Abstract

As the current CMOS technology behind computing devices is scaled smaller and smaller it becomes less practical and will soon be unable to continue the current trend in size reductions and speed improvements. New technology is emerging that operates on a nanoelectronic scale and in a fundamentally different way from current devices. Simulations and modeling of this new technology will be a large part of its design and implementation. The Nanoelectronics Theory and Simulation Laboratory at the University of Massachusetts Amherst is developing a simulation environment called NESSIE that is capable of such simulations and modeling for arbitrary devices. We are creating an extension to this environment to calculate electron transport properties through arbitrary open systems. To solve such an open system boundary conditions must be included in the finite element mesh used by the framework to effectively include the solution in the leads. Knowing the form of the solution in the leads we are able to produce the mesh used by the framework to effectively include the solution in the leads. Results found using this method are still preliminary but seem to agree with experimental and simulative results.

Research Objectives

• Accurately simulate electron transport properties through arbitrary nanoscale potential systems such as single molecules within the NESSIE framework.
• Perform simulations using full 3D mesh structure and all electron calculations derived from first principle equations (the Schrödinger equation).
• Corroborate results for electron transport through single molecules with experimental results and simulations performed using different methods.

Methods

• Within the NESSIE framework the calculations are performed using the finite element method (FEM) to discretize the system. The Non-Equilibrium Green’s Function (NEGF) along with the density functional theory are used in solving the many electron system.
• Here this is expanded from a closed system to an open one through the inclusion of proper boundary conditions at the system edges. These boundary conditions describe the solution in the leads attached to the system including injection, reflection, and transmission of electrons into, from, and through the system.
• Once the system is solved, current can be found through the Landauer formula:

\[ I(V_{sd}) = \frac{2e}{\pi h} \int T(E,V_{sd}) dE \]

Figure 1: An overview of the capability of the NESSIE framework from single atoms on the left to single molecules to complete nanostructures on the right.

Progress and Results

• A proof of concept simulation in 1D was performed using the methods described. The resulting current voltage characteristics for a double barrier (resonant tunneling diode) are shown in Figure 3.
• The full 3D simulation is still being developed. Preliminary results for a simple system with no atomic structures can be seen in Figure 4.

Future Work

• Complete the full 3D framework so it is capable of performing simulations with arbitrary potentials caused by atoms within the system.
• Perform simulations using the completed framework on real life systems and corroborate results, experimental and simulative, found by other groups.

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