Fast Self-Energy Calculations & Point Charge Implementation in ELEQTRONeX

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Abstract

The Non-Equilibrium-Green's Function (NEGF) technique is used in Carbon Nanotube (CNT) simulations. We build on ELEQTRONeX, a fast, parallelizable NEGF framework. Our work has two major aspects: **implementing fast methods for computationally complex self-energy calculations and adding external charge sources to allow for broader applications.**
Our existing ELEQTRONeX framework uses an analytical self-energy solution, valid specifically for CNTs with basic lead configurations. To calculate more general self-energies, we use a tight-binding approximation, leading to an iterative and eigenfunction-based self-energy approach. Using randomly generated matrices, we show our methods are much more efficient than alternative direct inversions, allowing for faster and more complex NEGF geometries.
Motivated by discrepancies with experimental results, we also implement point charges as external boundary conditions, which we demonstrate to have drastic impacts in our simulations.

Motivation

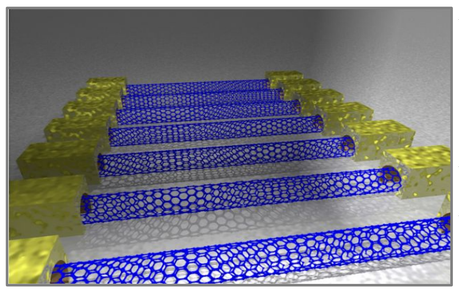

Figure I: Parallel CNT array

- **ELEQTRONeX is a framework for ELEctrostatic-Quantum TRansport modeling Of Nanomaterials at eXascale**
  - Using NEGF formalism, it has been applied to misaligned CNT arrays, with applications in photon detection
- **Extending solver for intricate materials requires faster self-energy calculations**
- **Point charge implementations are relevant for expanding modeling capabilities**
  - Effects of isolated charges near CNTs
  - Effects of charged impurities within gate-oxide in topgate experiments

ELEQTRONeX Workflow

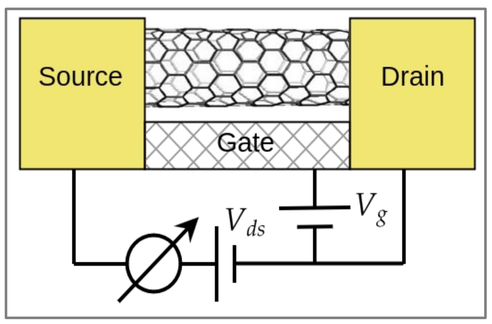

Figure II: Planar CNT configuration

- **CNT is a conductor between source and drain V_{ds}, and over gate V_g**
  - Current and conductance modified by varying V_g
- **ELEQTRONeX couples NEGF and electrostatics recursively**
  - Poisson's equation finds potential U from charge distribution ρ_{in}
  - NEGF calculates charge distribution ρ_{out} from potential U
  - Coupled via Broyden's 2nd Algorithm
- **At convergence, current I and conductance G are found**
  - Inputs: Boundary Conditions (BCs), external charge densities ρ, and material transmission operators τ_j

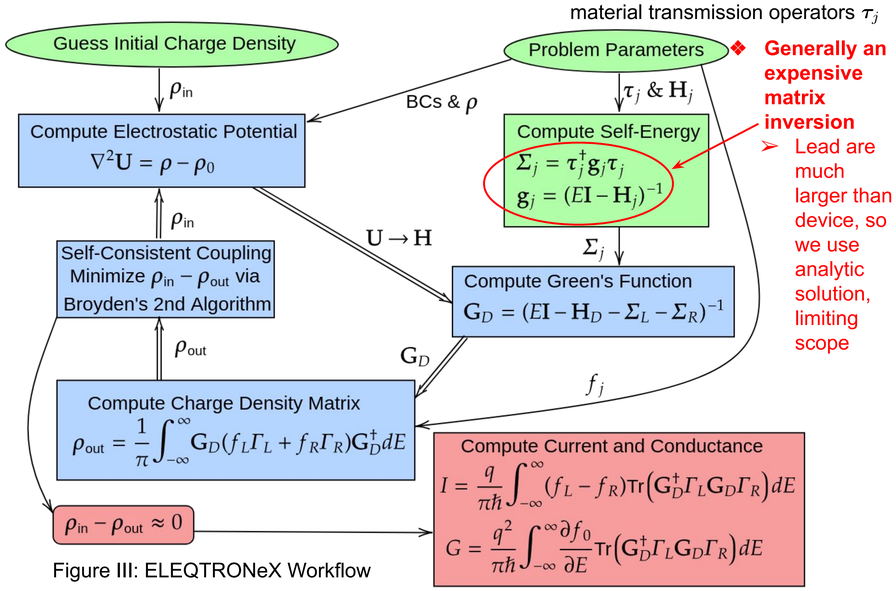

Figure III: ELEQTRONeX Workflow

- **Generally an expensive matrix inversion**
  - Lead are much larger than device, so we use analytic solution, limiting scope

Fast Self-Energies

- **2 methods to calculate faster based on tight-binding approximation**
  - Assume CNT layers affect only nearest neighbors
- **I. Decimation Method**
  - Recursive calculation to invert tridiagonal $(EI - \boldsymbol{H}_j)^{-1}$ quickly
  - Desirable convergence for random matrices

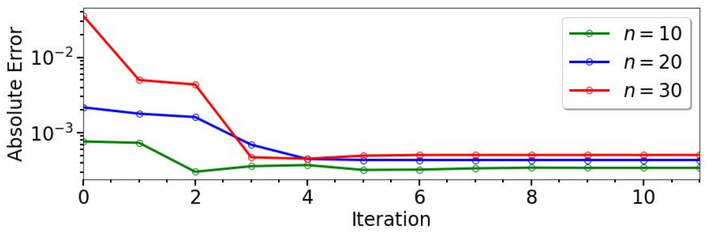

Figure IV: Error of decimation technique for random matrices of varying size

- **II. Eigenfunction Method**
  - Uses periodicity of CNT to write Bloch wave solutions;

$$\boldsymbol{H}_{R\,\text{cond}}(p) = \boldsymbol{H}_{R\,\text{cond}}(p+P) \rightarrow |\psi_j(p+P)\rangle = \lambda\,|\psi_j(p)\rangle$$

  - Solves eigenfunction problem to decompose: $g'_{P,0} = \boldsymbol{UC}$
  - Generalizable to any material via Hamiltonian condensation

	Time Complexity
Decimation Method	$(P-1)\,\mathcal{O}(n^3) + (M+1)\,\mathcal{O}(n^3)$
Eigenfunction Method	$(P-1)\,\mathcal{O}(n^3) + \mathcal{O}(2^3 n^3) + \mathcal{O}(n^3)$
Inversion of $\boldsymbol{H}_{\text{R cond}}$	$(P-1)\,\mathcal{O}(n^3) + \mathcal{O}(P^3 n^3)$
Inversion of $\boldsymbol{H}_{\text{R}}$	$\mathcal{O}(N^3 P^3 n^3)$

	$P=2$	$P=4$	$P=8$
Decimation Method	0.0184	0.0117	0.0159
Eigenfunction Method	0.0117	0.0148	0.0294
Inversion of $\boldsymbol{H}_{\text{R cond}}$	0.5753	0.7039	1.583
Inversion of $\boldsymbol{H}_{\text{R}}$	3.146	20.64	136.2

- **Both methods are independent of N, the number of layers, instead they depending on the period size P and layer size n**

- **Faster surface Green's function calculations significantly accelerate NEGF method and allow for more complex materials**
  - Modeling arbitrary lead geometries
  - Different material lead and device layers
  - Phonon transport
  - Device defects and errors

Point Charge Implementation

- **We model external point charges as steep Gaussians**
  - Using Poisson's equation, we solve for potential U
  - Only one calculation per simulation, allows for any configuration without slowing iterative procedure
  - Ability to handle large number of charges

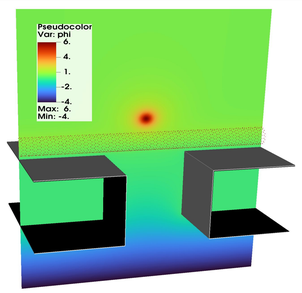

Figure V: CNT with point charge

Figure VI: ELEQTRONeX logo written with 200 point charges

Digital poster **Research Report** **Contact**

Point Charge Results

- **We test a single point charge above a 100 nm CNT at equilibrium, varying V_g from -2 V to 2 V**

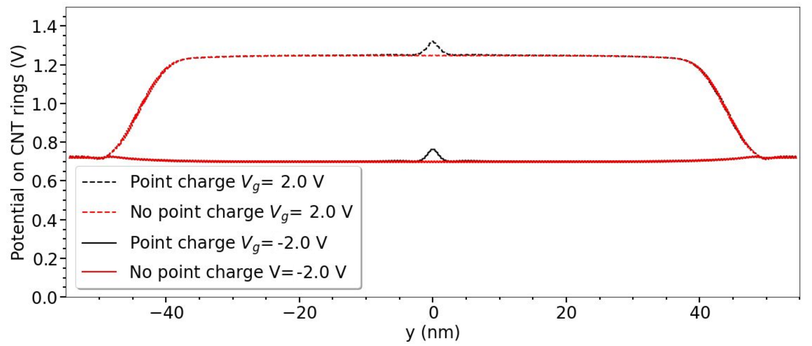

Figure VII: Potential distribution over 100 nm CNT

- **Point charges create result in large SS differences**

CNT Geometry	G_{ON} (μS/μm)	G_{OFF} (μS/μm)	SS (mV/dec)
10 nm	64.61	9.869	1912
10 nm Point Charge	197.7	33.26	2641
100 nm	16.76	1.215e-3	22.852
100 nm Point Charge	324.3	45.82	499.35

- **Topgate configuration, with gate above CNT separated by oxide region, is common in experiments**
  - Discrepancy between simulated and experimental results due to trapped charge impurities in gate oxide
  - Simulate charge distribution in oxide region
  - Point charge density causes shift in G
- **We suspect charge dependence on electrostatics affects slope**

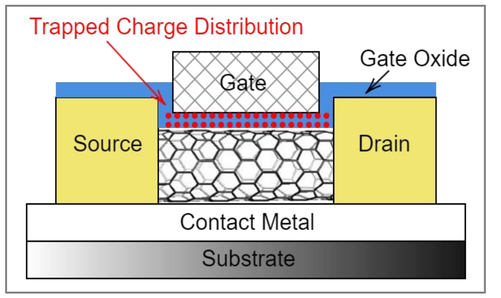

Figure VIII: Topgate CNT with trapped charges

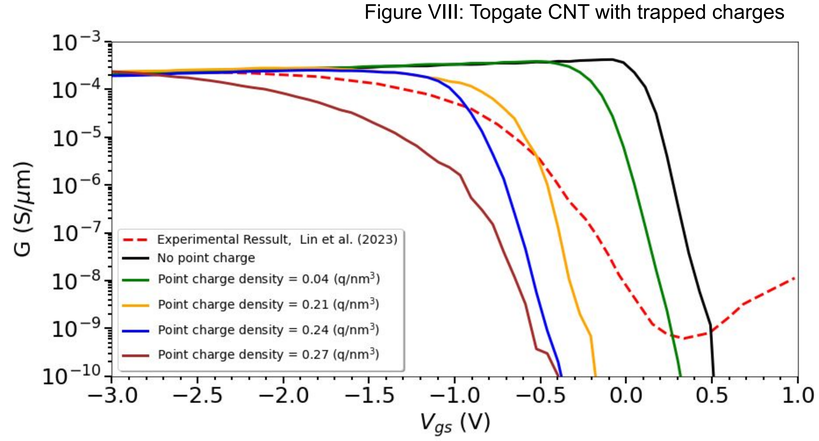

Figure IX: Conductance plot for topgate configuration, V_{ds} = -0.1 (V)

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