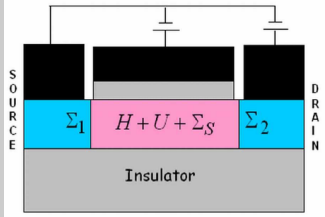
# The NEGF Approach to Nano-Device Simulation




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**

- S. Datta, “Nanoscale Device Simulation: The Green’s Function Method,” Superlattices and Microstructures, *28*, 253-278 (2000).
- S. Datta, “Non-Equilibrium Green’s Function (NEGF) Formalism: An elementary Introduction,” *Proceedings of the International Electron Devices Meeting (IEDM),* IEEE Press (2002). (preprint)-
- S. Datta, “Electrical resistance: an atomic view,” *Nanotechnology,* **15**, S433-S451 (2004).
- M. P. Anantram, M. S. Lundstrom and D. E. Nikonov, “Modeling of Nanoscasle Devices,” http://arxiv.org/abs/cond-mat/0610247v2 (2007). -
- M. Paulsson, “Non Equilibrium Green’s Functions for Dummies: Introduction to the One Particle NEGF equations,” arXiv.org cond-mat/0210519 (2002). -
- E. Polizzi, and S. Datta, “Multidimensional Nanoscale device modeling: the Finite Element Method applied to the Non-Equilibrium Green’s Function formalism,” *IEEE-NANO 2003. Third IEEE Conference on Nanotechnology,* **2**, 40-43 (2003). -
- A. P. Jauho, “Introduction to the Keldysh nonequilibrium Green function technique,” -

**Online Seminars**

- 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

**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:***


- Gerhard Klimeck, Roger K. Lake, R. Chris Bowen, William R. Frensley and Ted Moise,, "Quantum Device Simulation with a Generalized Tunneling Formula," *Appl. Phys. Lett.*, **67**, 2539, 1995.

- R. C. Bowen, G. Klimeck, R. Lake, W. R. Frensley and T. Moise,, "Quantitative Resonant Tunneling Diode Simulation," *J. Appl. Phys.*, **81**, 3207, 1997.
- R. Lake, G. Klimeck, R. C. Bowen and D. Jovanovic, "Single and multiband modeling of quantum electron transport through layered semiconductor devices," *J. Appl. Phys.*, **81**, 7845, 1997.
- J. Guo, S. Datta, M.S. Lundstrom and M.P. Anantram, "Towards Multiscale Modeling of Carbon Nanotube Transistors," *International J. on Multiscale Computational Engineering,* special issue on multiscale methods for emerging technologies, ed. N. Aluru, **2**, 257-276, 2004. *(a treatment of carbon nanotube transistors by a pz orbital, tight-binding method)*-
- M. Paulsson, F. Zahid, and S. Datta, "Resistance of a Molecule," chapter in *Handbook of Nanotechnology,* ed. S. Lyshevski, Press, 2002, ISBN: 0-849312000. *(Huckel approach for molecules)*-
- F. Zahid, M. Paulsson, and S. Datta, "Electrical Conduction in Molecules," chapter in *Advanced Semiconductors and Organic Nano-Techniques,* ed. H. Morkoc, Academic Press, 2003, ISBN: 0-12-507060-8. *(Huckel approach for molecules)*-


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

- Z. Ren, R. Venugopal, S. Goasguen, S. Datta and M. S. Lundstrom, “nanoMOS 2.5: A Two-Dimensional Simulator for Quantum Transport in Double-Gate MOSFETs,” *IEEE Trans. Electron. Dev.*, special issue on Nanoelectronics, **50**, 1914-1925, 2003. -
- R. Venugopal, Z. Ren, S. Datta, and M. S. Lundstrom, “Simulating Quantum Transport in Nanoscale Transistors: Real versus Mode-Space Approach,” *J. Appl. Phys.*, **92**, 3730-3739, 2002. -
- R. Venugopal, S. Goasguen, S. Datta, and M. S. Lundstrom, “A Quantum Mechanical Analysis of Channel Access, Geometry and Series Resistance in Nanoscale Transistors,” *J. Appl. Phys.*, **95**, 292-305, 2004. -
- J. Wang, E. Polizzi, and M. S. Lundstrom, “A Three-Dimensional Quantum Simulation of Silicon Nanowire Transistors with the Effective Mass Approximation,” *J. Appl. Phys.*, **96**, 2192, 2004. -


***NEGF simulation at the ab initio level***


- P.S. Damle, A.W. Ghosh, and S. Datta, “Nanoscale Device Modeling,” chapter I in *Molecular Nanoelectronics,* ed. M. Reed and T. Lee, Scientific Publishers, 2003, ISBN: 1-58883-006-3.
- P.S. Damle, A.W. Ghosh, and S. Datta, “First-principles Analysis of Molecular Conduction Using Quantum Chemistry Software,” *Chem. Phys.*, **281**, 171-188, 2002.
- P.S. Damle, A.W. Ghosh, and S. Datta, “Unified Description of Molecular Conduction: From Molecules to Metallic Wires,” *Phys. Rev. B*, **64**, Rapid Communication, 201403-1-201403-4, 2001.


***NEGF in Phonon Transport***


- N. Mingo and Y. Liu, “Phonon Transport in Amorphous-Coated Nanowires: an Atomistic Green Function Approach,” *Phys. Rev. B*, **70**, 249901, 2004.


**Related Ph.D. Theses**


- Roger Lake, “Application of the Keldysh Formalism to Quantum Device Modeling and Analysis”, Ph.D. Thesis, Purdue University, 1992. -
- Gerhard Klimeck, “Electron-Phonon and Electron-Electron Interactions in Quantum Transport” Purdue University, 1994. -
- Zhibin Ren, “Nanoscale MOSFETs: Physics, Simulation, and Design,” Ph.D. Thesis, Purdue University, December 2001. -
- Prashant Damle, “Nanoscale Device Modeling: From MOSFETs to Molecules,” Ph.D. Thesis, Purdue University, May 2003.. copy)-
- Ramesh Venugopal, “Modeling Quantum Transport in Nanoscale Transistors,” Ph.D. Thesis, Purdue University, August 2003. copy)-
- Jing Guo, “Carbon Nanotube Electronics: Modeling and Physics,” Ph.D. Thesis, Purdue University, August 2004. copy)-
- Jing Wang, “Device Physics and Simulation of Silicon Nanowire Transistors,” Ph.D. Thesis, Purdue University, August 2005. -
- M. Luisier, “Quantum Transport for Nanostructures,” (2005) -

### 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:***


- Martin, P. C. and Schwinger, J., "Theory of many-particle systems," *Phys. Rev.* **115**, 1342, 1959.
- Kadanoff, L. P. and Baym, G., *Quantum Statistical Mechanics,* Frontiers in Physics Lecture Note Series, WA Benjamin, New York, 1962, now published by Perseus Books, ISBN: 020141046X
- Keldysh, L. V., "Diagram technique for non-equilibrium processes," Sov. Phys. JETP, 20, 1018, 1965.
- Danielewicz, P., "Quantum theory of non-equilibrium processes," Ann. Phys., 152, 239, 1984.
- Rammer, J. and Smith, H., "Quantum field-theoretical methods in transport theory of metals," *Rev. Mod. Phys.*, **58**, 323, 1986.
- Mahan, G. D., "Quantum transport equation for electric and magnetic fields," *Phys. Rep*, **145**, 251, 1987.
- Khan, F. S., Davies, J. H. and Wilkins, J. W., "Quantum transport equations for high electric fields," *Phys. Rev. B*, **36**, 2578, 1987.


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


- E.V. Anda and F. Flore, "The role of inelastic scattering in resonant tunneling heterostructures," *J. Phys. Cond. Matt.*, **3**, 9087, 1991.
- C. Caroli, R. Combescot, P. Nozieres and D. Saint-James, "A direct calculation of the tunneling current: IV. Electron-phonon interaction effects," *J. Phys. C: Solid State Physics*, **5**, 21, 1972.

- Y. Meir and N.S. Wingreen, “Landauer Formula for the Current through an Interaction Electron Region,” *Phys. Rev. Lett.*, **68**, 2512, 1992.
- S. Datta, “A simple kinetic equation for steady-state quantum transport,” *J. Phys. Cond. Matt.*, **2**, 8023, 1990.
- A.P. Jauho, N.S. Wingreen and Y. Meir, “Time-dependent transport in interacting and non-interacting resonant tunneling systems,” *Phys. Rev. B*, **50**, 5528, 1994.
- H. Haug and A.P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors,* Springer, Berlin, 1996, ISBN: 3540616020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