2015

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Lundstrom, Mark S., "Computational Electronics for the 21st Century: Reflections on the Past, Present, and Future" (2015).
Department of Electrical and Computer Engineering Faculty Publications. Paper 151.
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Computational Electronics for the 21st Century:

Reflections on the Past, Present, and Future

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Abstract—The author’s career has coincided with the development of numerical simulation into an essential component of semiconductor device technology research and development. We now have a sophisticated suite of simulation capabilities along with new challenges for 21st Century electronics. This talk presents a short history of the field and a description of the current state of the art, but it concentrates on lessons learned and thoughts about how computational electronics can continue to contribute effectively to the development of new electronic device technologies. The author will argue that electronics is changing, and that computational electronics can play a key role in this evolution. In addition to supporting the continuing development of a small suite of physically detailed / first principles tools, he will argue for more emphasis on analytically compact, strongly physical, conceptual models. Such models help guide the development of physically detailed models, connect to circuit and application designers, and advance device science itself.

Keywords—semiconductor devices; simulation; TCAD; nanoelectronics; cyberinfrastructure;

I. INTRODUCTION

The invention of the transistor and the integrated circuit transformed the world, and progress in semiconductor electronics continues to shape the world we live in. Theory, modeling, and simulation played a key role in the development of microelectronics, in its evolution to nanoelectronics, and they will be critical to continued progress in semiconductor technology. In this talk, the author will reflect on the history of computational electronics from the perspective of someone who has been watched and participated in the evolution of the field for almost 40 years. The focus will be on the theory, modeling, and simulation of transistors - only one aspect of computational electronics, but an important one that has driven much of the research in the field. The main goal of the talk is to discuss lessons learned and to spark discussions as we prepare for a new era of electronics.

II. A VERY BRIEF HISTORY

The device that made microelectronics possible is the transistor, and the history of computational electronics is closely connected with the history of the transistor. When I began my career as an integrated circuit process engineer, MOSFET channel lengths were five micrometers (5000 nanometers). Researchers were just beginning to develop the

kinds of computational tools that would later become part of every engineer’s toolkit. Simulation played little role in technology development in the 1970’s, but by the end of the 1980’s, sophisticated simulation tools had become an essential part of technology research and development. One of the lessons learned was the impact that modeling and simulation can have when simulation tools are placed in the hands of those with problems to solve.

Computational electronics began with the so-called semiconductor equations as formulated by von Roosbroeck are [1]:

$$\begin{aligned}\nabla \cdot \vec{D} &= \rho \\ \frac{\partial n}{\partial t} &= \frac{1}{q} \nabla \cdot \vec{J}_n + G_n \\ \frac{\partial p}{\partial t} &= -\frac{1}{q} \nabla \cdot \vec{J}_p + G_p\end{aligned}$$

When constitutive relations for the displacement field, $\vec{D}$, the electron and hole current densities, $\vec{J}_n$ and $\vec{J}_p$, and the electron and hole generation rates, G_n and G_p , are inserted, these equations become three equations in three unknowns, the electrostatic potential and the electron and hole concentrations. These three coupled, non-linear partial differential equations are by no means easy to solve. The development of accurate, fast, robust solutions for dc, transient, and small-signal ac conditions in one, two, and three-dimensions was a major accomplishment with critical contributions from engineers and applied mathematicians [2-8]. These equations continue to describe a large number of devices of current interest, but the ability to solve these equations is becoming a lost art as students are trained on more advanced methods.

As transistor channel lengths shrunk, a more detailed description of the internal device physics became necessary, and drift-diffusion approaches began to be supplemented by advanced methods. In the presence of high electric fields that vary rapidly in space and time, so-called “off-equilibrium” transport effects such as velocity overshoot occur. The classic semiconductor equations can be supplemented by higher moments of the Boltzmann Transport Equation, and much work in the 1990’s was directed at developing and solving

these “energy transport” equations. Developing these equations, however, entails many simplifying assumptions the validity of which is hard to assess [9]. Full, numerical solutions of the Boltzmann equation eliminate most of the simplifying assumptions, but the “curse of dimensionality” (the six-dimensional phase space) makes a direct discretization of the Boltzmann equation very difficult, which led to the development sophisticated Monte Carlo simulations [10]. At Illinois, Hess and colleagues first demonstrated “full band” Monte Carlo simulation [11] and Fischetti and Laux at IBM Research extended this approach to treat realistic bandstructures and scattering processes in realistic device geometries [12]. By the end of the century, however, the increasing importance of quantum mechanical effects demanded new simulation approaches. While several different approaches to quantum transport exist, the non-equilibrium Green’s function (NEGF) approach has become the most widely used [13]. The first, true NEGF CAD tool was developed at Texas Instruments [14]. Driven by research on molecular electronics, the NEGF approach was coupled with ab initio quantum chemistry simulations [15, 16]. Most recently, the development of tools like NEMO5 has produced an industrial strength quantum tool for quantum transport [17].

It has been more than 30 years since numerical device simulation entered the mainstream of device research. We now have available to us a set of sophisticated device simulation tools that range from drift-diffusion, to full Boltzmann transport (Monte Carlo), to full quantum transport (NEGF). Complementing these tools are a set of first principles materials simulations tools based on density functional theory (DFT) and molecular dynamics (MD). It is interesting, however, that the new, more sophisticated tools now available have not supplanted the simpler tools. Each technique has its limits and its own role in device research. Questions facing us now include: 1) Do we focus on improving and extending these tools? 2) Do we develop new simulation capabilities, and if so, what capabilities are needed? or 3) Should we focus on better using the tools we have? The author will share some thoughts on these questions.

III. THE WWW AND COMPUTATIONAL ELECTRONICS

The author has been involved in initiatives that use the world-wide web in support of computational electronics. The first is the nanoHUB (www.nanoHUB.org). The nanoHUB was created for a specific purpose – to allow computational experts to easily share their simulation tools with others – not just to permit software downloads that can be installed (and maintained!), but also to give users the ability to operate software tools through any standard web browser with no need to download and install anything. The open-source platform that powers nanoHUB (www.hubzero.org) makes it easy to web-enable and deploy almost any application. Key to the success of nanoHUB was the deployment of supporting resources, such as seminars and tutorials that teach the fundamentals of the science and Matlab scripts that show how to implement the algorithms. Launched in a significant way in 2002, the nanoHUB now has more than 12,000 users running more than 800,000 simulations annually. More than 300,000 users per year come to the site for the supporting resources.

The nanoHUB has become a major, global resource for electronics and computational electronics. It played a major role in the rapid dissemination of the NEGF approach.

Fig. 1. The nanoHUB homepage (www.nanoHUB.org)

A related and more recent online activity is the nanoHUB-U initiative. nanoHUB-U aims to bring new educational resources to the electronics community. Although spearheaded by computational electronics specialists, the goal is to engage experimental as well as computational experts. A growing suite of freely available on-line short courses present the fundamentals of nanoelectronics in a broadly accessible way that does not assume a long string of prerequisites. The motivation is that electronics in the 21st Century will be much broader than in the past, and that students and working engineers will need technological breadth as well as expertise in a specialty. Since launching nanoHUB-U in the spring of 2012, more than 15, 000 students have registered for courses.

Fig. 2. The nanoHUB-U homepage (www.nanoHUB.org/u)

Although the WWW is now more than 25 years old, what we see today should be considered as experiments being conducted to determine how to most effectively use these new technologies. The author’s experience convinces him that cyberinfrastructure of the nanoHUB kind can play an important role in 21st Century electronics.

IV. DISCUSSION

Computational electronics has had an interesting ride for the past few decades. It has progressed from a curiosity to a core activity. As a community, we have developed powerful capabilities; what should we do next? In thinking about that question, it is worth thinking back to the early days of the field.

Much of the early development of computational electronics was done by people who considered themselves device scientists – not computational scientists or applied mathematicians. As the field developed, people with a more theoretical, mathematical, and computational expertise became involved, and our computational tools became much more powerful. But something was also lost – the close connection to the real problems that must be solved. As we look to the future, we could concentrate on improving the tools we have – there is certainly much that can and should be done. It is possible however, that new problems will require new tools, but to know what new tools to develop, we need a clear understanding of current research in electronic materials and devices. To ensure the success of computational electronics in the future, the connection to hands-on device research must be strengthened.

The continued down-scaling of device dimensions continues to provide a strong driver to computational electronics, but electronics in the 21st Century is changing; it is likely to be much broader. For example, there is more and more interest in energy generation (solar cells and thermoelectrics) and energy conservation (power electronics and solid-state lighting), and a tighter and tighter connection of electronic to biology and medicine. Spintronics, nanomagnetism, and multi-ferroics may lead to important new technologies. It is quite likely that addressing these challenges will require major extensions to current tools, or even completely new tools. To deeply understand what is needed, the computational electronics community must be actively engaged in device and materials research with the goal to solve problems with whatever tools are available or can be readily created. Only in the process of this activity will it become apparent what new tools are needed.

Analytically compact models and SPICE-compatible circuit models are not generally considered to be within the domain of computational electronics. This should change. These models connect physically-detailed simulations to circuits and applications, but they can do much more. The original device models were analytical models that were developed before numerical simulations were available. The authors of these models had deep insight into the physics of devices; they could distill the essential physics into an analytical model that did much more than enable circuit designs. These models provided the conceptual framework that the device community used to understand devices. When numerical simulations became available, they deepened our understanding of devices, but the simple models continued to provide the conceptual framework for thinking about devices. They help us interpret what we see in detailed simulations, and detailed simulations help us improve the model.

It is the authors' view that physics-based compact models should play a stronger role in computational electronics at this time. More and more, electronics research will be driven by new applications. Compact models connect work at the device level to applications, but physics-based compact models do more than provide the connection to applications - they provide a way of thinking about devices that is critical for device research.

In spite of the powerful simulation tools that we have created, most devices cannot be fully described with any one of the tools we have available. Rather, it takes a combination of simulations complemented by experiments to illuminate the physics of a device. Simulations should be excellent [18] and impact device research [19]. An analytical model that attempts to distill the essential physics into a simple form is a good starting point for excellent and impactful computational electronics. Questions about the physics in the simple model are addressed by physically detailed simulations and by experiments. The iterative process of developing a model and using detailed simulations to refine it leads to a physically sound, analytically compact model that provides the device community (not just simulation experts) with a conceptual understanding of the device. Some might argue that the physics is too complex to model simply, but it has been observed repeatedly that macroscopic performance is very often controlled by a few key parameter – despite the great complexity at the molecular scale [20]. Such models also provide a starting point for the creation of a SPICE-compatible compact model that can be used to explore applications.

The Nano-Engineering Electronic Device Simulation (NEEDS) initiative has a mission to advance device science and connect it to applications. The central focus is physics-based compact models. The initiative is funded by the U.S. National Science Foundation and by the Semiconductor Research Corporation and consists of teams at Purdue University, the Massachusetts Institute of Technology, the University of California at Berkeley, and Stanford University. The NEEDS website (Fig. 3) is built inside the nanoHUB and, as a result, it inherits the capabilities of the nanoHUB.

Fig. 3. The NEEDS website built inside nanoHUB.org (www.needs.nanoHUB.org)

The five major aspects of NEEDS are reflected in its website. The first is compact models. A growing suite of compact models for a very broad range of technologies is

available to download. The specification of standard release packages, licenses, and publication processes helps ensure a level of quality. A self-publishing capability allows anyone in the community, not just those involved in NEEDS, to publish models. A second aspect of NEEDS is the development and deployment of physically detailed simulations that support the creation of physics-based compact models. These physically-detailed models make use of nanoHUB capabilities so that users can operate them through a web browser. The third aspect of NEEDS is the development of an open-source, Matlab-based Model and Algorithm Prototyping Platform (MAPP). This platform allows users to create compact models and test them in simple circuits all within a Matlab environment. Verilog-A models can be translated to MODSPEC, the model description language, and debugged in MAPP in a Matlab environment. We are finding that this Matlab-based platform works well for physical scientists who only occasionally develop compact models. When Verilog-A models are needed, this MAPP workflow improves the quality of the final model.

A fourth aspect of NEEDS is training in the art and practice of compact modeling. The goal is to provide those who are brand new to compact modeling with the understanding they need to get started quickly and to write “simulation ready” compact models. The fifth and final aspect of needs is the nanoHUB-U initiative, which provides short courses on the science that underlies the various technologies for which NEEDS is developing compact models. These courses are designed to be broadly accessible to graduate students and working engineers and to provide them with the understanding they need to contribute to the evolution of electronics in the 21st Century. In short, NEEDS aims to be a driver for a new type of computational electronics for the 21st Century.

V. SUMMARY

Computational electronics has created a powerful set of simulation capabilities that are widely-used in electronics research and development. Electronics in the 21st Century is changing, and computational electronics can play an important role in this new era of electronics. To play a vital role in the new electronics, computational electronics must re-establish the intimate connection of modeling and simulation to device research and applications that launched the field of computational electronics more than three decades ago.

ACKNOWLEDGMENT

This work was supported through the NCN-NEEDS program, which is funded by the National Science Foundation, contract 1227020-EEC, and by the Semiconductor Research Corporation.

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