Course Topics

EEE 598: 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

- Schrodinger Equation
  - General Notation
  - Stationary States for a Free Particle
  - Bulk dispersion
- Discretized Schrodinger Equation
  - Method
  - Bulk dispersion
  - Comparison between continuum and discretized bandstructure
- 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

- Tunneling Theory - Continuum Semi-Analytical Method
  - Current operator
- Landauer Approach
  - Current expression
  - Charge expression
- Numerical Instability of Transfer Matrix Approach
- Physical Limitations of the Semi-analytical Tunneling Approach
  - different effective masses,
  - transverse momentum
  - finite bandwidth of a realistic semiconductor band
- 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

- Mixed States and Distribution Function
- Irreversible Processes and MASTER Equations
- 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