The non-equilibrium Greens function (NEGF) formalism provides a powerful conceptual and computational framework for treating quantum transport in nanodevices. It goes beyond the Landauer approach for ballistic, non-interacting electronics to include inelastic scattering and strong correlation effects at an atomistic level.

NEGF is generally regarded as an esoteric tool for specialists, but we believe it should be a part of the standard training of science and engineering students.

For the convenience of interested students we have set up a Q&A forum along with tutorial materials open to all.

**Tutorial Papers**

Simulators

- **Resonant Tunneling Diode Simulation with NEGF**: Compute charge and current through a resonant tunneling diode and multi-barrier heterostructures in a single band effective mass approximation.
- **NanoMOS**: 2-D simulator for thin body (< 5 nm), fully depleted, double-gated n-MOSFETs.
- **Nanowire**: Simulate electron transport in 3D through nanowires in the effective mass approximation subject to 3D Poisson solution.
- **Multi-gate Nanowire FET**: 3D Simulator for Silicon Nanowire Field Effect Transistors with Multiple Gates.

Research Publications

**NEGF simulation of semiconductor devices at the tight binding or Huckel level:**


**NEGF simulation of nanoscale transistor at the effective mass level:**

- Datta: *CQT: Concepts of Quantum Transport* (4 part lecture)
- Datta: *Nanodevices: A Bottom-up View*
- Klimeck: *NEMO 1-D: The First NEGF-based TCAD Tool and Network for Computational Nanotechnology*
- Klimeck: *Numerical Aspects of NEGF: The Recursive Green Function Algorithm*
- Lundstrom: *A Top-Down Introduction to the NEGF Approach*
NEGF simulation at the *ab initio* level


NEGF in Phonon Transport


Related Ph.D. Theses


Online Classes

- Datta: Atom to Transistor, earlier teachings: graduate level
- Datta: Fundamentals of Nanoelectronics, earlier teachings: undergraduate level

Downloads

- Datta: MATLAB Scripts for "Quantum Transport: Atom to Transistor"
- Koswatta/Nikonov: MOSCNT: code for carbon nanotube transistor simulation (Matlab)
- Nikonov: Scripts for “recursive algorithm for NEGF in Matlab”
- NanoMOS 2.5 Source Code Download

Standard References

Most device simulation is based on models that neglect interactions or at best treat them to first order, for which simple treatments are adequate. But here are a few standard references and review articles on the NEGF formalism all of which are based on the use of advanced concepts like the “Keldysh contour”, which are needed for a systematic treatment of higher order interactions.

Infinite homogeneous media:


Finite structures: Many authors have applied the NEGF formalism to problems involving finite structures.

THE NEGF APPROACH TO NANO-DEVICE SIMULATION


Additional nanoHUB Resources

- [Search for all NEGF related content](#)