**Course Topics**

**EEE 566: Advanced Device Modeling**

**Prerequisites:** EEE EEE434, EEE 534 or instructor approval

**Catalog Course Description:** Understanding semi-classical and quantum transport theory and device simulations

**Course Topics:**

Review of semiconductor physics and transport

o Semiconductor physics - basic concepts

o Review of drift-diffusion model

o Hydrodynamic model

The BTE and its solution

o Introduction of the BTE

o Derivation of the Fermi's Golden Rule

o Scattering mechanisms description

o Low-field and high-field transport characteristics calculation (Rode's Iterative Method)

o Single particle Monte Carlo description

o Ensemble Monte Carlo method

o Simulation examples

Solving the Poisson and the Maxwell's equations

o Field equations - Numerical solution techniques: finite difference in 1D-3D, direct vs. iterative methods, rate of convergence estimate, mesh generation, boundary conditions

o The multi-grid method

o Description of the Conjugate Gradient Methods

o Solution of the Maxwell Equations

Particle-Based device simulator

o Stability Criteria for time-step and mesh-size

o Particle dynamics with boundary conditions (modeling of the ohmic and Schottky contacts, artificial boundaries)

o Particle-mesh coupling techniques (NGP, NEC, CIC, etc.)

o Current calculation techniques

Examples of device modeling

o Si MESFET Simulations (Tarik Khan)

o SiGe devices - Full-Band Simulations (Santhosh Krishnan)

o FINFETs (Hasanur Rahman Khan)

Advanced Topics

o Many-Body Effects: Molecular Dynamics, P3M approach, Corrected Coulomb approach, FMM, application in device simulators

o Quantum corrections to semi-classical approaches:

 - Density Gradient Method

 - Quantum Corrected Hydrodynamics

 - Effective potential approach used in conjunction with particle-based device simulators

Quantum Simulation

o Schrodinger Equation

- General Notation

- Stationary States for a Free Particle

- Bulk dispersion

o Discretized Schrodinger Equation

- Method

- Bulk dispersion

- Comparison between continuum and discretized bandstructure

o Realistic Semiconductor Bandstructure Models

- Atomic cores impose a potential on the electrons

- Pseudopotential method

- k.p method method and treatment of strain

- Tight binding method and treatment of strain

Quantum Transport in a single band - Non-interacting Systems

o Tunneling Theory - Continuum Semi-Analytical Method

- Current operator

o Landauer Approach

- Current expression

- Charge expression

o Numerical Instability of Transfer Matrix Approach

o Physical Limitations of the Semi-analytical Tunneling Approach

- different effective masses,

- transverse momentum

- finite bandwidth of a realistic semiconductor band

o Tunneling Theory - Discretized Numerical Method

- Single Band, Single Effective Mass

- QTBM method

- Direct solution of the Schrodinger Equation through LU

- Current and charge expressions via Landauer approach

Non-Equilibrium Transport

o Mixed States and Distribution Function

o Irreversible Processes and MASTER Equations

o Green's Functions Approach

- Second Quantization of Particles

- Single particle and two-particle operators

- Schrodinger, Heisenberg and Interaction representation

- Wicks Theorem

- Feynman Diagrams and the partial summation method for the self energy

- Dyson Equation

- Definition of the six Green's functions

- Ballistic approaches for solving the Green's Function problem in devices

A. Recursive Green's function Approach

B. Contact Block Reduction method

Assignments:

1. Scattering rates derivation /10
2. Scattering Table Construction /10
3. EMC for Bulk GaAs /30
4. Poisson 2D Implementation/15
5. Modeling of GaAs MESFETs /35