partners re- defined their effort in these workpackages.

During the third year of the project, work on nonlinear and transients solvers concluded. UB demonstrated the effectiveness of the algorithms by solving a floating gate EPROM cell. Again, significant differences with the two-dimensional simulation results were found. Philips concentrated on combined stopping criteria for the linear and nonlinear systems, and achieved a considerable speed-up with this technique, as well as increased accuracy of results. The work on transient solvers mainly focussed on time stepping strategies, which is one of the most important factors determining the efficiency. Finally, tests using an AC-facility were conducted, showing that the techniques developed are indeed applicable to such problems. It should be remarked that some work on linear solvers had to be carried out in this context, since the linear systems involved contain complex matrices.

Most of the effort in the fourth year of the project has been on improvement of nonlinear solution techniques, whereas RAL has concentrated on improvement of the performance of the Project Research Code EVEREST on parallel and vector machines. Also, UB concentrated on speeding up the ICCG and CGS solvers on parallel machines. The main emphasis during the final year was on adaptive solution techniques, both for the steady-state, transient and the AC case. In all cases, methods were developed successfully. The most important step towards the solution of adaptively meshed problems was the development of a two-stage solution procedure. This procedure can only be used in programmes which use the subset solving algorithm; fortunately, this technique was used by all partners involved since it was a technique which was recommended during the first years of this project. Using this two-stage procedure has enabled the partners in this project to solve several advanced problems in an adaptive way, not only for the steady-state problem, but also for time dependent and AC problems.

2.4.3 Major achievements

In this project the work on linear solvers has been very successful. Since its start in 1986, the Project has always advocated the use of iterative linear solvers for the solution of device modelling problems. Gradually, other device modelling groups are recognising the importance of these techniques and over the past few years the number of groups switching to these methods is rapidly growing. The use of ICCG and CGS has enabled the partners in this project to indeed solve three-dimensional problems, a task which could not have been carried out without these techniques.

The main achievement in the development of nonlinear solution procedures is the two-stage solution technique for adaptively discretised problems. Conventional algorithms can not cope with such problems, but the two-stage procedure based on subset solving can. Both UB and Philips have used this technique for their device modelling problems. Furthermore, it has been implemented in the project research code EVEREST and used successfully for solving adaptive problems. Another important achievement on nonlinear solution techniques is the method of correction transformation. This method has been developed for use on the coupled problem and on the Poisson problem (decoupled solution), showing considerable speed-up in both cases. This method is new and is gradually becoming recognised by other groups working in the field of semiconductor modelling.

The main achievement on transient solution techniques is the development of an adapted Gear's method and a corresponding time stepping strategy. Also, an adaptive algorithms have been designed for transient and AC problems. The latter is unique and has not been noticed elsewhere in the literature.

2.5 Workpackage 5 – Project Research Program

Coordinator: RAL
Members: IMEC, Philips, RAL, STC, TCD, UCS

2.5.1 Introduction

A major deliverable of the project was a modular software system demonstrating a consistent set of techniques and algorithms developed during the project. This software was intended both as a test bed for work done during the project, but also as the basis for the development of a commercial three-dimensional device simulator. The activity in this workpackage was broken down into the following five tasks:

- Task 5.1 Design
- Task 5.2 Graphics
- Task 5.3 Serial Implementation
- Task 5.4 Advanced Post Processing
- Task 5.5 Validation The work of this Workpackage required the very close collaboration of six partners in the project. During the implementation phases this required meeting on a very regular basis and exchanging staff. As part of the software strategy common development standards were adopted.

2.5.2 Summary of Activities

The first six months of the workpackage were devoted to the assessment of the task and the definition of requirements. This included the production of a number of initial reports on geometric modelling, mesh generation, post processing and data bases. At the end of this period it was concluded that there was a serious short-fall in the effort allocated to the workpackage to enable it achieve its goals. An outline plan with man power estimates was prepared and presented to the project.

The second period of the first year saw a re-allocation of effort to the workpackage and the production of the first detailed plan. Each partner involved in the workpackage was given responsibility for a specific area: pre-processor and mesh generation (TCD); impurity profiles and post processor (UCS); solver module, infrastructure and coordination (RAL). Other partners involved in the design phase were SGS and GEC. A specification of the overall software framework was produced and the necessary background and third-party software gather and distributed. The framework was based on two pieces of common software: the command parsing environment and the neutral files data base. These elements of software would help the software integration process.

The major goal of the second year was to implement a full three-dimensional off-state solver using the techniques developed in the other workpackages of the project. The elements of the suite that were completed during the year were: a basic geometric modelling with integrated mesh generator, an impurity profile generator, the three-dimensional off-state solver module and an initial post processor. In parallel with these developments a number of test problems were defined to be used in the validation process. These included both very simple tests such as a block of silicon to a high voltage reference diode with a recessed contact. The end of the second year saw the successful demonstration of the off-state solver.

Even at this early stage the needs of device engineers were taken into account. The initial geometric modeller was found to be difficult to use and time consuming. To help over come this problem a library of standard devices was developed. This library provided a way in which commonly used device structures could be concisely presented to the designer. Each device was characterised by a number of critical parameters which the user provide and the rest of the geometric description was generated by the pre-processor.

Once the complete off-state solver had been implemented effort in the workpackage was directed toward the on-state solution. Using the same basic software framework the solver module was extensively enhanced to include new linear algebra, a library of physical models, discretisation schemes for the continuity equations, and an implementation of both the Gummel and full Newton linearisation schemes. Each element used a consistent set of results from the other workpackages. By the end of the second year a basic on-state solver had been prepared.

The third year of the project centred about the testing, validation and assessment of the three-dimensional on-state solver. As part of this task a comprehensive set of test problems was developed. This ranged from simple one-dimensional diodes to full three-dimensional bipolar devices. During this period both Philips and STC took an active part in the validation and assessment process. This work resulted in the production of a large validation document and a set of recommendations for improving the suite.

The other major developments of the third year were the implementation of the transient solver and the laying of the foundations for adaptive mesh generation. Each of these objectives required considerable development and revision of the solver module. The basic initial mesh generator was re-written and new data structures included using the results of Workpackage 3. A adaption module was written for the solver and adaptive solution strategies developed. In parallel with this a Gear-type solver was introduced into the solver for transient problems. This was based on work from Workpackage 4. The major importance of this developed was that it would enable the solver to simulate device behaviour such as latch-up.

The final year of the project was taken up with the development and improvement of the adaptive solver. The work originally plan on a parallel implementation of the solver was abandoned in favour of applying more effort to adaptive solutions. Although some major difficulties were encountered in geometric modelling and mesh generation by the end of the project a fully adaptive three-dimension solver was demonstrated. A second, but just as important, strand of the work in the final year was the application of the suite to industrial problems. This led to a very careful assessment of the suite in the simulation of industrial devices such as a power MOSFET and a CCD. This work produced an extensive list recommendations for future developments.

2.5.3 Major Achievements

The most important achievement of Workpackage 5 within the project was to bring together many of the different ideas and techniques proposed by the other four workpackages into a fully adaptive three-dimensional simulator. This simulator is viewed as being one of the best in the world.

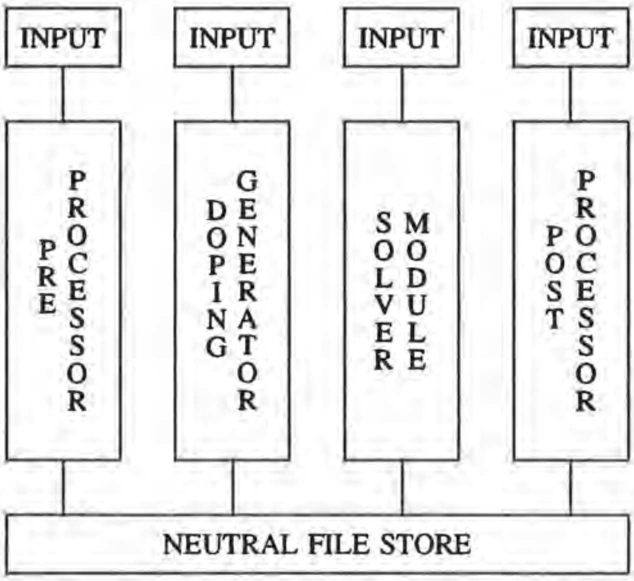

Figure 1: Structure of EVEREST Suite

3 EVEREST Software Suite

3.1 An Overview

EVEREST is the software package developed under Workpackage 5 for the simulation of three-dimensional semiconductor devices under steady state and time dependent conditions. The simulation is performed by the numerical solution of the fundamental partial differential equations which describe the electrical behaviour of semiconductors using the techniques developed in the other workpackages in the project. It has been designed to meet the needs of a device physicist, and provides total flexibility in device geometry definition, impurity profile generation and offers a selection of mathematical models to describe the physical processes. The suite contains a post-processor to enable the user to view primary quantities such as potentials and carrier densities and derived quantities such as currents, space charge, and recombination rate.

The complete software package consists of four stand alone modules: the pre-processor, the doping generator, the solver module and the post-processor each with its own command parsing environment and on line help system. The modules communicate via a set of neutral files and are used interactively or in background mode.

3.2 Capabilities and Limitations

As described above the EVEREST Suite consists of four main modules. In this section a brief indications of the capabilities and limitations of each is given. The full specification of the modules is given in the user documentation and the associated project reports.

The Pre-processor Module This module performs the geometric modelling and the mesh generation. The user can describe the geometric model in terms of a set of basic primitives; points, lines, surfaces and volumes or in terms of a set of high-level primitives; bricks, prisms and tetrahedra. In addition, there is a library of *standard models* containing the skeletons of device structures which can be extended by the user. The mesh generator fills the model with a mixture of hexahedral and tetrahedral elements and computes the quantities necessary for the simulation.

The Doping Generator This module enables the user to implant impurities into silicon, in a uniform profile, a Gaussian profile or a profile generated from another package. The uniform profiles are applied to defined geometric volumes and the Gaussian and external profiles are implanted through windows on the surface.

The Solver Module This module solves the coupled time dependent drift-diffusion semiconductor equations, using the control region method in space and the Gear method in time. The nonlinear systems of equations are solved by a modified damped Newton method and the linear systems are solved by the incomplete Choleski conjugate gradient method and the preconditioned conjugate gradient squared method.

The user is given a choice of models to describe the bandgap narrowing, the recombination rate and the carrier mobility, and control over some parameters in the numerical techniques to improve computational speed.

The Post-processor module This final module provides a facility to view the output from all the other modules. It will display the geometry, the mesh, the impurity distribution and various aspects of the solution in variety of ways; one dimensional graphs, contour plots, isometric projections, vector plots and I-V graphs.

Documentation In addition to the on-line help system provided by EVEREST full user documentation is available for all the modules giving details of all the commands and their associated parameters together with worked examples.

3.3 Benchmark Results

During the EVEREST Project a large benchmarking suite of devices was developed. These were used in all the assessments and testing of the programs. In this section the results from three typical semiconductor device structures are presented. These are selected to show the advantages of the adaptive solution of the problems over solution on static meshes.

The first example is a two-dimensional diode. The geometry is a $50\mu m \times 50\mu m \times 1\mu m$ brick, the front face of which is shown in Figure 2 together with the initial mesh. One contact extends along the bottom edge while the other extends $1.25\mu m$ along the top edge from the top left corner. The doping gives a circular junction of radius $30\mu m$ centred on the top left-hand corner. Three passes of refinement are carried out on doping to give the second mesh shown in Figure 2 with 872 nodes. Even with a locally structured mesh our technique captures the circular doping profile automatically. We also show the meshes after successive refinements on potential which contain 1504 and 2286 nodes respectively. In Figure 3 we show the electrostatic potential, ψ, on the line $x = 0$ for each of these meshes, illustrating the convergence of the solution.

The second device is a more complicated bipolar junction transistor. Here there are two electrical junctions which need to be resolved. Details of this device can be found in [2]. The quantity of major interest in such devices is the current-voltage characteristic, particularly the variation of emitter and base currents as the voltage between the base and emitter is changed. An adaptively generated

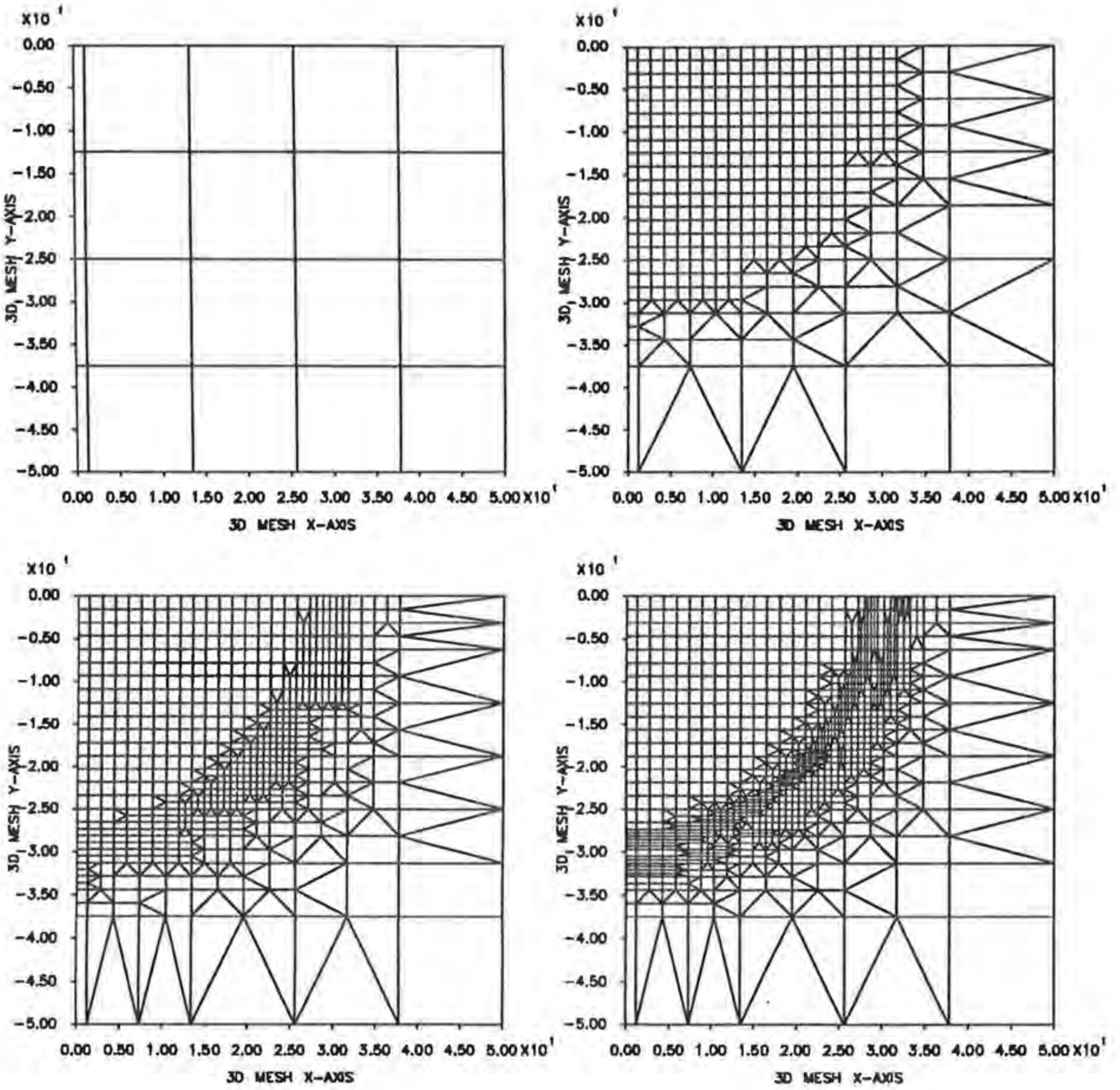

Figure 2: The initial mesh for the two-dimensional diode, the mesh after three passes of doping refinement and after each of two refinements on potential.

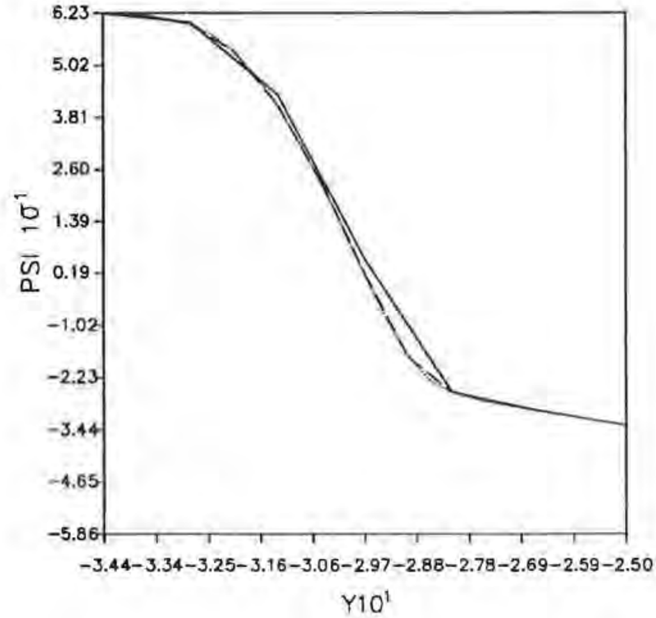

Figure 3: The electrostatic potential ψ, along the line $x = 0$ for the three refined meshes shown in Figure 2 (solid line: 872 nodes;dashed line: 1504 nodes; dotted line: 2286 nodes).

mesh for this device is shown in Figure 4 along with a plot of the calculated I-V characteristics. The high density of mesh lines near the top of the mesh indicates the location of the electrical junctions. The final mesh contains 2692 nodes. The I-V characteristic for this device has also been calculated using a static, user-generated mesh of 3300 nodes. Even for a two-dimensional device a considerable amount of time and effort is required to produce such a mesh by hand. The comparison of the I-V results in Figure 4 shows that good agreement is obtained between the results from the adaptive and static meshes. It should be noted that the present refinement criteria is based only on variation in the potential ψ. As mentioned in [1], it is expected that extending the criteria to include variation in current between elements will allow accurate I-V data to be obtained with fewer nodes and we are investigating such extensions.

The above examples are two-dimensional for ease of presentation and comparison with other device modelling software. Finally we present results for a three-dimensional MOSFET device. In such a device there are four basic regions of interest: the highly doped regions around the source and drain contacts, the lightly doped channel under the gate contact and the region under the field oxide. When a voltage is applied to the gate the potential rises in the channel region. This needs to be well resolved, since it is in this region that the bulk of the current flow occurs. The field oxide region is used to isolate the transistor from the influence of neighbouring devices and it is critical that this isolation is accurately modelled. This device thus illustrates the need to adapt both on doping (to identify source and drain regions) and on solution (to model the channel and isolation regions).

Figure 5A shows the geometry of the device. Dimensions are in μm. The dimensions of the MOSFET have been chosen in order to provide readily understandable meshes, since real devices often have a much higher aspect ratio. EVEREST has no difficulty in solving such problems, and

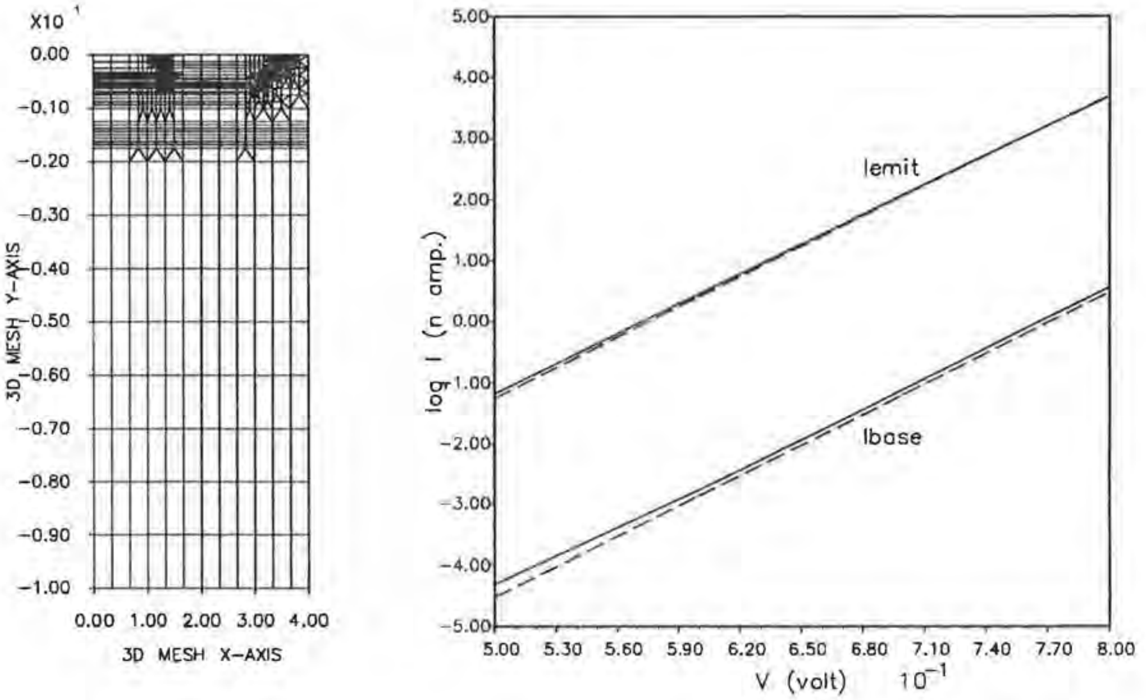

Figure 4: The adapted mesh for the two-dimensional bipolar transistor (left) and the calculated I-V data for this device (right). The emitter and base currents are shown as a function of the emitter-base voltage for the adapted mesh (solid lines) and the static mesh (dashed lines).

in particular in adapting the mesh. For illustrative purposes, however, a low aspect ratio device is preferable. The three other parts of Figure 5 show the mesh after refinement to completion, first on doping; secondly on potential first with $V_{gate} = 2V$ and $V_{drain} = 0V$, and finally on potential with $V_{gate} = V$ and $V_{drain} = 2V$. Figure 5B shows the mesh on the plane $x = 0$. Here the refinement which has taken place around the edge of the source and drain regions can be seen. Figure 5C shows the mesh on the plane $y = 2$ which is the plane in which the major part of the MOSFET action can be seen. Again the source and drain implants have been well resolved and in addition the channel under the gate contact has been enriched. Lastly, Figure 5D shows the mesh on the plane $x = 0$ and here we can see the resolution which has been added in order to resolve the effects of the convex corner of the gate contact which extends over the field oxide.

3.4 Industrial Results

As much modern device design has elements of three-dimensional behaviour, the programme should be judged on its behaviour for real three-dimensional examples. It should be stressed, however, that the research code developed in Workpackage 5 was intended to demonstrate the effectiveness, robustness and reliability of the algorithms in Workpackages 2, 3 and 4. Since most of the effort spent in Workpackage 5 has concentrated on achieving this goal, it is clear that several facilities which may be important to future users of the code have not yet been incorporated. Thus, many facilities which are available in commercial packages are not yet available in EVEREST. This means that the number of real examples which can be run using the code is slightly limited at the moment. Nevertheless, several examples can be simulated using the present version of the code.

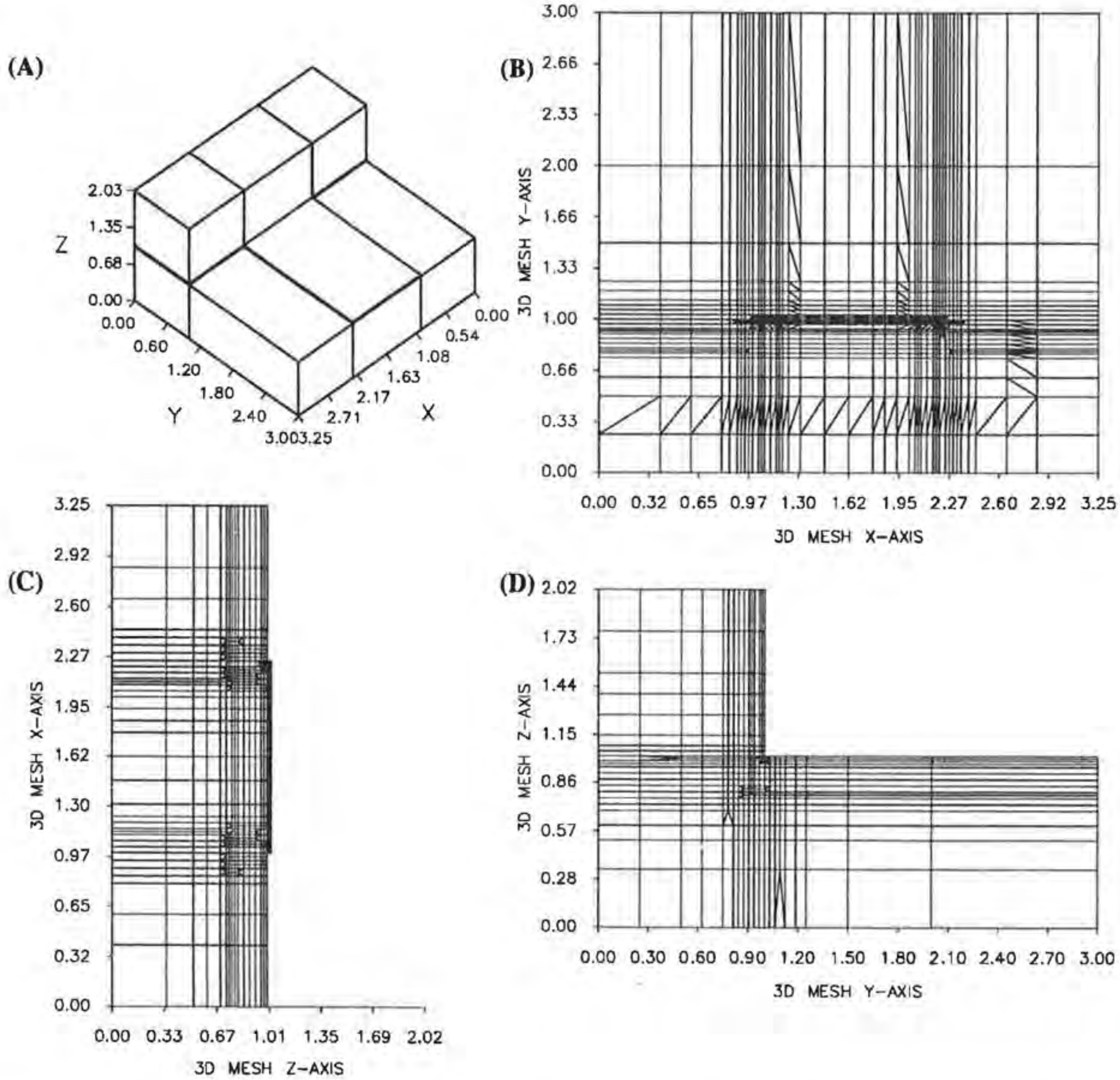

Figure 5: The geometry of a three-dimensional MOSFET and three cut planes through the mesh after refinement.

The first is a polysilicon emitter transistor with a fully three-dimensional structure around the emitter. Figure 6 shows the basic geometry of the device with the base and raised emitter contacts. The collector contact is on the back face simulating a buried collector layer. This is a device for which experimental results and two-dimensional simulations are available for comparison. SIMS profiles were used to define the doping for emitter, base and collector regions. Two stages of refinement are carried out, first on doping to ensure that features above $10^{14} cm^{-3}$ are resolved to within $0.033\mu m$ followed by a further three levels of refinement on potential with a collector bias of $2V$. The final mesh has 12163 nodes. This mesh is then used in all subsequent simulations. The predicted currents and Early voltage have been compared with measured data and with the two-dimensional simulator HFIELDS [4]. The same physical models were used in both simulations so that any differences are attributable to the methods used to solve the device equations. The two simulations agree well but the base currents are over-estimated compared with measurements. However, accuracy is consistent with two-dimensional simulators.

Figure 6 shows the logarithm of the net doping across the base region. The doping gradient has been well captured by the mesh used. Note that the isometric projection software is based on triangular elements so that diagonals have been inserted on quadrilaterals. In Figure 7 we show the electrostatic potential, ψ, on the plane $z = 0\mu m$. This shows how well the depletion regions around the base-emitter and base-collector junctions have been resolved.

The second device is based on a $1.25\mu m$ gate length n-MOS structure. The doping profiles were obtained from SUPREM [3] simulations with lateral diffusion of the source and drain implants approximated by a lateral error function with $\sigma_{\perp} = 0.04\mu m$. In this device we are looking for refinement of three features: the source and drain junctions, the channel under the gate and the spreading of the drain depletion region at high source-drain bias. The field oxide is approximated by a step as the isolation edge effects are not investigated. A schematic of the geometry in which the y-coordinate has been shrunk by a factor of 0.1 is shown in Figure 8. In this case the refinement is performed in three stages. Following refinement on doping to locate the source and drain junctions, $1.45V$ is placed on the gate so that refinement on potential captures the inversion layer. Then the gate is turned off and the drain biased at $2V$ to perform extra refinement around the drain depletion region. The final mesh contains 22731 nodes. Again, reasonable agreement with experiment is found, particularly given the uncertainties in the exact channel length and mobilities for the measured device. In particular the threshold voltage agrees well, although the drain current is greater than measured. This discrepancy could be due to an error in the channel length or in the mobility value used, or it could be due to not refining on current. However, the correct prediction of threshold indicates that the adaptive refinement has adequately described the channel doping and the inversion layer location.

In Figure 8 we show the customary MOS cross section on the end plane of the device where nearly two-dimensional behaviour is to be expected. For these simulations the mesh generated by the above technique was used but the bias conditions were $V_g = 1.95V$ and $V_d = 0.05V$. It can be seen that the source and drain regions and the channel are well resolved and a careful examination shows that there has been some extra refinement around the drain end depletion region. In Figure 9 we show a section through the centre of the gate contact. The use of a step field oxide introduces rapid curvature into the potential since it poses a Laplace problem with a Dirichlet boundary condition on an internal corner. The refinement has coped well with this difficult problem, although it could be argued that it has gone too far in trying to resolve the corner.

Thirdly we have simulated a charge-coupled device used in imaging applications. The compli-

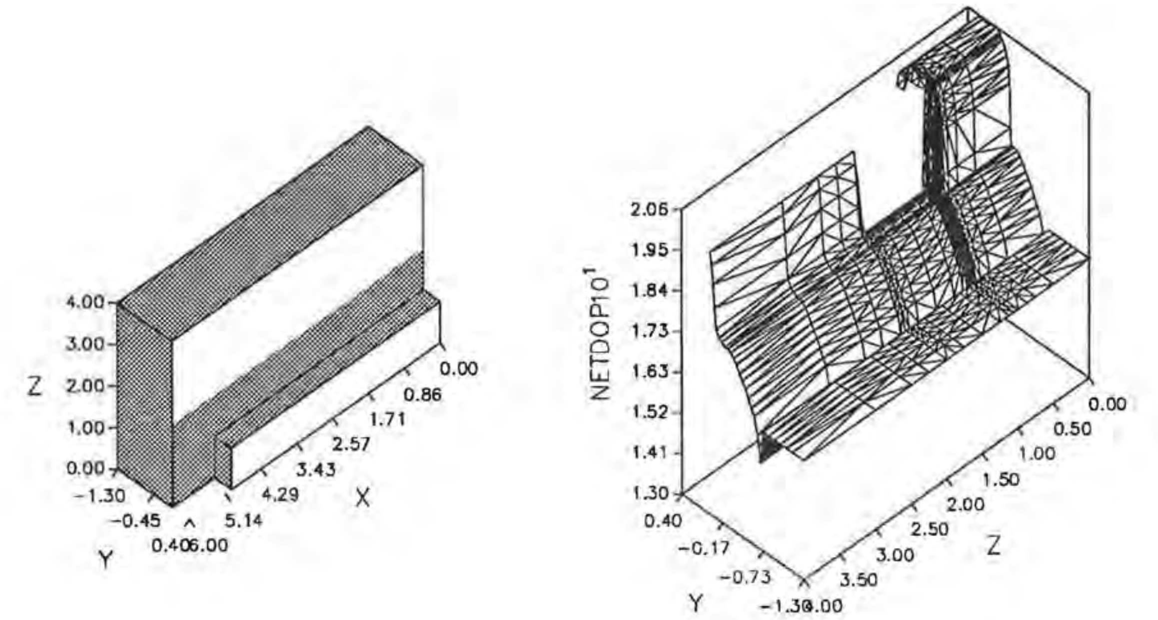

Figure 6: Geometry of the 3D *npn* bipolar (left). The white areas are the base and emitter contacts. An isometric view of the net doping ($\log|N_A - N_D|$) on the plane $x = 0\mu m$ is also shown (right), showing good resolution of the base doping.

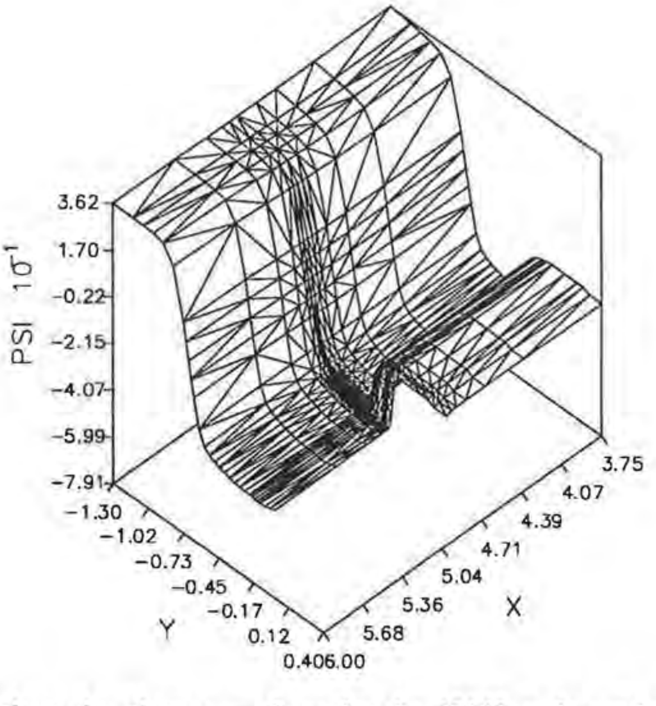

Figure 7: Potential on the plane $z = 0\mu m$ for the 12163 node mesh with $V_e = -0.8V$ and $V_c = V_b = 0V$.

cated doping profile for this device is incorporated into EVEREST by means of a Fortran subroutine. It consists of a background dope and several implantations leading to a three layer structure on one side of the device and a four-layer structure on the other. There are five gate contacts as well as contacts on an n-channel, a p-well and the substrate. In operation the two outer gates are held at $0V$ and the remaining three gates at $10V$. The substrate is biased at $15V$, the p-well at $4.5V$ and the n-channel at $10V$ reducing to $7V$.

Figure 10 shows three levels of mesh on the centre plane of this device. Top left is the initial coarse mesh of only 784 nodes where only minimal user input has been used to place nodes close to the gate contacts. Top right is the mesh following refinement on doping, which now contains 6027 nodes and is beginning to display features of the device. Then $2V$ is applied to the inner gates and the mesh refined to 9459 nodes as shown at bottom left. Now we can begin to see the gate structure emerge, particularly the high field region between the outer and inner gates. Finally the full $10V$ potential is applied to the inner gates and the mesh refined to 16609 nodes. An isometric plot of potential is shown bottom right. Some of the further refinement visible on this plot arises from the need to resolve potential features in other regions of the device and so appears not to be necessary on this plane. It is a feature of the restrictions which we place on the mesh that refinement spreads through the device until it can heal sensibly by a transition to a larger hexahedron or until it reaches the device boundary.

It is expected that the currents will increase exponentially as the p-well voltage is reduced and this is seen. In fact, the height of the potential barrier experienced by the carriers in the device can be calculated and the current shows an exponential dependence on this barrier height. Finally it is worth noting that the simulations have shown discrepancies with the one-dimensional based rules of thumb commonly used to explain the operation of such CCD-cells. Clearly the three-dimensional nature of the device is manifesting itself at a fundamental level and the use of simulators such as EVEREST will be valuable in understanding how such devices work and can be optimised.

3.5 Status, Availability and Maturity

The development of the EVEREST Suite has been continued by a number of partners, notably by RAL. Through its contacts in the academic community EVEREST has been applied of several new device structures. The solver module and post processor have been improved and the range of device simulated by the suite increased. Mesh adaption has been extended in include adaption of current densities and electric fields.

The suite is available from all partners but the most up to date version is only available from RAL. A version can be obtained by writing to the RAL contact name given in Appendix I.

4 Project Software Development

In the following section a brief description is given of the other software developed within the EVEREST Project. Readers should approach the specific contact person at the institution producing the software for further details.

4.1 NMRC

Two specific programs in the area of parameter extraction were developed at NMRC. These were:

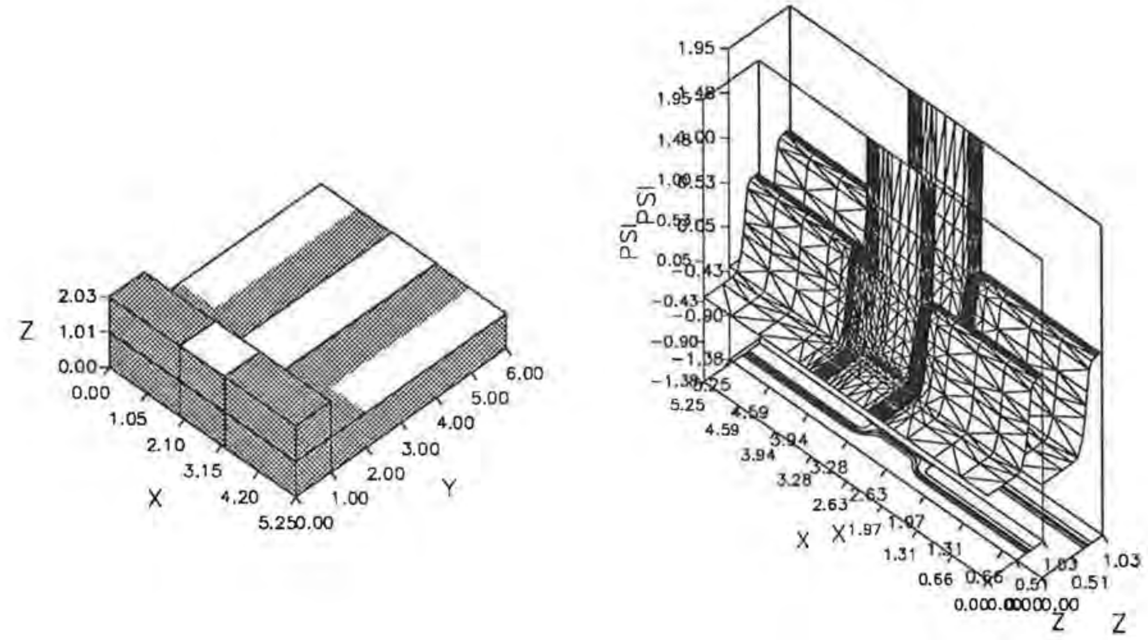

Figure 8: Geometry of the MOSFET (left, in μm, except the y-axis which is compressed by a factor of 10). The central white strip is the gate contact with source and drain to either side. The block of field oxide extends from 0 to $10\mu m$ in y. To the right is shown the potential on the face $y = 60\mu m$.

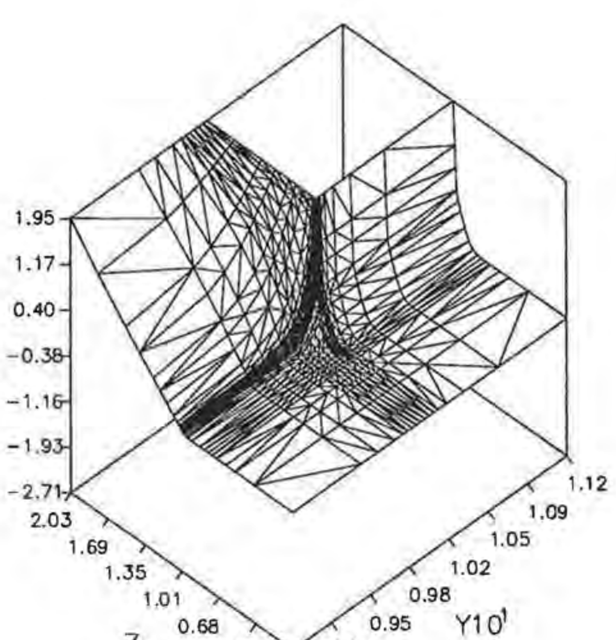

Figure 9: Potential on the plane $x = 2.625\mu m$, along the centre of the gate. Only the region around the field oxide corner is shown. Solution with $V_g = 1.95V$ and $V_d = 0.05V$.

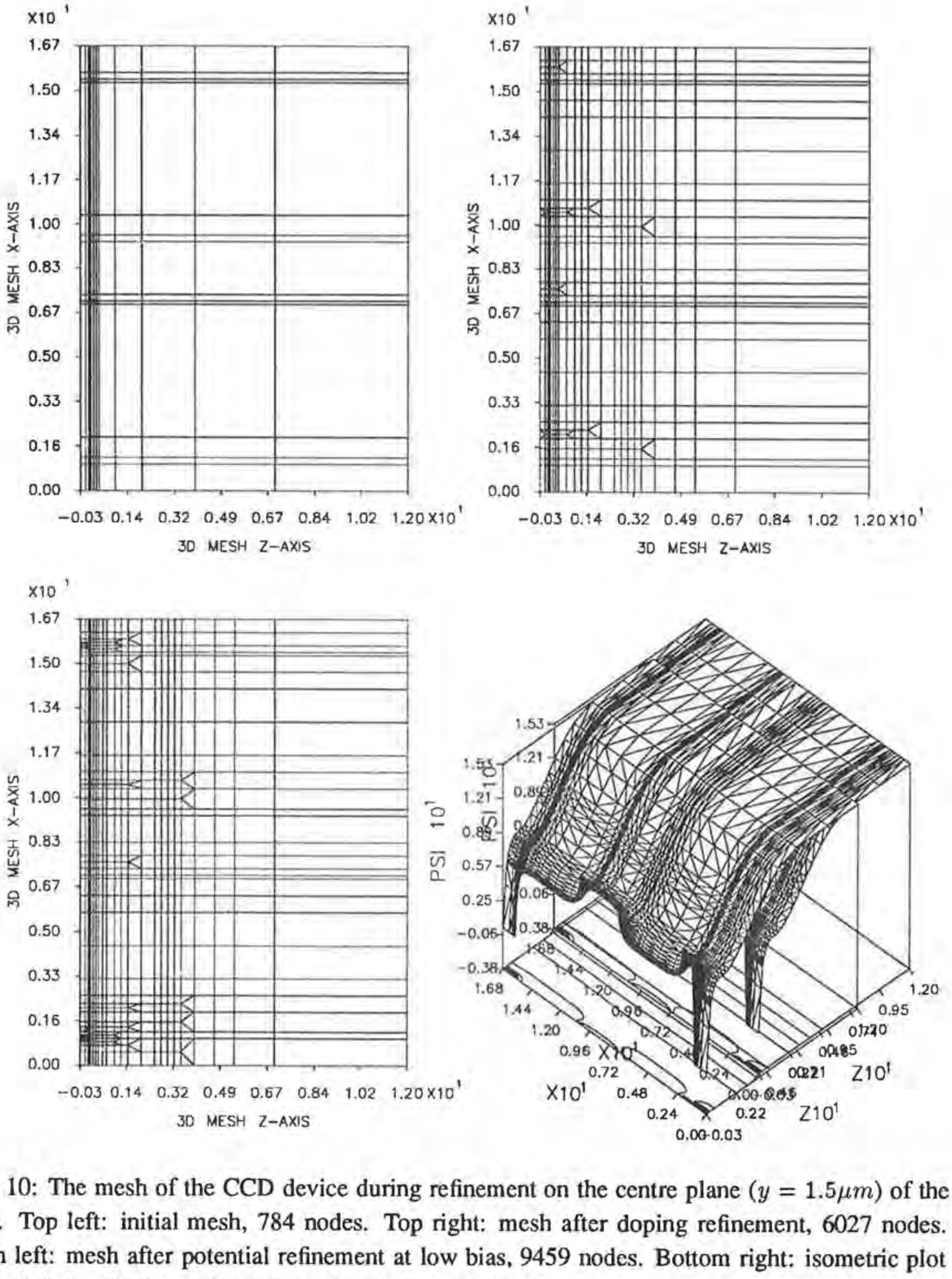

Figure 10: The mesh of the CCD device during refinement on the centre plane ($y = 1.5\mu m$) of the device. Top left: initial mesh, 784 nodes. Top right: mesh after doping refinement, 6027 nodes. Bottom left: mesh after potential refinement at low bias, 9459 nodes. Bottom right: isometric plot of potential after further refinement at high bias, 16609 nodes.

ADEPT: Completed parameter extraction program. In use in NMRC and installed in ADBV. The program is available but not marketed.

CACPAR: MOSFET parameter extraction from MINIMOS is in use in NMRC but not in a condition to deliver to third parties.

4.2 Philips

No specific software packages have been developed within the project. However, several techniques developed in this project were implemented in our in-house device simulation programme CURRY, which can handle both off-state and on-state problems, adaptive and non-adaptive, steady-state, transient and AC.

These algorithms have shown a considerable speed-up of the performance of CURRY and the range of applicable problems has also been extended considerably. The programme is available within Philips, and as such has been used by quite a large number of researchers and development engineers over the past six years.

The linear solution techniques have also been implemented in our off-state 3D semiconductor simulation package PADDY, which has been used predominantly for the design of charge coupled devices. The on-state simulation of such devices has recently been performed using the project research code EVEREST.

4.3 STC

STC developed no packages as part of this project. Minor modifications were made to the HFIELDS two dimensional device simulator to include the recommended intrinsic carrier and band gap narrowing models. All other physical modifications were obtained by adjusting input parameters. HFIELDS is available from University of Bologna, details of the physical models and modifications to the code are available from STC.

4.4 University of Bologna

A large number of programs were developed or enhanced under the EVEREST project. These included:

ATMOS-3D: A three-dimensional grid generator based on prismatic, triangular-base elements. Development of this program has continued and its has been used for a number of internal tests.

HFIELDS-3D: A three-dimensional device-analysis code for solving the Poisson equation and the electron-continuity equation based on the drift-diffusion model. Physical model for impact ionization based on the mean energy of the carriers, and its one-dimensional implementation. The development has been continued after the end of EVEREST and a number of improvements have been added. The activity on the code is still ongoing.

HIPPO-3D: Graphic postprocessor for the three-dimensional device-analysis code. This software tool allows for different representations of the simulation results, namely: colour maps of the unknown values over non-planar surfaces representing either the exterior or any internal portion of the device, and three-dimensional plots on arbitrary "cut planes".

The policy of the University of Bologna on releasing versions of these programs will be on similar lines already adopted for the two-dimensional versions, i.e. the system may be released under License Agreement to non-profit Institutions. It should also be mentioned that the three-dimensional system is rather less "user-friendly" than its two-dimensional counter-part.

4.5 SGS-Thomson

SGS-Thomson has not been involved in specific software development. However the mobility and the ionization energy models developed within the have been implemented and validated on the SGS-THOMSON version of the simulators MINIMOS4 and HFIELDS-2D. Most of the results have been published and the relative enhancements to the above programs are available. In order to carry on the activities on "Statistical Analysis" some dedicated software has been developed based on our user interface IDAD and on the SAS package but it must be considered as α-test code.

4.6 University College, Swansea

As part of the project UCS developed in-house a mesh generator for testing algorithms and strategies. This is a research code used as a vehicle for testing mesh generation algorithms. All other code developed under the project was for EVEREST Suite and is now incorporated there.

The status of the mesh generation code is that it has served its purpose as a vehicle for algorithmic testing. The option in the project to use this in EVEREST was not taken up. The status of the code is such that no further development is presently contemplated. This is not presently in a form where release to other parties could be contemplated.

5 State–of–the–Art

The demand for three dimensional simulation gave rise to first extensions of device simulations into three dimensions in the early eighties. These codes were written by the larger semiconductor manufacturers and were thus proprietary and required considerable CPU time on large computers to solve. One of the first of these codes was IBM's FIELDAY [6, 7, 8] which in 1981 applied the finite element solution procedure methods. In 1981 problems of about 2100 nodes were solved on an IBM 370/168 in hours of CPU time. Concern was raised at this time that the solution of the linear equation systems was a severe restriction as both the solution time and memory requirements increase rapidly as the problem grew. In 1985, the simulation was running on an improved processor, the IBM 3081, which enabled larger problems (some 5,000 nodes) to be solved in hours of CPU time. By 1989 the IBM code had moved onto a vector machine the IBM 3090/600, and the numerical procedure was based on a control volume approach and a bi-conjugate gradient method was adopted for the solution of the linear equations. Problems of up to 100,000 nodes were now possible.

In the late 80's there was a general push towards numbers of nodes in the range ten to one hundred thousand. Toyabe [9] of Toshiba was solving MOS devices with 21,000 nodes using a finite difference mesh, Kircher [10] of Siemens was using meshes of 40,000 nodes also on a finite difference mesh and Selbeherr [11] had updated MINIMOS to solving MOSFET devices in three dimensions on a 60,000 node finite difference mesh. Three points can be deduced from the literature of the late 1980's, these are:

- To accurately solve realistic three-dimensional problems, tens of thousands of nodes are required. This has a direct consequence on managing data size.

- Meshing such problems is very difficult and the success to date has been mainly with the simple finite difference meshes, or with two-dimensional finite element meshes pulled out into the third dimension using prismatic elements.
- The problem size has forced the use of iterative linear solvers which are faster, more economic on memory and more readily implemented on vector or parallel computers.

Of the simulators discussed so far, only the MOS specific simulator MINIMOS is available in the public domain. In 1990, the American company TMA announced that they were marketing a three dimensional device simulator, da Vinci, which is a commercial version of the Texas Instruments in-house simulator SIERRA. SIERRA was described by Chen [12]; it uses prismatic elements, the incomplete LU CGS linear solver (referencing work of the Philips group in ESPRIT 962) and was solving problems with 3,550 nodes but claims were that its capacity could be extended to one hundred thousand nodes.

The problem of generating the mesh to represent a device in three dimensions is a severe one. Of the codes discussed so far only MINIMOS has demonstrated a capability to generate its own mesh adaptively, and this is restricted to MOSFET devices. In March 1991, at the CeBIT trade fair in Hanover, a general purpose three dimensional device simulator with adaptive meshing was announced by a group at Zurich's Federal Institute of Technology. This code uses a mixture of hexahedral, pyramidal, prismatic, and tetrahedral elements and allows local mesh refreshment to occur as demanded by the solutions. This code is now available publicity and represents the state-of-the-art outside ESPRIT 962.

The ESPRIT 962 code, EVEREST, compares favourably with the state-of-the-art throughout the world. Like other codes it is using iterative linear solvers based on preconditioned gradient methods. In fact papers published from the group work is within ESPRIT 962 are often cited for the use of preconditioned schemes for non-symmetric systems.

Problem size has been carefully considered and by using hexahedral elements for filling the bulk of the device and tetrahedral elements to represent non- rectangular geometries and to allow local mesh refinement, efficient use of memory has been made. Within the project tests have been performed on an MOS device with 22,700 nodes. This use of a mixture of hexahedra and tetrahedra represents a level of sophistication only found elsewhere is the recently announced code by the Zurich group.

Furthermore, the code has a fully adaptive mesh generation capability with mesh line termination in all three dimensions which means that nodes will be placed more effectively than in other codes, thus 20,000 nodes in the EVEREST code may be expected to produce as accurate a result as 40,000 distributed according to a finite difference grid (though this number is very problem dependent). Such an adaptive feature is again only available in the code from the Zurich group.

From the algorithmic approach, this clearly places EVEREST close to, if not at the, state-of-the-art.

The physical models in EVEREST also compare favourably with other codes. This is summarised in the table below:

Thus from both the algorithmic and the physical model perspectives the EVEREST code compares favourably with the state-of-the-art. Moreover the independent development of similar meshing strategy at Zurich, reinforces the suitability of the approach taken in the EVEREST code and the recent announcement of three dimensional simulators available on the open market by other organisation around the world also supports the timeliness of one of the major results of ESPRIT

Physical model	da Vinci (TMA)	Minimos (Vienna)	Second (Zurich)	Everest
Temp dependent mobility	Y	Y	Y	Y
Doping dependent mobility	Y	Y	Y	Y
E field dependent mobility	Y	Y	Y	Y
MOS surface mobility	Y	Y	Y	N
Auger Recombination	Y	Y	Y	Y
Shockley-Read-Hall Recombination	Y	Y	Y	Y
Band gap narrowing	Y	N	Y	Y
Magnetic field effects	N	N	Y	N
Impact Ionization	Y	Y	N	N
Surface Recombination	N	Y	N	N
Hot carrier modelling	N	Y	N	N
Photogeneration of carriers	Y	N	N	N

962. It only now remains for suitable exploitation.

6 Exploitation Plans

The EVEREST project has given rise to a large number of results and ideas. All of these have been documented in the project reports and in conference and journal papers. The results of project have been and are being exploited by the partners in a variety of ways. Some of these are: publications, in-house software development, use of simulation packages in device design, distribution of software developed within the project to national communities and use of results as background to new projects.

As part of the project management and monitoring, the workpackage coordinators produced on a six-monthly basis a detailed progress report on each task being performed by the workpackage and collated this with technical reports from each partner participating. These reports were grouped in three volumes by workpackage: Volume 1, Workpackage 1; Volume 2, Workpackages 2, 3 and 4; and Volume 3, Workpackage 5. There are reports for each six month period of the project, twenty-four in all.

These reports and the open publications (over fifty listed in Appendix II of the Final Report) provide the main way in which the results of the project have been disseminated to the community. The distribution of the software developed within the project is a second way in which the results are being disseminated. This is on a more limited scale since much of this software is experimental in nature.

A list of the software developed within the project is given in Section 4.

More detail on the exploitation plans of each partner is given in the Exploitation Report.

7 Conclusion

During the life time of the project many elements required for the effective design and fabrication of semiconductor devices have been advanced. In particular modelling has progressed from the realm of two-dimensional analysis to that of full three-dimensional analysis in both steady state and transient conditions. The physical models required to achieve this have been assessed and developed and their capability validated against measurements on test devices.

The whole realm of physical modelling has been review and advanced for both MOS and bipolar devices. The sensitivity of the models to changes in process parameters has been considered and methods have been developed to link the variations in process parameters to the expected electrical behaviour. The linking of device simulators to circuit simulators has been explored and new methods of deriving the necessary parameters developed.

Robust and efficient algorithms for the discretisation of the three-dimensional semiconductor device problem have been developed successfully. Considerable progress has been made from the start of the project on a variety of techniques, the most important being that, for the first time, three-dimensional semiconductor problems have been solved adaptively. The algorithms developed have enabled this major breakthrough.

Robust and efficient algorithms for the solution of the discretised three-dimensional semiconductor device problem have been developed successfully. Without exaggeration it can be stated that this project has been a trendsetter in the area of solution techniques. Gradually, other device modelling groups are starting to use the methods developed in this project: the use of ICCG and CGS is already commonly recognised as being the only way to solve three-dimensional problems, whereas the technique of correction transformation is recently receiving more and more attention. Finally Gear's method for the solution of the time dependent problem has been shown to be far superior to the techniques commonly used in device modelling, and it is to be expected that this method will also be used by other groups in the near future. Needless to say, the adaptive solution of semiconductor problems is still unique, especially in the field of three-dimensional modelling.

Finally the project has proven its developments in an implementation of a fully coupled three-dimensional simulation suite, EVEREST. This suite integrates all the elements required to perform a device simulation over a common data base. Tested and validated on a library of twenty benchmark problems the EVEREST suite has been demonstrated in solving a number of industrially important device problems.

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Appendix II — List of Workpackages and Tasks

Workpackage 1: Physical Models and Validation

- 1.1 Validation
- 1.2 Physical and Analytical Models
- 1.3 Parameter Extraction
- 1.4 Fabrication & Measurement of Test Structures

Workpackage 2: Discrete Problem Formulation

- 2.1 General Discretisation Schemes
- 2.2 Special Discretisation Schemes
- 2.3 Error Analysis and adaption
- 2.4 Discretisation with Parallel Hardware
- 2.5 Discretisation with Hot Electron Effects

Workpackage 3: Mesh Generation and Refinement

- 3.1 Manual and Automatic Schemes
- 3.2 Adaptive Refinement
- 3.3 Exploitation of Advanced Hardware

Workpackage 4: Solution Procedures

- 4.1 Linear Solvers
- 4.2 Non-Linear Solvers
- 4.3 Transient Solvers

Workpackage 5: Project Code

- 5.1 Design
- 5.2 Graphics
- 5.3 Serial Implementation
- 5.4 Advanced Post Processing
- 5.5 Validation

Appendix III — List of Publications and Reports

III.1 Published Papers: Conferences and Journals

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III.2 — Project Reports

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