
Hierarchical simulation of quantum circuits

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ABSTRACT: The focus of the present project is to develop the fundamentals of quantum circuit modeling. Quantum circuit modeling will enable us to describe the integration of quantum nanodevices into circuits and the simulation of the circuit as a whole for novel applications. These models are essential if one is to anticipate novel computing architectures where molecular devices may function far differently from modern transistors and where optimized circuit design may entail radically different patterns of device interconnections.

INTRODUCTION

Within the framework of the IREE award Brandon Cook, who is a graduate student at Vanderbilt spent three month (May 2008-July 2008) in Prof. Hong Guo's group at McGill, Montreal, Canada. Prof. Hong Guo is a world leading expert in quantum transport theory working on wide variety of important problems including description of spin-injections, inelastic electron tunneling, spin polarized transport and field effect transistors within the framework of the Non-equilibrium Green's Function method.

The aim of this collaboration is to develop a unified framework to couple quantum devices into circuits. The quantum devices will be connected by quantum wires forming circuits that will be modeled by interfacing the Boltzmann transport description of the wires and the engineering device models.

RESEARCH ACTIVITIES AND ACCOMPLISHMENTS OF THE INTERNATIONAL COOPERATION

Brandon Cook spent the summer at McGill learning techniques used to study quantum transport in nanoscale spintronic devices. The exploitation of electron spin in addition to charge has the potential of a new paradigm for electronic devices. *Ab-initio* spin-polarized transport calculations are generally needed to capture more than qualitative features of such systems. MATDCAL is a code developed at McGill that implements density function theory (DFT) within a non-equilibrium Green's function (NEGF)

framework to allow calculations in realistic devices. Our goal for the summer was to understand the NEGF-DFT theory and the implementation in MATDCAL. In parallel to learning the techniques and code we would be testing that knowledge by investigating the properties of a Fe/ Carbon nanotube magnetic tunnel junction.

Several example calculations are discussed in the literature and provide instructive examples. These include Ni/BDT/Ni, Fe/MgO/Fe and ZGNR/C60/ZGNR (Zigzag Graphene nano ribbon). As a sample system to study I worked with Fe/(5,5)Carbon nano-tube junctions (Figures 1 and 2). This system was chosen because nanotubes have promising properties for use in spintronic devices and ferromagnetic contacts are present in several experimental setups. The main purpose of the calculations was to familiarize myself with the software and the practical aspects of using it. A sample result of a transmission calculation is shown in figure 3.

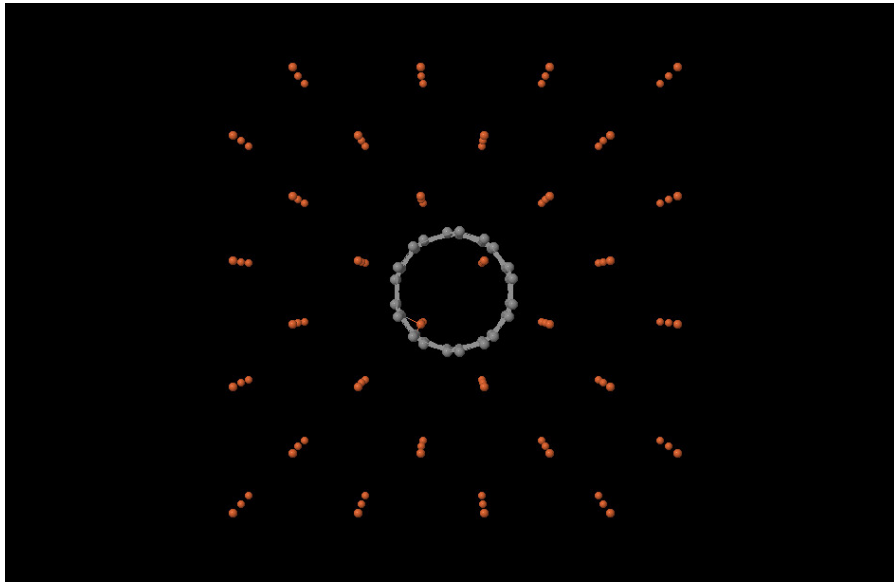


Figure 1: Front View of a Fe/CNT magnetic tunnel junction

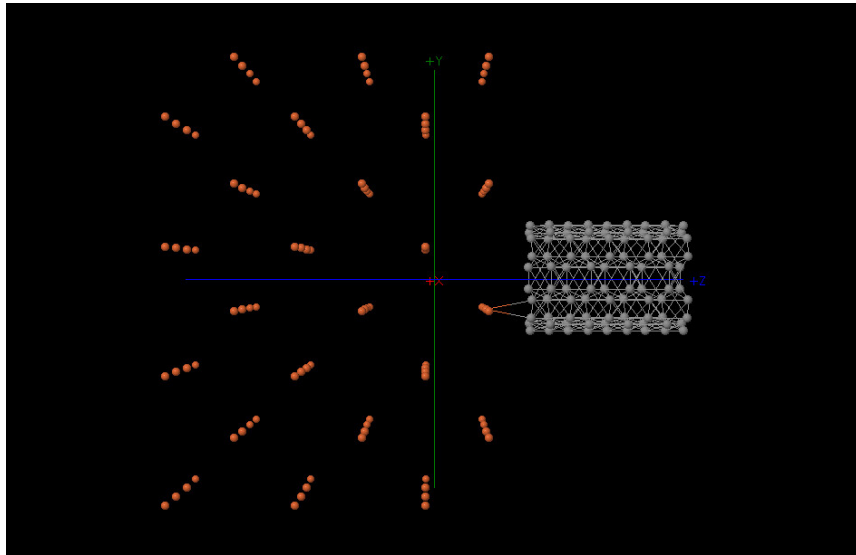


Figure 2: Side View of a Fe/CNT magnetic tunnel junction

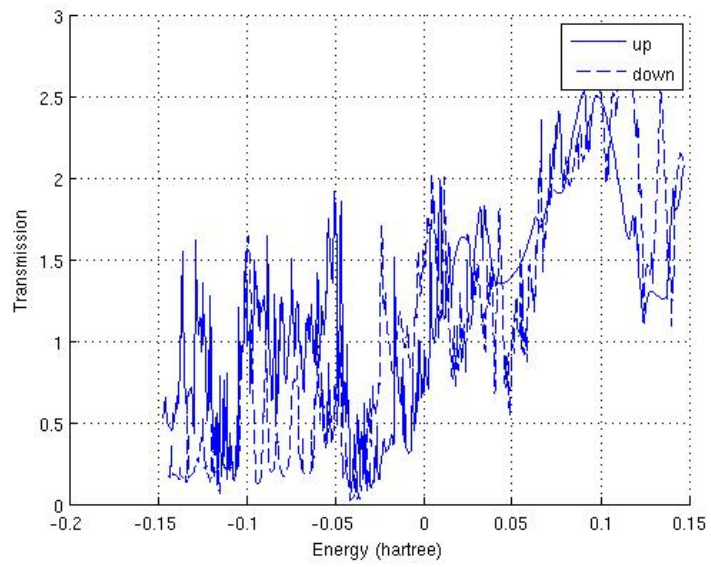


Figure 3: Transmission in Fe/CNT magnetic tunnel junction

BROADER IMPACTS OF THE INTERNATIONAL TRAVEL

Collaboration with Prof. Hong Guo's group greatly enhanced our capability to simulate nanodevices especially. Graduate student Brandon Cook spent three month in Montreal and learned how to use the McDcal device simulator. The McDcal is based on the Non-equilibrium Green's function theory. The efficient implimentation of this theory is a non-trivial task. Prior to calculation with MATDCAL an external program such as Siesta, VASP, WEIN2K or OpenMX is used to optimize the device geometry. Typically this is done with a full-potential linear augmented planewave method (FLAPW) to ensure accurate total energies. Matrix inversion is a computationally expensive operation and necessary to construct the Green's function. This imposes limits on the size of basis set that can be used. A typical calculation is done with linear combination of atomic orbitals (LCAO) basis sets optimized to accurately reproduce the electronic structure found in FLAPW calculations. The potential is obtained from a real space solution to the poisson equation. The K-point integration needed to accurately get the denisty from the Green's function is a computational intensive part of the calculation as many points are needed for the result to converge. However this represents an opportunity for parallelization as each k-point can be evaluated independently. Efficient matrix inversion is key for a fast implimentation of this theory; MATDCAL uses a partitioning algorithm exploiting the block tridiagonal structure of the Hamiltonian to obtain solutions. This techniqe allows for calculation time that scales with $O(N)$ with respect to the device length. The other main bottleneck is the conversion of densities and potentials from orbital to real space representations. In MATDCAL this is handled by a caching algorithm where a subset of the most frequently used orbital overlaps are kept in memory. MATDCAL is implimented in Matlab with bottlenecks impimented in Java and calls to MPI for parallization contained in C wrappers. Finally there are several other relevant aspects to the computation, convergance criteria and further opportunities for parallel computing.

DISCUSSION AND SUMMARY

More detailed and accurate calculations for the system in question are ongoing and will be published. There are now several running serial installations of MATDCAL at Vanderbilt and plans for a full parallel instalation. Further projects would include optimization of the code, integration with other common tools and the study of other systems of interest. This work will be part of Brandon Cook's PhD thesis.

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BRIEF BIOGRAPHIES OF RESEARCHERS

Kalman Varga, Assistant Professor of Physics. Kalman Varga received his PhD in 1996 at the University of Debrecen, Hungary. His research interests include computational nanoscience, molecular dynamics simulations, density-functional and time dependent density functional calculations, electron transport, and the development of linear scaling first-principles approaches. He has published more than 100 papers, co-authored two books, and currently serves as Condensed Matter Field Editor on the editorial board of Few-Body Systems (Springer). He is member of the Vanderbilt Institute of Nanoscale Science and Engineering (VINSE).

Brandon Cook received his BS in Mathematics and BS in Physics from Lynchburg College in 2003. He is a second year graduate student at Vanderbilt University. His research interests include first principles calculation for nanoscale devices and quantum molecular dynamics, and improving the scaling of current approaches.