SINIMS Workshop on Applications of Mathematics and Computing in the Semiconductor Industry

Wednesday 24th April 2002
International Centre for Mathematical Sciences
Edinburgh

The workshop programme and the list of participants are respectively given in Appendices A and B.

1 Welcome and introduction to the Smith Institute Faraday Partnership (Dr Paul Moseley, Smith Institute)

Paul Moseley welcomed the participants and described the aims of the meeting as being i) to promote Faraday Partnerships (and in particular the Smith Institute Faraday Partnership) to industry as a good way of engaging with the academic community, ii) to promote understanding of how mathematics is being applied in the Semiconductor industry and iii) to identify potential opportunities for new collaborations.

Paul Moseley first gave an outline of the Faraday Partnership scheme. There are currently 18 Faraday Partnerships with a further 6 expected before the end of 2002. The Faraday Principles, which all 18 of the Faraday Partnerships work to, are

1. To promote active flows of people, industrial technology and innovative business concepts amongst the science and technology base and industry,
2. To promote the partnership ethic in industrially relevant research organisations, business and the innovation knowledge base,
3. To promote core research that will underpin business opportunities,
4. To promote business-relevant post-graduate training, leading to life-long learning.

The main characteristics of the Faraday Partnerships are that they focus on industrial sectors of national or regional economic importance as identified by Foresight (a DTI agency), they have core funding from government (DTI/DEFRA) and research councils (EPSRC/PPARC), they are structured around hub partners sharing a common vision, and they employ Technology Translators to ensure the selective exploitation of research. The Faraday Partnership web site is at http://www.faradaypartnerships.org.uk/, which has links to the web site of each of the Faraday Partnerships.

Paul Moseley then described the aim of the Smith Institute Faraday Partnership (www.smithinst.ac.uk) as being to enable companies of all sizes to benefit from the commercial potential of mathematics and computing in their industrial activity and planning. Overall, activity involves 30 current and planned projects, 70 companies and 25 universities, with a value over $3M in excess of DTI investment in the Faraday Partnership and contributing to both emerging and traditional technologies. Industry-driven core research programmes have been established with core EPSRC funding. Some 14 research proposals, designed to create long-term advantages for industry, had been submitted to the EPSRC, a number of which were now underway. Dissemination of the results of the research would be through publication and open meetings. Other mechanisms available are the DTI core funding, responsive and managed mode EPSRC proposals, CASE projects, TCS (formerly Teaching Companies Scheme), direct industrial funding, SMART awards, LINK, workshops (open or closed) and Study Groups. Workshops held so far reflected the diversity of applications of mathematics and had included the topics of Food, Weather forecasting for risk management, Resource management in distributed environments, Guided wave photonics, Electromagnetic compatibility, Tissue engineering, Violent mechanics, Microwave cooking, Nonlinear signals, Inverse Problems, Dynamical Instabilities in Lasers and Applications of Mathematics in Technical Textiles. More recent and forthcoming events were outlined, including the SINIMS series of 6 workshops on: Technical textiles, Optoelectronics, Health, Medicine and Biotechnology, Food and Agriculture, Oil and Gas, Semiconductors. The recent 43rd European Study Group with Industry (2-5 April, 2002 at Lancaster University) had provided an opportunity for industry to have problems worked on by over 50 mathematicians. There had also been recent workshops on Particulate Flows and Flexible Photovoltaics during the last two months. Planned workshops include: Transport Environments and the Practices of Scheduling, 24 June 2002, at Canterbury and Low Temperature Industrial Plasmas,17-18 December 2002, at Culham in Oxfordshire. Looking further into the future, the Smith Institute had recently launched an industrial roadmap for mathematics and computing (http://www.smithinst.ac.uk/news/RoadmapLaunch) , which presents a vision for the application of the mathematical sciences to industrial competitiveness over the next 10 years.

2 The design of quantum well material for semiconductor lasers (Prof. John Arnold, Glasgow University)

John Arnold explained that semiconductor lasers for the optoelectronics and semiconductor industry were fabricated using expitaxial growth methods in the Optoelectronics Group at Glasgow. Quantum wells, residing between the valence and conduction bands and created by the use of Ga/Al/As doping, result in discrete energy states in which valence band electrons may be trapped. Photon resonances with the energies between these discrete states provide the mechanism for lasing. In order to control the quality and specification of such semiconductor lasers, it is necessary to control the shape of the quantum well by a process known as quantum well intermixing. This is a process of material (eg Ga) diffusion between the well material and the surrounding materials which, encouraged by the introduction of 'holes' in the well material, gradually makes the quantum well shallower until it ultimately disappears. Stopping the diffusion process early provides a mechanism for controlling laser properties by changing quantum well eigenstates. Laser properties are also determined by a process of selective bombardment to create degrees of disordering in materials adjacent to the well. This mechanism allows the production of monolithic wafer lasers by selective disordering and so also allows production of passive waveguides, modulators, and 2nd harmonic generators.

John Arnold then described two important areas for the application of mathematics:

i) *Modelling of material diffusion processes for improved quality control of standard quantum well designs*

Although quantum well intermixing involves the diffusion of discrete entities, mathematical modelling is currently based upon homogenisation and the use of Fick's law for the diffusion current and a species conservation equation. The diffusion coefficient is dependent upon the species concentration. The aim is to predict the behaviour of the diffusion process and thus the determination of when it should be stopped in order to minimise residual losses. Mathematical methods are required to improve the modelling of this process to achieve improved empirical correlations with experimental results and so improve the quality of the production process.

ii) *Designing new quantum well shapes to specification*

The quantum cascade laser and its relative, the quantum fountain laser, work using electrons only (not holes). In the former, a cascade of 20-30 quantum wells is immersed in a potential gradient such that on emission of a photon in each well, the energy lowered electron tunnels through to a high electron state in an adjacent well so affording emission of a further photon in a similar fashion. The process then proceeds 'in cascade'. Three eigenstates in each well require precisely defined spacing for the required phonon and photon resonance and, moreover, precise inter-well energy level alignment is required to achieve an efficient cascade. This is a severe design problem in well shaping and spacing. The design issues are eased somewhat, though still challenging, in the case of the (single well) fountain laser, which is optically rather than current pumped. In this latter case the challenge is limited to designing a well with the required eigenstates to meet a given laser specification. Theoretically, this problem is well known as an inverse scattering problem and there are mathematical methods (Backlund & Darboux transformations, eg see recent paper by Tomic) for determining potentials to achieve the required eigenspectra. However, given such a 'design' potential how does one define the initial monolithic structure, the bombardment processes and the diffusion process such that the design potential is faithfully manifested? This is a (fabrication process) inverse problem. A connection was made with process of bread making which is a topic of one of the Smith Institute's 2 year post-doctoral research projects.

In response to questions, John Arnold explained that the motivation for improved laser design capability was provided by the strong demand for improved atmospheric environmental sensing (eg for methane in the far infra-red 5-20 micron wavelength range). Semiconductor devices were substantially smaller than CO2 devices and so offer enormous portability and packaging advantages.

3 Applications of data mining in the semiconductor industry (Mr Phil Darby, Napier University)

Phil Darby explained that, at Napier University, statistical methods and more recently data mining methods are applied to a wide range of areas in including the semiconductor industry (within which he has considerable experience), health, demography and forecasting.

Phil Darby presented the aim of data mining as the discovery of hidden patterns (nuggets) in large volumes of data and referred to database knowledge fusion methods. He quoted the 'beer and nappies' legend of data mining, whereby unforeseen valuable correlations are exposed to the benefit (in this case) of retail markets. Parallel diagnostic benefits were also anticipated in other fields. He gave examples of object oriented interfaces for search definitions quoting the wryly named 'Clementine' software. The motivation for increasing interest in this rapidly developing field, was the huge amount of data now being generated (claimed to be doubling every 20 months). Exemplar sources were satellite sensing, astronomic observations, computer processing etc. Reference was made to various inference methods: neural nets, decision tree partitions, webmaps and Kohnen networks (a data condensation method whereby neural nets are used to group together related data which is also similar to clustering methods familiar in statistics).

There has been little published literature on the application of data mining in semiconductor manufacturing, perhaps because of confidentiality. However, the field is full of promising opportunities and several semiconductor support companies offer this capability. An important aspect in developing applications of data mining, particularly in the semiconductor manufacturing industry, is the provision of realistic data, the sources of which are indeed sometimes inhibited by issues of confidentiality. Phil Darby reported work on the application of these new techniques in which anonymous factory data had been used. No useful results were found from the factory data so test data with the same structure as the real factory data was constructed. This approach proved a valuable method of exploring data mining in semiconductor manufacturing. An important parameter is the minimum lot size required to resolve the cause (amongst many possible causes) of a given fault from a set of possible fault conditions in the product. One example, in this case, was the identification of the minimum number items that had to be produced before a poorly performing machine could be found. Such diagnosis of production faults from observed semiconductor wafer faults requires production line simulation and models of potential machine failure modes.

Phil Darby concluded that data mining was not a miracle method but with realistic data, good process characterisation and simulation it could bring substantial benefits to the semiconductor industry.

4 Automated yield pattern and cross-section generation (Dr Raymond Bienek, Motorola)

Raymond Bienek explained that on a plant with which he was concerned, 6" diameter wafers, of 3mm square bi-CMOS 0.5 micron chips, are produced at the rate of 2,500 per week. Their production involves 400 different processes. The length of the fabrication process is 7 weeks. After fabrication, tests are carried on (up to 3,000) circuits on each chip and faults and their type are recorded. Early signals are sought of fault types and rates outside the normal limits of expectation. Yield rates are a direct measure of chip performance.

There are two areas where the application of mathematics could bring important improvements:

i) Analysis of yield patterns

Yield patterns are the patterns of faults and fault types observed upon wafers of chips at the end of the production process. Yield patterns are currently analysed by methods which rely upon human classification and interpretation. A substantial amount of statistical information has been compiled on the types of fault. However, there is a need for an automated method to match up fault types and their patterns to root-causes in the production process in order to obtain correct problem diagnosis and rectification. Each plant uses different production technologies and so any new method would need to be sufficiently general to be applicable to different plant types. As the semiconductor is now moving towards the production of 12" diameter wafers, the need for automated methods of yield pattern analysis and root-cause diagnosis is becoming more urgent.

There was some discussion amongst the audience of possible approaches to this problem, including data mining methods, Bayesian analysis and also Markov-Monte Carlo approaches currently used for analysis and prediction of disease epidemics.

ii) Cross-section generation

Integrated circuits are constructed from many layers of material and undergo numerous photolithography stages to create the appropriate patterns in these layers. SEM cross-sections through circuit features reveal the end product of fabrication and are an important component of failure analysis. These can reveal missing or extra layers, layer-to-layer misalignments etc. Sophisticated commercial packages are available for process simulation, which produce process cross-sections, however these tend to be aimed more at the development arena, rather than wafer production. A faster way to generate realistic cross sections would be of benefit. The aim would be to have the ability to generate the cross-section from the 2-D photomask layer data for a given process. These would aid the failure analysis process, especially if combined with the ability to simulate the removal of certain layers or modify layer thickness, since the actual features observed (SEM) could be compared to those expected from correct layer processing.

5 Analogue-digital conversion in resistive networks (Mr Alan Gillespie, Analog Devices)

Alan Gillespie explained how Analog Devices use transistor switched resistive networks to generate very high-resolution A/D and D/A conversion devices for a range of applications including digital storage and retrieval of analogue physical signals. The design problem is to determine the (set of) network configuration(s) meeting design constraints which give the required resolution of A/D conversion in particular.

While at first the design problem seemed to be one of integer arithmetic, Alan Gillespie explained that the resistive networks contain intrinsically non-linear elements such as transistors and switches (also made of transistors). Field effects in the resistive network devices are a further source of non-linearity; each resistance element being a function of the voltages of nodes in a local neighbourhood of the element. Moreover, there are tolerances on the design of the elements, which can limit the resolution of an otherwise effective network. The functional dependence of the (sparse) resistance matrix element non-linearities and their uncertainties are (at least approximately) to be determined from measurements of the device voltagecurrent characteristics in all the switching modes. The analysis of these networks presently is prosecuted using the industry standard code called SPICE.

Currently, to estimate the distribution of the errors in a network circuit, SPICE is used to do a "Monte-Carlo" analysis. This consists of running the same simulation over and over again, with the parameters of the devices "randomized" by an amount consistent with the estimated production variations. Circuit performance parameters can then be extracted from the results of these simulations and the discrete values of these results can be put into a statistical package to estimate their distribution. With this approach, it takes a whole afternoon to evaluate a given the network. As a simple example, for a 16-bit digital to analogue converter, there would be 65,536 output values to check. If each of these needs to be simulated, say 100 times, to get a meaningful output distribution, then 6,556,600 simulations are required, which can take a long time. Usually not all states are checked but this is a short cut, which it ideally would not be taken. A faster method of analysis is therefore required to remove this bottleneck in the design process.

In posing one approach to the problem, Alan Gillespie asked if SPICE could somehow use the statistical data about the parameters which make up the circuit to directly estimate the variance of the simulation results, then the "100" simulations would become just one. Is there a way to solve a system of equations whose coefficients all have some variance associated with them, and directly find the "distribution" of the solutions for the "unknown" variables?

It was also suggested in discussion, that perhaps because general matrix methods were used in SPICE, its (almost certainly iterative?) methods might not be optimised to the resistive networks of the general type designed by Analogue Devices (with up to 65,000 nodes). If that were indeed the case then the adoption of more appropriately tuned/pre-conditioned sparse matrix methods might also provide the required speed advantage. There was also concern that over-optimisation of such methods might lead to loss of required scope for flexibility in the network design. It was suggested that after closer inspection of this problem, an appropriate first contact might be Prof. Iain S. Duff, CSE/Numerical Analysis Group, Rutherford Appleton Laboratory.

6 Virtual Component Co-design (Mr Elias Biris, Cadence Design Systems)

Cadence is a large supplier of software products, methodology services and design services used to accelerate and manage the design of semiconductors, computer systems, networking and telecommunications equipment, consumer electronics and a variety of other electronics-based products.

Elias Biris explained the challenges of optimally realising design functionality in physical devices. Given a functional requirement and a set of physical devices and their operating constraints, optimal (re-)configuration of devices and their processes poses problems in physical arrangement, optimal scheduling, data transfer and communications control. Cadence aims to produce software tools that enable system designers to overcome these challenges.

Elias Biris said that while SystemC (http://www.systemc.org), a language and modelling platform based on C++, has provided some simulation facilities, there is still little progress in providing automatic optimization capabilities to system designers. Cadence therefore sought advice on general methods that would be appropriate for exploring and optimising integrated systems to meet functional specifications subject to diverse physical and process constraints. In brief discussion, it was suggested that perhaps genetic algorithms might provide the required level of generality to handle the sometimes discrete optimisation problems and rule based constraints that might be involved. It was clear that more detailed discussion of the application area would be required before potential solution avenues could be proposed for this challenging question.

7 Close

Paul Moseley thanked the speakers for preparing and presenting stimulating presentations and thanked all for their participation in the workshop. He also thanked ICMS staff for their pivotal support in organising the event. He explained that notes recording the event would be circulated to all who had attended and that he would write to the companies represented to explain opportunities for follow-on collaborative activities. Paul Moseley closed the meeting with an invitation to stay on for drinks.

Melvin Brown
Smith Institute
9/5/02

APPENDIX A

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Programme

10:30 *Registration / Coffee*

11.00 Welcome & introduction to the Smith Institute Faraday Partnership
(Dr Paul Moseley, Smith Institute)

11:30 "*The design of quantum well materials for semiconductor lasers* "
(Professor John Arnold, Glasgow University)

12:15 *"Applications of data mining in the semiconductor Industry"*
(Dr Phil Derby, Napier University)

13:00 *Buffet Lunch*

13:45 *"Industrial Perspective - Motorola"*
(Dr Raymond Bienek)

14:30 *"Industrial Perspective – Analog Devices"*
(Mr Alan Gillespie)

15:15 *Tea*

15:45 "*Industrial Perspective – Cadence Design Systems*"
(Dr Elias Biris)

16:30 Concluding Remarks
(Dr Paul Moseley, Smith Institute)

16:45 Close

APPENDIX B

Workshop Participants

Arnold, Prof J.M., University of Glasgow

Bienek, Dr R., Motorola

Biris, Mr. E., Cadence Design Systems

Brown, Mr. M., Smith Institute

Carr, Prof J, Heriot-Watt University

Dagpunar, Dr J, Edinburgh University

Darby, Mr P., Napier University

Dart, Miss T., ICMS

Duncan, Dr D., Heriot-Watt University

Gibson, Prof G., Heriot-Watt University

Gillespie, Mr A., Analog Devices

Mackay, Dr T., Edinburgh University

McKee, Prof S., Strathclyde University

Moseley, Dr P.G., Smith Institute

Parker, Dr D., Edinburgh University

Qiu, Dr Y., Heriot-Watt University

Rees, Prof E.G., Edinburgh University