The future with computational electronics: a new golden age?

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Abstract

The advent of low cost high performance workstations and new visualisation tools is coincident with a growth of new problems in electronics ranging from large scale power devices to nanometer dimensions. The rise of molecular electronics and bioelectronics points to new regimes for the device modeller to explore. It is argued that some software discipline especially standards and portability is required if the modelling community is to be effective. Lessons may be drawn from successes in other fields such as quantum chemistry and molecular modelling.

I. Introduction

Just seven years from the twenty-first century it is perhaps a good time to reflect on the future of computational electronics. The modelling and simulation of solid-state devices is at an important watershed in its history because for the first time it is possible to imagine universal access to software and mathematical techniques which will allow any experimentalist, theorist, industrialist, whatever, access to knowledge which was at one time the select speciality of a few groups around the world. The changes are being brought about by the microelectronics revolution which now provides the power of 1980s mainframes and early supercomputers in relatively cheap workstations - with promises of more to come. There is a similar change in software habits; in the last few years industrial employers of our engineering and science graduates have begun to expect proficiency in languages such as C rather than the traditional FORTRAN; and some nodding acquaintance is now expected with the concept of "user-friendliness". It is no longer fashionable to log up hours of Cray time to produce a couple of numbers. There are expectations aroused that something better is required. Explanations, interpretations, insight, visualisation, projections are required quickly, graphically and easily. Computer scientists are devoting time to topics such as persistent programming which addresses the issues of 25 year old and older software. Computation is now one strand of more complex activities; any computed data is to be regarded as part of a rich interacting hierarchy of

knowledge which can be used by different people for different reasons. In computational electronics we have only just begun to realise what these changes might entail and it is the purpose of this paper to give a personal view of what we have to look forward to. I want to start by first looking back to the beginnings of the subject(for me anyway) in the 1960s.

2. Some history

Coincidentally, it is also a quarter of a century since the first conference on computational electronics held at the Culham laboratories in 1968. At that meeting were some of the first papers on computational electron transport theory including one by myself and Cliff Hearn which dealt with self-scattering in a Monte Carlo simulation of photo excited hot electrons and which used propagator techniques to prove that the Monte Carlo solutions were equivalent to solutions of the Boltzmann equation. At that time Culham was a centre for computational work, mainly due to the intense interests in plasma physics and to a lesser extent neutron transport theory. Culham provided an educational distribution point with series of weekly lectures on computational physics organised by Potter. The smallness of the computers of those days made the use of compact ingenious algorithms the order of the day rather than brute force number crunching. It is not surprising that Potter went on to develop the Psion organisers and other compact systems.

By 1969 much of the familiar theoretical base of computational electronics was already in place. JFET theory had been set up in 1947, Bipolar transistor theory by 1952, MOSFET theory by 1960, MESFETs in 1966. Of the computational techniques, drift-diffusion theories dated from 1952, hydrodynamic models from 1962, the Gummel algorithms from 1964 and the first solid state electron transport theory handled by Monte Carlo was reported by Kurosawa in 1966(the latter work was part of the inspiration that guided me into transport theory especially hot electron theory in 1967). But many of these techniques were really derivative: Monte Carlo studies were enjoying extensive use in neutron transport theory (although Lord Rayleigh was doing much the same thing without computers in the last century); and the influence of hydrodynamics (particularly driving the aerospace industries from WWII onwards) and plasma physics cannot be under-estimated. There were already major forays into quantum kinetic theories although these were still of a formal rather than practical nature.

What really limited practical applications was computing power . The really interesting (as well as applicable)problems were either highly complex or non-linear or both. Looking back I am still amazed by the lack of imagination we all had. "You are only limited by your imagination" is the proud boast of many a computer advertisement in the 1990s. Well, my limit was a factor between 3 and 10. In 1967 I developed code (ALGOL 60) for simulating the time evolution of Gunn domains and similar effects in photoconductors using an Elliot 803 computer with 32K

core memory. A little later the offer of time on the national ATLAS computer at Harwell brought the luxury of 90K memory but entailed a two day wait to receive the wad of data (mainly error messages and core dumps) from the post. That extra factor of 3 in memory seemed impressive, and every few years we in the computational sciences looked forward to that extra factor of ten or so which would bring the biggest of problems into our control. It is perhaps fortunate that the compute did not exist because the control and detailed understanding of solid state device materials was not sufficent for realistic modelling. Not only was compute power singularly poor, but means of handling the output data were primitive. In 1968 I spent maybe one week at a time collecting plotter pictures on large rolls, selective frames of which were placed along a corridor to facilitate a "computer movie" of Gunn domain dynamics. Today, that entire problem, including symbolic manipulation and computer movies can be handled using Mathematica on a Macintosh computer in a few minutes. It is this simple reminiscence which brings home the immense opportunities that we now have for unleashing computational electronics from the grip of computational poverty. But others have been there first: the computational chemists have achieved a close partnership with their industry which has produced an effective, widely shared approach to applicable computational science which we in computational electronics could learn from.

III. Physical modelling versus equivalent circuit

There has always been a division between those advocating the empirical approach to device and particularly circuit modelling and those favouring the development of physical models. The advantages and limitations of the two approaches are well known: industry, especially given the exponential pace of integrated circuit technology, has needed data quickly and cost-effectively; empirical or equivalent circuit models do the trick - in the short-term. But, that approach and a poor investment in physical models led one well-known review paper in the late 1970s to state that it was highly unlikely that silicon transistors could be manufactured with design rules less than 10 microns. It is also true that physical models give the best route to device understanding and to devising new device concepts - provided the underlying physical model is reliable. The latter case is still a problem because we do not usually know how to model surface and interface charge very readily. Indeed, the whole problem of physical modelling of real devices is bound up with understanding and developing models of the underlying technological processes.

The physical modellers have often dealt with the esoteric: the spate of quantum "devices" investigated in the 1980s would have achieved short shrift with the empiricists had they followed the literature. After all it is assumed that devices should be interconnectible, isolatable and designed to function at room temperature not milli-degrees Kelvin. Again due to a certain

innocent over-familiarity with the field many advocates of quantum devices fail to point out the frequent necessity to use lock-in amplifiers in operating the devices. The real lesson here is not that work on quantum devices is only of academic interest: it is that the science required to achieve engineering goals is not necessarily the same science that drives the physical scientist to investigate phenomena within devices. This problem did not arise with the quantum chemists. Over the last 25 years the chemistry community has mutually developed molecular modelling, drug design and molecular graphics/design software which is not only relevant to science and industry but mixes the empirical and physical to advantage; is also readily available and widely used. My own interests in molecular electronics have led me to have a healthy respect for the sheer accessibility of computational techniques and databases to the chemistry community.

There are distinct signs now that the physical modelling/empirical industrial rift is healing within the electronics community. This is coming about partly because of better control and understanding of real materials and the need to include "esoterics" in device design e.g. hot electron effects. There are also questions of "attitude": we have all heard of the physical scientists easy dismissal of engineering problems as containing no interesting physics. Often this is misleading and in our own recent work (with Asenov and Brown) on applying (technology transfer ?) microscopic device modelling techniques to large power transistors (200 A switches) we have developed considerable respect for the complexity and subtlety of the underlying physical problem. More significantly, the immense complexity of realistic quantitative as opposed to qualitative physical device simulation such as Laux's Monte Carlo models of MOSFET devices is becoming manageable with the advent of very high power workstations.

IV. Machine power I: workstations

Early next year my University will relinquish its three mainframes (including an IBM 3090 vector processor) in favour of a distributed system of workstations inter-connected by fast networking. Other Universities here and abroad have already experienced this trauma - and survived. The argument is compelling: why share a 126 Mbyte mainframe with 400 other people when you can have a cheap 256 Mbyte workstation, with instant on-line colour graphics for yourself . For a little more money one can expect to have 100 MFLOP workstations for use within modelling groups over the next few years. If the dreams of modellers from the 1970s are to be believed this already is extreme overkill for computational electronics problems. Of course that is not the case, but it is the case that this development should lead to very much closer links between academics and industry on grounds of cost alone.

There are questions of fashion however. There is still some cachet in using SUN workstations. My own pedestrian approach is to use networked Apple Quadras running Unix,

X-Windows and Mac environments(and even DOS!) concurrently, which at lower cost and some performance penalties allows everyday word-processing, graphics, movie making, e-mail and so on to be integrated with the normal workstation role. The catch of course is that the system is linked to a large transputer array for compute-intensive tasks. This example raises the issues of hardware and operating system standards. My own solution is partly cost based (more for less) and partly with an eye on upgrade routes and inter-working with IBM systems, UNIX, DOS and MAC. It also raises the issue of the human interface: should we be developing specialist code or code that is easily used within familiar environments by non-specialists? If the answer is yes we have to confront the problem of huge software design costs and that extra memory and power starts to look less effective.
What power do we really need? As we shall discuss later some problems require GFLOP -> TFLOP power and > GBytes memory. How do we get it? National super computers or local solutions?

V. Machine power II: vectorisation and parallelisation

Even with the projected advances in integrated circuits it is unlikely that desktop single processor GFLOP power is imminent. Parallel processing in the widest sense of the word is usually advocated as the way ahead and of course forms the basis of many super computer approaches.Vectorisation is the least flexible in one sense and so is easier to use, full-scale parallelisation, for example in a software configurable transputer array is often highly efficient in run-time but may be costly in development time. If the new found universality offered to computationalists by the workstation revolution is not to be over-turned it is essential that some order and standardisation is brought into parallelised codes for general and local use. Our own approach at Glasgow is to cut development time and improve portability by re-generating all our codes in common parallelisable format, for which we have chosen finite-element algorithms as the main format which can cover classical device modelling through to many electron quantum transport. These codes are designed to run on arbitrary numbers of transputers and so can be developed in simple workstations before transfer to the main cluster. It appears at present that the main lesson is to use the workstation as the main hardware tool but supplemented by networking to compute intensive local parallel machines of intermediate power.
These arguments for the workstation approach pale into insignificance when we consider the opportunities that workstations now offer for visualisation.

6. Visualisation

The chemistry community was quick to develop visualisation tools, many of which are now available in the public domain for quite ordinary workstations. It is thus possible to put on appropriate goggles(plus IR sensor) and guide the viewer through a colour stereo journey through a molecular structure on a Silicon Graphics workstation. Virtual reality systems have been pioneered by the computational chemists. In a sense this is obvious, the complexity of molecular design is in direct space: it is three-dimensionally geometrical and topological.. In device modelling the effective parameter spaces are less physically obvious and often high dimensional. We have yet to learn how best to represent dynamic data for real devices. The 3D representation of electron and hole trajectories colour coded for temperature is already good practice and drawing a leaf from quantum chemistry the use of 3D transparent (cloud representation) colour contours for potentials of temperature surfaces should be manageable. This requires 24 bit colour high resolution workstations and of course soaks up memory and CPU time (graphics accelerators of course are a way out). At Glasgow we have been developing movie and graphics techniques to help us gain intuition into the transient few electron problem in quantum waveguides and single electronic systems. Like the mediaeval schoolmen there is nothing to be gained by not trying things out. I believe that visualisation is crucial to the development of computational electronics especially if the aim is to provide access to general designers and experimenters. Multiple displays with friendly interfaces will be essential. This route should not be left to chance it should be organised and draw on the experience of other communities. In particular the input/output of visualisation should be linked to other software such as CAD codes where possible.

VII. Software

The demands of visualisation, operating systems, portability, parallelisation bring us to the prospects for the software side of the business. It also raises the issue of what level we should develop our computational models. First some generalities. It is becoming obvious that computational electronics involves large codes which are both continuously developing and meeting new demands from interface and visualisation requirements. Although there is huge investment in it, FORTRAN is not the best medium for managing and verifying large quickly developable, de-buggable codes (my own bias was already admitted earlier - I was brought up on ALGOL). C, C^{++}, PASCAL all have their merits especially in object oriented forms. The answer is not to choose the best (I actually am attracted to functional programming languages) but to choose the best for the community.

On visualisation should we be developing our own codes or providing hooks into public domain or commercial software? I would argue for both because today's best visualisation software has evolved from earlier scientific studies.

One of the most interesting developments has been the spread of software such as MATHCAD and MATHEMATICA which provide highly simplified frameworks for quickly solving what used to be formidable problems (with excellent graphics thrown in). The use of symbolic techniques and functional programming make these approaches very attractive for certain problems (for example simple 1D tunnelling simulations). But they have little efficiency and it is often difficult to program them for efficiency. Nevertheless these approaches do provide universality.

VIII. Organised modelling

Like synchronised swimming I believe that organised modelling will eventual appear sensible and exciting. We need to learn from communities like the chemists that there is mutual advantage in sharing, documenting and jointly developing community codes for device modelling. There are too many stand-alone operations to bring the promise of universal access to modelling closer.

There is a great deal of in-house expertise which is fiercely guarded (not always with justification). I would like to see this type f workshop develop into a forum that aims to set standards, goals, achieve inter-working and sharing of knowledge so that full attention can be paid to applications driven research. Paradoxically some organisation is necessary because of the problems of diversification which come from the freedom brought about by the workstation revolution. How this should be achieved is a subject for debate.

IX. New opportunities

Finally, let us turn to a selection of the new opportunities for the core of computational electronics - the models, applications and tools themselves. Many of these are represented at this workshop, some are steeped in antiquity, others are striving for birth.

In classical/semi-classical models the challenges are in TeraHertz high frequency device modelling, the inclusion of thermal effects, the incorporation of process models. Despite the complexity it is becoming possible to devise physical models which quantitatively describe real devices. These will be essential as integrated circuit technology heads into the fully sub-micron regime. The advent of surface probe technology (STM, AFM etc.) and on-chip electrometry and capacitance techniques will open up the hitherto problematic surface and interface charging problems which will underpin the model development. There are considerable opportunities for modelling which is designed to interpret the new atomic scale probes.

The same on-chip techniques have recently allowed direct observation of the ubiquitos fluctuation potential which bedevils quantum devices and the direct observation of many

electron states and their filling in quantum dot structures. The application to ultra-small commercially oriented devices will be challenging and will require active modelling work. The aim is to understand and control the intra- and extra-device environment in detail.

The shift to ultra-small devices and devices with ultra-small capacitative regions brings up the issue of quantum charging effects: Coulomb blockade, correlated tunelling, macroscopic quantum tunneling, telegraph and shot noise effects associated with the discreteness of the electronic charge. The modelling required here and for the now extensive range of single electronic systems is non-trivial.. Single electronics is scaleable to high temperatures by fabricating sufficiently small capacitative tunnel junctions. It is already integratable. Techniques from the charge density matrix , the quantum Langevin equation, Monte Carlo, Traffic theory and linear programming are all being brought to bear. The single electron problem actually turns out to be a many body problem and much remains to be discovered. Device-device coupling is an unavoidable reality in such systems and extended systems of devices need to be modelled. Control of killer efects such as quantum fluctuations, charge-trapping de-trapping and cross-talk can in principle be handled by designing the substrate electrostatic environment correctly: 3D modelling on heterostructres is essential here.

There is now enormous scope for quantitative quantum modelling but we should be careful to distinguish the physically interesting from the engineering possibilities. To restore some balance I should remark that my own interests prtly involve studying quantum device systems fabricated within two-dimensional electron gases which can act as atomic scale instrumentation for exploring hithto intractable regimes of quantum physics such as delayed-choice, empty wave and quantum measurement problems. In this context we have been recently successful in modifying the Bohm pilot wave version of quantum mechanics in setting up and solving problems in quantum transport theory.

If we pursue the limit of miniaturisation of devices to its logical conclusion we encounter structures on molecular scales. The problems of bioelectronics, biosensors, molecular sensors, molecular electronics and nanoelectrochemistry all converge with device electronics at nanometre scales. Even the techniques in quantum chemistry for studying the STM tunnel curent and energy spectrum of a small molecule bound to a surface bear striking resemblance to quantum dot modelling. The long range tunnelling of electrons through polymer chains, redox centre arrays and enymes is closely related to the electronic soliton dynamics of single electronic systems.

The future then is rich in promise, quantitative models, evolving interdisciplinarity and a chance to develop a strong mature modelling community properly integrated with industry. I look forward to a new golden age.