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Modeling and Numerical Challenges in Nanoscale Device Engineering

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In spite of considerable research effort and progress, high quality simulation-based design of nanoscale emerging devices still presents formidable modeling and computational challenges. Characterization of nanoscale emerging devices needs to be addressed via quantum simulations that need to account for: (i) information of the material at the atomistic level, (ii) multiscale aspects of electron transport modeling and electrostatics effects, (iii) high-fidelity treatment of the contact regions, and (iv) efficient methodology for dissipative scattering. For enhanced reliability and accuracy of the simulation of transport phenomena, one needs detailed knowledge of the electronic structure of the materials. Ab-initio calculations have been, so far, restricted to the simulations of small two-probe molecular systems, that does not consider the coupling with the surroundings such as electrostatics gate effects [1]. In practice to reduce the computational costs, one needs to use simplified electronic structure models such as effective mass type-models for semiconductors [2], or semi-empirical and tight-binding methods for molecules and nanotubes [3-4].

Given the advances in the-state-of-art of computer architecture, processor and memory technology, underlying system software, and parallel algorithms, computational scientists and engineers can now expect to solve large-scale nanoelectronics problems using real-space mesh techniques for atomistic ab-initio simulations. These techniques that were thought to be intractable in the not-too-distant past, will result in fundamentally superior accuracy to address a combination of the two following challenging problems: (i) a comprehensive description of the transport problem, (ii) a fully atomistic description of the materials.

In material sciences, real-space mesh techniques such as the finite difference method (FDM) [5], and the finite element method (FEM) [6-7], were proposed in the early nineties, for the simulation of electronic structures. In contrast to the Linear Combinations of Atomic Orbitals (LCAO) methods (along with the dominant use of Gaussian basis sets), or plane waves expansion schemes, they offer significant advantages that have been summarized in [8]. They also produce very sparse matrices and can be cast as linear scaling electronic structure methods. These advantages, in turn, enable the use of multiscale and multilevel methods, and other sophisticated parallel numerical techniques on high-end computing platforms [9-10].

In principle, it is possible to extend the capabilities of an effective mass-based transport simulation code such as NESSIE (see Fig. 1), to account for higher degree of details of the electronic structure. The Kohn-Sham/DFT equation is then expected to replace the Schrödinger equation, and a pseudopotential approach may be used to remove the core electrons and the singularities in the discretization [11]. These simulations pose, however, significant challenges in developing robust and efficient large sparse linear system solvers and eigenvalue problem solvers resulting from the numerical handling of the transport problems [14-16].

This work aims to explore strategies that will result in fundamentally superior modeling accuracy and will enhance our ability to handle multiscales to achieve high-fidelity simulations of materials and transport problems. We propose to review the associated challenges in modeling, mathematical and numerical techniques, and the needed parallel algorithms.

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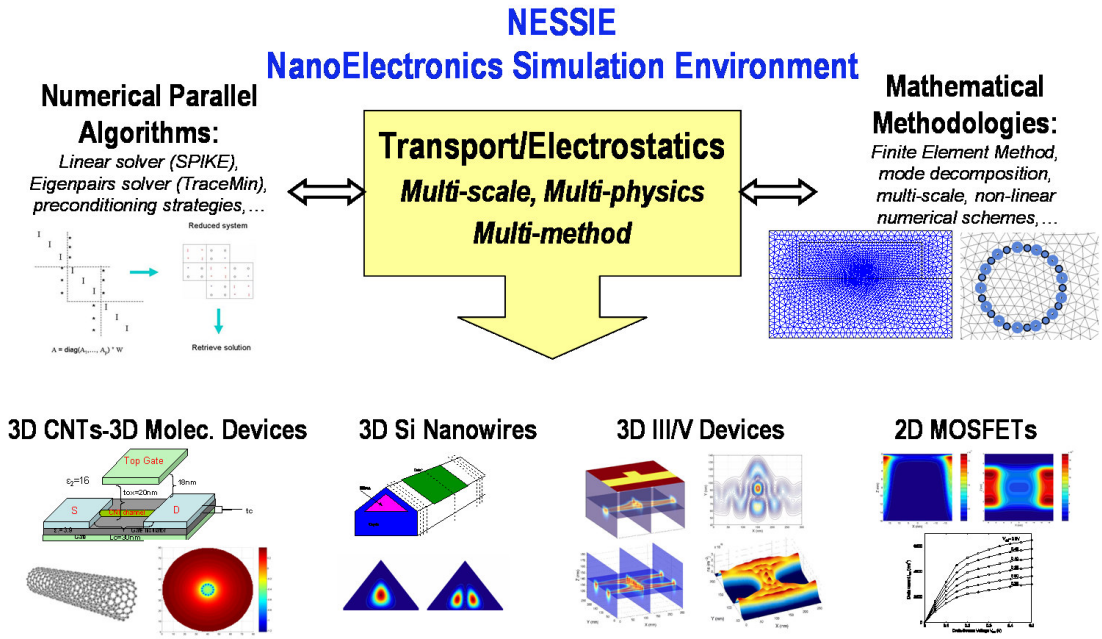

Fig. 1. This figure summarizes the capabilities of NESSIE (1998-2006), that is currently using real-space mesh techniques for performing nanoelectronics simulations on the following devices: 2D-MOSFET and 2-D DGMOSFET [12], 3-D Silicon Nanowire transistors [13], 3-D electron waveguide devices (III-V heterostructure) [2], and electrostatics calculations of molecular transistors and carbon nanotube devices [3], [4]. In carbon nanotube simulations, the transport phenomenon is localized in the nanotube while the coupling with the surroundings is achieved by considering only the electrostatics. Within our simulations, the atoms inside the device are considered as localized point charges, while FEM is needed for solving the Poisson equation in the overall transistor [3], [4].

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