ECE 593 Advanced Topics in ECE
(Theoretical and Computational Nanoelectronics)
Spring 2010

Instructor:

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new course!

Lecture: MWF 4:00–4:50 PM

As semiconductor devices shrink into the nanoscale regime, there arise problems related to not only understanding the device operation but the complicated manufacturing processes also. This fact signifies that the traditional *trial-and-error* approach of device optimization by actually *making* the devices will no more be feasible since it is both time-consuming and too expensive. Since computers are considerably cheaper resources, simulation is becoming an indispensable tool for device engineers. Besides offering the possibility to test hypothetical devices which have not (or could not have) yet been manufactured, device simulation offers unique insight into device behavior by allowing the observation of internal phenomena that can not be measured. Thus, a critical facet of the nanodevice development is the creation of simulation tools that can quantitatively explain or even predict experiments.

The need for simulation tools can also be justified from another perspective: It is felt that contemporary nanoscience is divided between two coexisting yet disparate worlds—the world of *academic science* and the world of *commercial science*. While academic science is mainly knowledge-oriented, commercial science focuses on marketable products. The product could even be software! From our experience, we have observed that only few students have necessary skills to build *reliable* scientific software. Matlab has become the students' tool of choice, whereas high-performance parallel computing is fairly unknown!

Motivated by these facts, we have planned to develop and offer a new course on Computational Nanoelectronics in spring 2010 semester. This course will, essentially, incorporate elements that are common practices in most of the semiconductor industries' TCAD divisions. While giving a general introduction to essential theories in nanoelectronics, this course will emphasize on learning how to model (solve equations) using high-performance (super) computers and translate those theories into reliable and efficient scientific software.

Tentative Course Outline

PART A Nanoelectronics theory within a bottom-up framework—quantum mechanics, molecular dynamics, electronic structure, phonon modes, scattering and collisions, electron interactions with electric and magnetic fields, spin, current conduction, heat conduction, and optical responses.

PART B Numerical techniques—Monte Carlo, non-equilibrium Green's function, PETSc package, and various iterative methods.

PART C Scientific software development techniques—computer organization, Linux, software carpentry, object-oriented programming, time and memory efficiency, optimization, portability, documentation, useful tools (MPI, subversion, Netlib, GAMS, Rappture, debuggers, valgrind, Tcl/Python), presentation skills (LaTeX, gnuplots, Adobe Illustrator, IEEE author guides).