COMPUTATIONAL NANOELECTRONICS

Eric Polizzi
polizzi@ecs.umass.edu

University of Massachusetts, Department of Electrical and Computer Engineering,
100 Natural Resources Road, Marcus Hall, Amherst, MA 01003-9292

August 28, 2006

Abstract

Mathematical modeling and computational simulations constitute critical elements of nanoscience research. They augment detailed experimental studies regarding fundamental limitations of traditional devices (such as nanoscale transistors MOSFETs) beyond which quantum effects become important. Modeling and simulations are also vital in focusing experimental investigation for the exploration of new classes of devices whose functionalities rely primarily on quantum effects; examples include: silicon nanowire transistors, carbon nanotubes transistors, molecular electronics transistors, and spintronics. Consequently, a full quantum description of the electron transport problem using a non-linear self-consistent Schrödinger/Poisson-type model, is necessary to address realistic three-dimensional nanoscale device simulations. Furthermore, the immense complexity of the mathematical and geometric models coupled with the multitude of underlying physical phenomena necessitate the development of advanced mathematical methodologies and numerical algorithms that are suitable for high performance computing platforms.

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. In particular, the hybrid banded parallel linear system solver SPIKE, will be presented as a new numerical component for the nanoelectronics simulator NESSIE for addressing large-scale nanoelectronics problems.