

**Computational Electronics: From Semi-classical to Quantum Transport Modeling**  
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The continued scaling of semiconductor devices and the difficulties associated with time and cost of manufacturing these novel device design has been the primary driving force for the significantly increased interest in Computational Electronics which now, in addition to theory and experiments, is being considered as a third important mode in the design and development of novel nanoscale devices. In addition to its significant role in industrial research, modeling and simulation also brings into the picture alternative education modes in which students, by running certain subset of tools that, for example, the nanoHUB offers, can get hands-on experience on the operation of nanoscale devices and can also look into the variation of internal variables that can not be measured experimentally, like the spatial variation of the electron density in the channel in the pre- and post-pichoff regime of operation, electric field profiles which can be used to tailor the electron density to avoid junction breakdown, etc. In summary, Computational Electronics is emerging as a very important field for future device design in both industry and academia.

The purpose of this tutorial is to introduce interested scientists from Academia and Industry in advanced simulation methods needed for proper modeling of state-of-the-art nanoscale devices. We give an overview of the basic techniques used in the field of *Computational Electronics* related to device simulation. The multiple scale transport in doped semiconductors is summarized in Figure 1 in terms of the transport regimes, relative importance of the scattering mechanisms and possible applications.

	$L \ll l_{e-ph}$			$L \sim l_{e-ph}$	$L \gg l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L \gg l_{e-e}$		
<b>Transport Regime</b>	Quantum	Ballistic	Fluid	Fluid	Diffusive
<b>Scattering</b>	Rare	Rare	e-e (Many), e-ph (Few)		Many
<b>Model:</b>					
Drift-Diffusion					
Hydrodynamic		<a href="#">Quantum Hydrodynamic</a>			
Monte Carlo					
Schrodinger/Green's					
Functions	Wave				
<b>Applications</b>	Nanowires, Superlattices	Ballistic Transistor	Current IC's	Current IC's	Older IC's

Figure 1. Relationship between various transport regimes and significant length-scales.

In the first half of the tutorial we cover semi-classical methods for semiconductor device modeling, beginning with the simplest one (the drift-diffusion model), then moving into a description of the hydrodynamic and energy balance transport and concluding the discussion on semi-classical transport modeling with a comprehensive discussion on particle-based device simulation methods. In addition to focusing on the theory, equal emphasis is placed in this tutorial on the description of the numerical solution approach used for particular method being described. For example, when talking about drift-diffusion model and its derivation from the Boltzmann transport equation, we will also discuss the Sharfetter-Gummel discretization scheme that relaxes some constraints on the mesh size and leads to improved convergence of either the Gummel or the Newton method used for solving the coupled set of Poisson and current continuity equations.

The second part of the tutorial begins with a discussion for the need for quantum transport, the description of various quantum effects that appear in current and future devices that are being either mass-produced or being fabricated as a proof of concept. In this context, we will describe the density gradient method, quantum hydrodynamics and we will also introduce the concept of effective potential used to include approximately quantum-mechanical space-quantization effects in a semi-classical particle-based device simulation scheme. Moving into the next topic, where we talk about open systems, we will introduce tunneling as a purely quantum-mechanical concept and we will discuss ways of calculating the tunneling coefficient for arbitrary piece-wise constant and piece-wise linear potential barriers. The Landauer-Buttiker formula for the calculation of the conductance will be introduced next as a way of studying quantum-mechanical systems in a linear-response (near-equilibrium) regime of operation.

The last part of this tutorial is dedicated to the far-from equilibrium quantum transport, where we will introduce the concept of pure and mixed states and the distribution function. Several methods, with different level of complexity and accuracy will then be explained in details when solving the far-from equilibrium quantum transport problem including the density matrix method, Wigner functions and Green's functions method. Since the emphasis in this tutorial will be placed more on the Green's function method for solving the quantum transport problem, we will describe in details the recursive Green's function method and its variant, the Usuki method. Then we will move on and describe the Contact Block Reduction method as the most efficient and most complete way of solving the quantum transport problem since this method allows one to simultaneously calculate source-drain current and gate leakage which is not the case, for example, with the Usuki and the recursive Green's function techniques that are in fact quasi-1D in nature for transport through a device. We summarize this tutorial with some open questions related to quantum transport, others areas of transport such as spin transport, not covered in this tutorial, and new computing paradigms such as quantum computing.

Tutorial covers the following:

- What is Computational Electronics?
- Semi-Classical Transport Theory
- Drift-Diffusion Simulations
- Hydrodynamic Simulations
- Particle-Based Device Simulations
- Inclusion of Tunneling and Size-Quantization Effects in Semi-Classical Simulators
- Tunneling Effect: WKB Approximation and Transfer Matrix Approach
- Quantum-Mechanical Size Quantization Effect
- Drift-Diffusion and Hydrodynamics: Quantum Correction and Quantum Moment Methods
- Particle-Based Device Simulations: Effective Potential Approach
- Quantum Transport
- Direct Solution of the Schrodinger Equation: Usuki Method
- NEGF (Scattering): Recursive Green's Function Technique and CBR approach
- Atomistic Simulations - The Future

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**Dragica Vasileska** received the B.S.E.E. (Diploma) and the M.S.E.E. Degree from the University Sts. Cyril and Methodius (Skopje, Republic of Macedonia) in 1985 and 1992, respectively, and a Ph.D. Degree from Arizona State University in 1995. From 1995 until 1997 she held a Faculty Research Associate position within the Center of Solid State Electronics Research at Arizona State University. In the fall of 1997 she joined the faculty of Electrical Engineering at Arizona State University. In 2002 she was promoted to Associate Professor and in 2007 to Full Professor. Her research interests include semiconductor device physics and semiconductor device modeling, with strong emphasis on quantum transport and Monte Carlo particle-based device simulations. She is a Senior Member of both IEEE and APS. Prof. D. Vasileska has published more than 140 publications in prestigious scientific journals, over 80 conference proceedings refereed papers, has given numerous invited talks and is a co-author on a book on Computational Electronics with Prof. S. M. Goodnick. She has many awards including the best student award from the School of Electrical Engineering in Skopje since its existence (1985, 1990). She is also a recipient of the 1998 NSF CAREER Award. Her students have won the best paper and the best poster award at the LDS conference in Cancun, 2004. Dragica Vasileska is a Senior Member of IEEE and is listed in Strathmore's Who's-Who.

**[ The tutorial fee is 100 Euro for each attendant ] (separated from the conference fee)**