

## Chapter 4

# High-Performance Computing for Theoretical Study of Nanoscale and Molecular Interconnects

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### ABSTRACT

*Interconnects in semiconductor integrated circuits have shrunk to nanoscale sizes. This size reduction requires accurate analysis of the quantum effects. Furthermore, improved low-resistance interconnects need to be discovered that can integrate with biological and nanoelectronic systems. Accurate system-scale simulation of these quantum effects is possible with high-performance computing (HPC), while high cost and poor feasibility of experiments also suggest the application of simulation and HPC. This chapter introduces computational nanoelectronics, presenting real-world applications for the simulation and analysis of nanoscale and molecular interconnects, which may provide the connection between molecules and silicon-based devices. We survey computational nanoelectronics of interconnects and analyze four real-world case studies: 1) using graphical processing units (GPUs) for nanoelectronic simulations; 2) HPC simulations of current flow in nanotubes; 3) resistance analysis of molecular interconnects; and 4) electron transport improvement in graphene interconnects. In conclusion, HPC simulations are promising vehicles to advance interconnects and study their interactions with molecular/biological structures in support of traditional experimentation.*

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## INTRODUCTION

Silicon technology and nanoelectronics have provided vast opportunities to advance the technology, including the advances in supercomputers and stream processors<sup>1</sup>. While the International Technology Roadmap for Semiconductors (ITRS, 2010) predictions suggest a silicon future of at least ten more years, the device, interconnect, or process technology to be used to advance us towards such predictions is not rigidly defined. Devices with gate lengths as small as few nanometers are actively researched, though it is not certain whether much smaller devices will be connected with each other with copper interconnects, or will indeed require integration with nanotube-based interconnects. Furthermore, requirements for low-cost and small medical devices, and bio-integrated sensors stimulate researchers towards integrating nanoelectronics with molecules (Birge, 1994; Stan et al., 2003). It has become indispensable to utilize supercomputers, which were manufactured through the utilization of the latest silicon-technology, to further the lifespan of silicon and integrate or replace copper interconnects with nanotubes, nanowires, or molecular interconnects towards the realization of systems that are low cost and error resilient.

Electronic characterization of devices of such small scale requires analysis and understanding of many nanoscale effects. These nanoscale effects, such as surface scattering<sup>2</sup> and quantum confinement<sup>3</sup>, are related to atomic interactions. For a given effect, the number of atoms involved in a region of a device can exceed thousands. Due to the nanoscale nature of the problem, effects that were not considered appreciable, such as quantum capacitance and contact resistance (Wang et al., 2009), may actually become important. While techniques such as continuum simulations, where groups of atoms are treated as one continuous medium, are possible for certain problems, most accurate results can be obtained through truly-atomic simulations.

At nanometer scales, electronic structure-based simulations are frequently used. There are two aspects to such simulations. First, the physics behind the molecule placement and interactions needs to be solved. This involves solving the Schrödinger equation, for which an exact analytic solution is not available for most systems. The solution can be quite complex. The next aspect is the visualization of molecular structures or the obtained solutions. Real-time, high-speed, and realistic visualization enables analysis and understanding of the physical effects. Both of these aspects require high-performance computing (HPC) for feasible turnaround time.

There are many HPC tools in the area of molecular dynamics. The complexity and implemented methods have been improved over time. Some examples of tools used for classical MD simulations are CHARMM (Brooks et al., 1982), LAMMPS (Sandia National Laboratories, 2011; Plimpton, 1995), NAMD (Phillips et al., 2005), and GROMACS (Van der Spoel et al., 2005; Hess et al., 2008) to name a few. Another molecular dynamics software package Desmond (Desmond, 2011), developed recently by D. E. Shaw Research, provides high-speed molecular dynamics simulations for biological systems that are highly scalable with the number of processors on conventional compute clusters (Bowers et al., 2006). However, when Desmond is used on the special-purpose supercomputer Anton, also designed by D. E. Shaw Research, speeds that are orders of magnitude faster can be achieved (Shaw et al., 2009). For the visualization aspect, Visual Molecular Dynamics package (VMD) (University of Illinois at Urbana-Champaign, 2011) is widely used. Advances are continually being made to improve existing visualization tools by using novel HPC methodologies and algorithms (Stone et al., 2009). In this chapter, we provide examples of more recent molecular dynamics and electronic transport simulation packages. Next, we give an overview of semiconductor interconnects and how high-performance nanoelectronic com-

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