

Drift-Diffusion and computational electronics – Still going strong after 40 years!

Reflections on computational electronics and the equation that started it all

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Abstract—The field of computational electronics began in a serious way when the so-called semiconductor equations were numerically solved in one, two, and three dimensions. The result was a new tool in the device engineer’s toolkit, and the impact was profound. Much of the subsequent history of the field has consisted of working to improve the description of carrier transport as provided by the drift-diffusion equation. Much has been accomplished, but drift-diffusion based simulations continue to be the mainstay. One reason has to do with the computational burden of more advanced techniques, but another is that drift-diffusion equations have proven to be surprisingly effective even in situations where there were expected to fail. This talk is a brief history of computational electronics with an emphasis on the unreasonable effectiveness of drift-diffusion equations. The talk concludes with thoughts on where things stand and on how computational electronics can best position itself to contribute to a new era of electronics.

Keywords— *Integrated circuit technology; Semiconductor devices; Semiconductor device modeling; Transistors;*

I. INTRODUCTION

Advances in semiconductor technology over the past 50 years have shaped the modern world, and numerical simulation of semiconductor devices and processes have played a critical role in these advances. The full, numerical solution of the van Roosbroeck “semiconductor equations” was a major advance, and numerical solutions to these equations still dominate (although only a few specialists remember how to solve them!). Much of history of computational electronics is a story of trying to do better than drift-diffusion. Using this as a theme, I’ll trace the history of our field from the simple drift-diffusion equation to full, numerical simulations of dissipative quantum transport, which is now the cutting edge of device simulation. Along the way, I’ll illustrate some unexpected examples of where drift-diffusion works surprisingly well and try to explain why. I’ll conclude with some thoughts on where our field is heading as we enter a new era of electronics and on the role computational electronics can play in this exciting future.

II. A BRIEF HISTORY

The device that dominates modern electronics is the transistor, and understanding electron transport in transistors has driven much of the work in computational electronics. The three,

coupled equations that describe semiconductor devices are the continuity equations for electrons and holes and the Poisson equation. When augmented by constitutive relations for the electron and hole currents, recombination and generation rates, etc. a system of three, coupled non-linear partial differential equations in three unknowns, the electron and hole densities and the electrostatic potential, results. By 1950, the equations had been clearly formulated with the currents described by drift-diffusion equations [1].

Before there were drift-diffusion simulations, device researchers developed analytical, compact models for transistors. Semiconductor device modeling consisted of appropriately simplifying the semiconductor equations and solving them analytically for specific devices (see [2, 3] for two early examples). This was all done without the aid of computer simulations. Looking back, it is remarkable how good the pioneers of our field were at understanding the essential physics and distilling it into models that engineers could use. One must admire their insights and intuition. Many of the models they formulated still form our conceptual picture of semiconductor devices.

By the 1960’s, computers had advanced to the point where the full set of coupled, nonlinear equations could be solved numerically. Beginning with the “Gummel method” [4] and the “Scharfetter-Gummel technique” [5], the solution of these equations became practical. Others followed by extending the solutions to 2D [e.g. 6,7]. A major step was the public release of codes designed to be used by device engineers rather than by experts in numerical simulation [8, 9]. Applied mathematicians became involved, and the codes became faster and more robust [10]. By the 1990’s, numerical device simulation had become a practical, everyday tool for device engineers and scientists (e.g. [11]).

Electronic devices continued to shrink in size as computational electronics entered the mainstream. Concerns were raised about the validity of drift-diffusion equations in the presence of high electric fields that varied rapidly in space and time. The obvious choice was to add higher moments of the Boltzmann Transport Equation using so-called energy transport and hydrodynamic approaches. Formulating these equations always involved, however, numerous simplifying assumptions that were difficult to justify in general [12]. In the

search for more accurate solutions to the BTE, Monte Carlo techniques were developed – first for high-field transport in the bulk or large devices [13, 14], and then in devices [15]. Sophisticated Monte Carlo simulations that could accurately treat so-called off-equilibrium transport and breakdown were developed and became widely used for scientific studies. Device engineers continued, however, to rely on drift-diffusion based PDE approaches informed by the more rigorous but more computationally demanding Monte Carlo simulations.

As the 20th Century ended and the 21st Century began, the continued downscaling of device dimensions led to concerns about the validity of semi-classical descriptions of carrier transport. A need for simulations that captured quantum transport arose, and many techniques were explored. Today, the mainstay of quantum transport is the Non-Equilibrium Green’s Function (NEGF) approach [16, 17], and sophisticated, industrial strength codes are available [18]. This approach not only describes nanoscale transistors [19], but also much smaller molecular device [20, 21].

Looking back over the past 50 years of computational electronics, it is amazing how far we have come. Our goal was general purpose, “predictive” simulations. This goal proved to be elusive and today, technology developers continue to rely heavily on drift-diffusion models complimented with more sophisticated simulations. Surprisingly, drift-diffusion models often work remarkably well. There seems to be an unreasonable effectiveness of diffusion equations at the nanoscale and this unexpected effectiveness can be explained.

III. THREE SIMPLE EQUATIONS

The celebrated drift-diffusion equation

$$J_n = nq\mu_n \mathcal{E} + qD_n \frac{dn}{dx} \quad (1)$$

continues to be widely-used in solid-state electronics. We understand, however, that the drift-diffusion equation can fail – especially in small devices. Even for near-equilibrium transport, it is widely felt that the drift-diffusion equation begins to break down in the quas-ballistic regime. This, it turns out, is not necessarily true.

The Shockley-McKelvey equations [22, 23]

$$\begin{aligned} \frac{dF^+(x)}{dx} &= -\frac{F^+(x)}{\lambda} + \frac{F^-(x)}{\lambda} \\ \frac{dF^-(x)}{dx} &= -\frac{F^-(x)}{\lambda} + \frac{F^+(x)}{\lambda} \end{aligned} \quad (2)$$

are a simple form of the Boltzmann Transport Equation. They describe the transport of a forward-directed flux of electrons, $F^+(x)$, and a reverse flux, $F^-(x)$. The two fluxes are coupled by backscattering. The probability per unit length of backscattering is $1/\lambda$, where λ is the mean-free-path for backscattering. Equations (2) describe transport from the ballistic to diffusive limits. For a very small mean-free-path, the forward and reverse fluxes are strongly mixed, and diffusive

transport results. For a very large mean-free-paths, the forward and reverse fluxes do not change – they are simply equal to the values that were injected from the two contacts. Surprisingly, eqns. (2) can be mathematically rewritten as eqn. (1) [23], which shows that at least under the right conditions, the drift-diffusion equation can describe ballistic transport.

The Landauer Approach [24, 25],

$$I = \frac{2q}{h} \int \mathcal{T}(E)M(E)(f_1 - f_2)dE \quad (3)$$

describes transport in terms of the quantum of conductance, $2q/h$, the transmission, $\mathcal{T}(E)$, the distribution of modes (or channels), $M(E)$, and the difference in Fermi functions of the two contacts, $(f_1 - f_2)$. Equation (3) is widely used to describe transport in nanostructures, but it can be derived from eqn. (2), which is not restricted to nanostructures. Equation (1) can also be derived from (3). We conclude that eqns (1) – (3) are, in some sense, equivalent and that they apply broadly to devices that operate from the ballistic to diffusive limits.

This talk will discuss several examples where “common sense” suggests that diffusion equations should fail, but where they turn out to work remarkably well for reasons that can be simply understood. Diffusion across the thin base of a bipolar transistor shows that Fick’s Law can work all the way to the ballistic limit. Heterojunction bipolar transistors with ballistic launching ramps show that far from equilibrium, near ballistic transport can appear diffusive. An emission-diffusion theory from the 1960’s reproduces the Landauer theory of the ballistic MOSFET. Turning to phonons, we find that steady-state heat transport at the nanoscale can be described by Fourier’s Law and that quasi-ballistic transient heat transport can be described by a diffusion equation. What is surprising is not that we can find conditions where drift-diffusion equations fail, but rather, how often they work. This talk will show that there are very good reasons for the broad applicability of drift and diffusion equations.

IV. DISCUSSION

Our field has witnessed remarkable advances over the past 40 years. We now have available a variety of tools to design and explore devices, but we still don’t have the single, broadly applicable solution that treats the wide variety of problems device researchers encounter. Today, we can see the end of Moore’s Law looming – at least in terms of device downscaling. Moore’s Law has driven much of the research in computational electronics. The future looks to be more diverse in terms of technologies, less predictable and “roadmapable”, and more driven by applications. What should we in computational electronics be doing to support the success of this new era in electronics? I argue that our focus at this time should not be on developing new simulation tools – rather, we should return to our problem-solving roots.

The great device physicists of the 1950’s, 60’s, and 70’s were remarkable people. Without numerical simulations to support them, they developed a deep understanding of the

essential physics of devices and translated that into models that had great impact. When simulations became available, we found that they got almost everything right. Today, we have a powerful set of computational tools and a new set of problem to address. Every tool has its limitations. The art and practice of modeling and simulation consists of understanding the science deeply, so that results from different simulations (complemented with carefully designed experiments) can be put together to solve problems. The challenge now is to use the excellent simulation tools that are available to do “excellent computer simulations” that address important problems [26, 27]. Analytically compact models, like the first generation device models, play an important role. They provide a concise description of the essential physics in a way that can be communicated to the broader device community. They help us interpret what we see in physically detailed simulations and experiments. The iterative back and forth between experiments and numerical simulations and simple, essentials-only models advances device science. Indeed, there appears to be a principle in science that things that look complex at the microscale can be simply described with only a few parameters at the macroscale [28]. Some examples of this style of computational electronics from the NanoEngineered Electronic Device Simulation (NEEDS – needs.nanoHUB.org) initiative will be presented.

V. SUMMARY

The first generation of computational electronics specialists was device scientists and engineers with problems to solve. They got the field started. Later on, when experts in theory, mathematics and computing joined the effort, the tools became much more powerful. There are some obvious ways that our current tools need to improve, and this important work should continue. It is not at all obvious, however, what new capabilities are needed to address the new problems of 21st Century Electronics. A problem-solving stage that largely makes use of the tools we have can set the stage for an exciting second act for computational electronics.

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