# Computational Electronics in the 21<sup>st</sup> Century:

Challenges, Opportunities, Issues

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*Abstract*—Semiconductor electronics transformed the 20<sup>th</sup> century, and computational electronics played an important role in its success. As we embark on a new century, it is worth reflecting on where electronics is heading and on how computational electronics can continue to play a vital role. This talk presents that author's personal reflections on this topic and will, he hopes, spark a discussion within the community.

Keywords-simulation; computing; semiconductor; microelectronics;nanoelectronics

### I. INTRODUCTION

Computational electronics began to emerge as a discipline in the 1960's and 1970's. It matured in the 80's and 90's, when conferences and workshops like SISDAD [1] and IWCE [2] were established, and a group of scholars and practitioners who thought of themselves as a community began to develop. Computational electronics is now integral to the practice of semiconductor and development. device research Semiconductor electronics based on processes and devices invented and developed into commercial technologies in the last century will continue to evolve and mature into increasingly powerful and sophisticated systems in the 21st Century. A major, international effort charts the future of semiconductor electronics and identifies critical needs for new modeling and simulation capabilities [3]. That is important and challenging work that will continue to require the support of a strong computational electronics community like ours, but that is not the subject of this presentation.

More than a decade ago, electronic device research began to explore new directions –examining novel devices based on using individual molecules, carbon nanotubes, semiconductor nanowires, and electron spin as well as charge. This research may lead electronics in new, and currently unforeseeable directions. What role will the computational electronics community play in defining new technologies for the 21<sup>st</sup> Century? The opportunities are great, but so are the challenges. In my view, computational electronics should play a vigorous role in defining and shaping new fields of electronic device technology. In the process, we will set the stage for a new generation of TCAD. The purpose of this talk is to present my thoughts on how we can do this.

## II. CHALLENGES

Silicon technology still has a long ways to go. As we explore new technologies, we should also look for creative, new ways to exploit silicon technology. It is an incredibly sophisticated technology that is primarily directed toward one thing – digital electronics. What else could we do with this existing, high volume manufacturing technology? Microelectromechanical Systems (MEMS) is an example of using silicon technology for purposes that were not originally envisioned. What other possibilities are there?

With regard to new electronic device technologies, the biggest challenge we face is uncertainty. Many technologies are being explored, but it is not at all clear what (if any) applications will emerge. The fact that experiments cannot always be trusted is another challenge. This is quite expected in new fields in which experiments are being done for the first time, but it creates uncertainty for those simulating experiments. A third challenge is the wide variety of devices and materials being explore and the fact that many of them require new conceptual, computational, and even theoretical approaches. That author will present his own thoughts on how challenges like these might be addressed.

#### III. OPPORTUNITIES

There are more than enough important problems in traditional semiconductor device technology to engage our community for the next two or three decades. We should address those problems and contribute to the continued evolution of semiconductor electronics. But I also hope that some part of our community accepts the challenge to play an active role in exploring new device physics, devising the new theories and computational approaches that will be needed, and also inventing and developing new devices and technologies. We have a real opportunity to play a leadership role in shaping 21<sup>st</sup> Century electronics, and we should seize it.

How can we contribute to the development of 21 Century electronics? It means much more than developing software. It means explaining new physical phenomena and then turning it into useful devices. As Richard Hamming famously said: "The purpose of computing is insight, not numbers." Writing a computer program to simulate a material or device is an embodiment of our understanding the problem. We don't really understand a problem unless we can program a computer

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to simulate it. We have an opportunity to develop the conceptual foundations for new fields of electronic devices - ones that will guide us as we develop simulation codes, but it will also guide experimentalists and designers just as much as our software tools (possibly even more).

When we simulate an experiment, we should not be content with "agreeing with the experiment." While that might be useful in benchmarking new simulations (recognizing that benchmarking against experimental data is much more involved that simply reproducing a curve in a paper), it is even more useful to clearly explain an experimental result. As Leo Kadanoff recently noted, pointing out when the experiment is incorrect, or incorrectly interpreted is just as important to the progress of science [4].

### IV. ISSUES

Although the challenges of 21st Century electronics are great, so are the opportunities. There are, however, a separate set of issues that we, as a community should think about. One set has to do with how we train our students. Greg Wilson has pointed out that the state of software skills in the computational community is a major factor in limiting progress [5]. Another issue has to do with the practice of computational electronics. Experimentalists insist that experimental procedures are documented; we do not insist on a clear and complete description of computational procedures [6]. Closely related is the question of open source software. Open source promotes the diffusion of knowledge and "documents" the computational experiment, but it conflicts with the desire protect intellectual property. And then there is the question of benchmarking simulation codes. To what extent do we, as a community, have a responsibility to those who read our papers and make use of our simulations to benchmark them against experiments and other codes? Finally, there is the issue of dissemination. Open source would facilitate broader dissemination, but we can do more to help others make use of our simulation tools by providing access to simulation services through the web. Several researchers have recently raised issues like these (e.g. [7, 8]). A workshop at the University of California at Berkeley addressed many of the same issues, and the lectures can be heard online [9].

The Network for Computational Nanotechnology established nanoHUB.org, a web-based science gateway to deliver simulation services through a standard web browser [10]. It allows computational researchers to web-enable an application with little effort and then to deploy it so that it can be used anywhere, by anyone. In addition to simulation services, nanoHUB also hosts a collection of tutorials and courses that convey the insights and understanding that are emerging in the course of developing and using computational tools. These services have proven to be extremely popular (more than 60,000 users per year as of May, 2008). The broader use of science gateways like nanoHUB could be useful in addressing some of the issues identified above. In that regard, the underlying software base, called HUBzero, is being developed as an open source platform [11].



Figure 1. The nanoHUB science gateway (http://www.nanoHUB.org), which hosts services for online simulation, education, and collaboration.

### V. SUMMARY

This is a period of great opportunity for computational electronics. It is worth taking some time to pause and reflect on where we are heading – to have some spirited discussions, and then to move forward into an exciting new century. My hope is that this presentation will be part of that process.

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