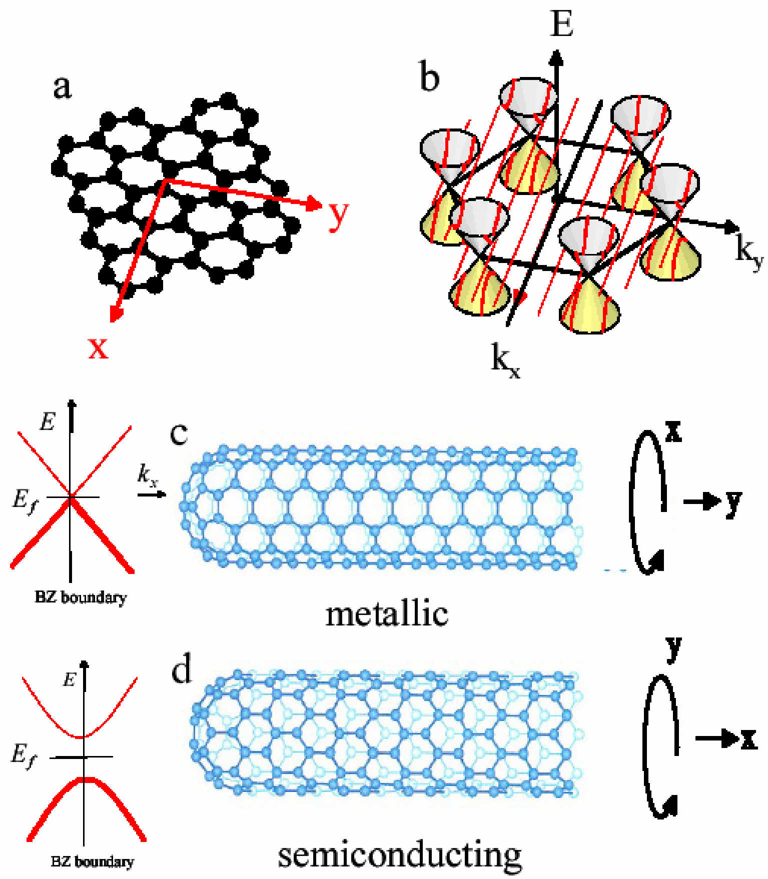
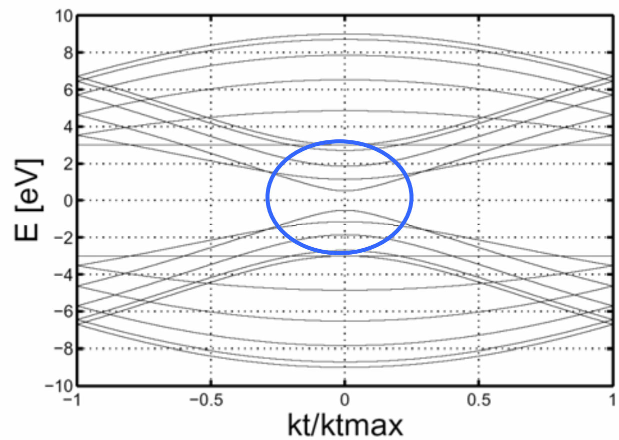
Atomistic Simulation of Carbon Nanotube FETs Using Non-Equilibrium Green's Function Formalism

Jing Guo[1], Supriyo Datta[2], M P Anantram[3], and Mark Lundstrom[2]
[1]Department of ECE, University of Florida, Gainesville, FL
[2]School of ECE, Purdue University, West Lafayette, IN
[3]NASA Ames Research Center, Moffett Field, CA

1. Introduction
2. NEGF Formalism
3. Ballistic CNTFETs
4. Summary

Introduction: carbon nanotubes





$$E(k) = \pm\left(\frac{E_G}{2}\right)\sqrt{1+(3kd/2)^2}$$

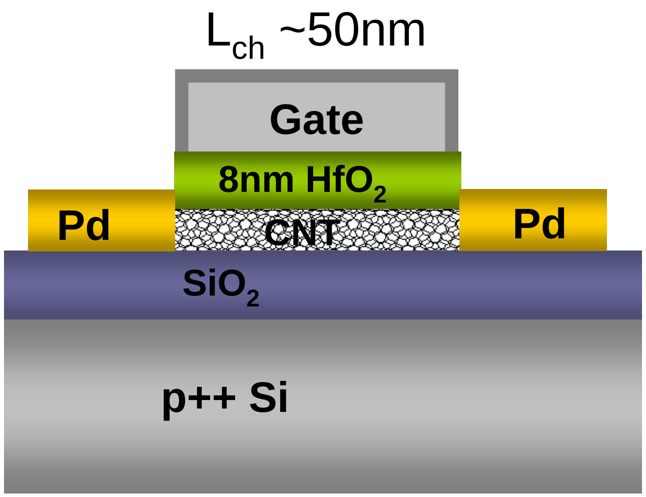
$$E_G \approx 0.8eV/d\,(\text{nm})$$

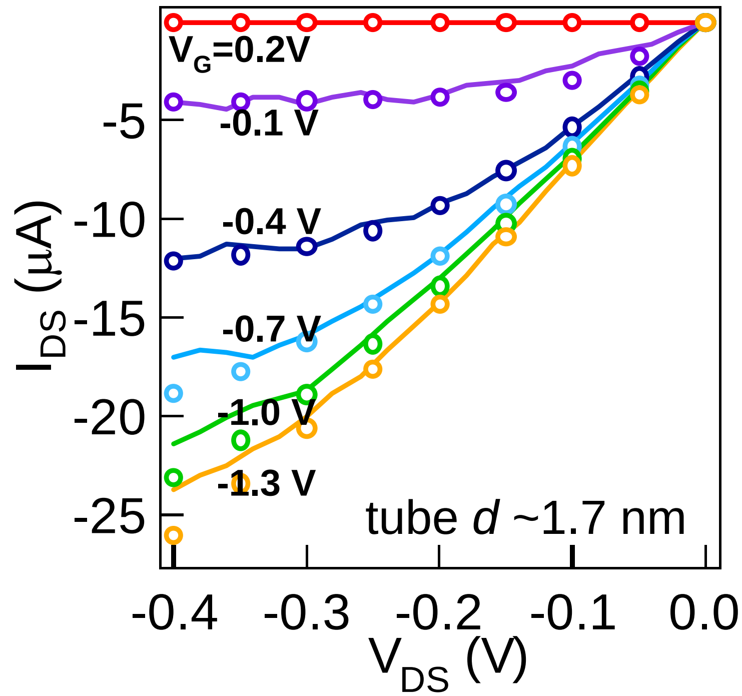
McEuen et al., *IEEE Trans. Nanotech*., **1** , 78, 2002.

(see also: R. Saito, G. Dresselhaus, and M.S. Dresselhaus, *Physical Properties of Carbon Nanotubes*, Imperial College Press, London, 1998.)

Introduction: device performance

nanotube diameter ~1.7 nm





$$G_D \approx G_B$$

$$I_{ON} \approx 3{,}000 \mu A / \mu m \qquad (W = 2d)$$

Javey, Guo, Farmer, Wang, Yenilmez, Gordon. Lundstrom, and Dai, Nano Lett., 2004

Outline

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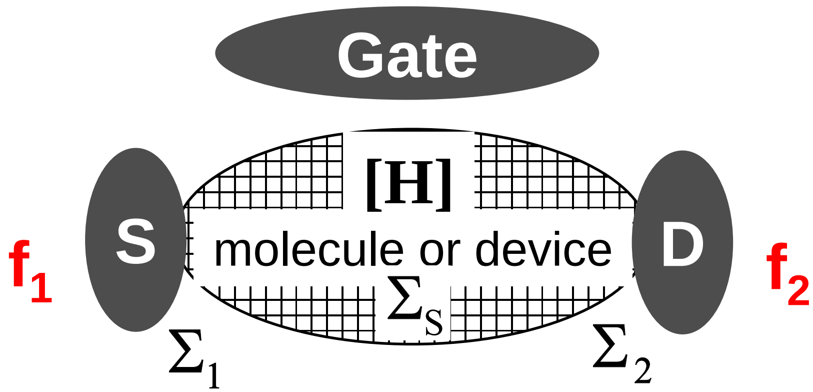
Nonequilibrium Green's Function (NEGF)



$$\mathbf{G} = \left[E\mathbf{I} - \mathbf{H} - \Sigma_1 - \Sigma_2 - \Sigma_S\right]^{-1}$$

device contacts scattering

Charge density (ballistic)

$$N = \int \left[D_1(E)\, f_1(E) + D_2(E)\, f_2(E)\right] dE$$

Current

$$I_D = \frac{2q}{h}\int T(E)\left(f_1(E) - f_2(E)\right) dE$$

$$D_{1,2}(E) = \frac{1}{2\pi}\mathrm{G}\Gamma_{1,2}\mathrm{G}^{+}$$

$$T(E) = \mathrm{Trace}[\Gamma_1 \mathrm{G} \Gamma_2 \mathrm{G}^{+}]$$

$$\Gamma_{1,2} = i[\Sigma_{1,2} - \Sigma^{+}_{1,2}]$$

Datta, *Electronic Transport in Mesoscopic Systems,* Cambridge, 1995

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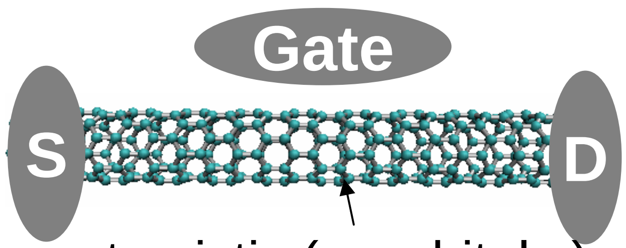
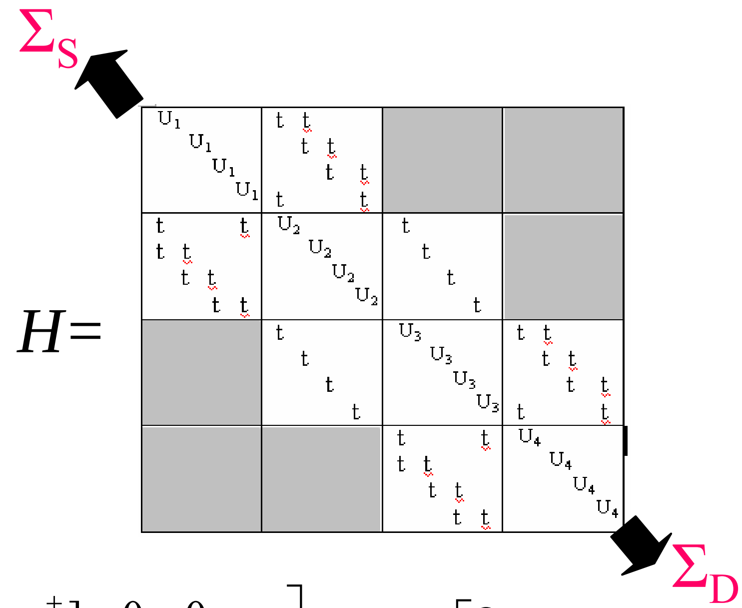
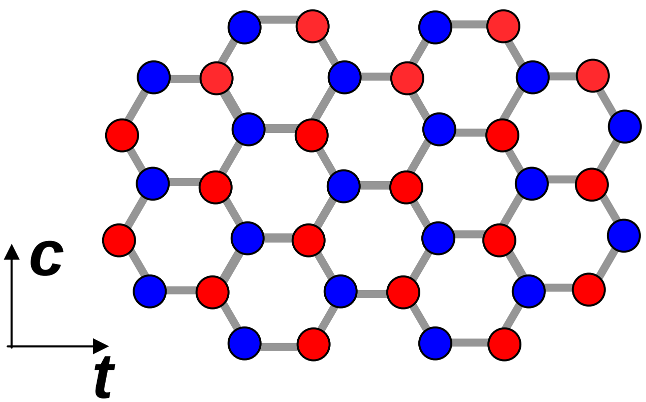
CNTFETs: real-space basis (ballistic)



atomistic (p_Z orbitals)





(m, 0) CNT

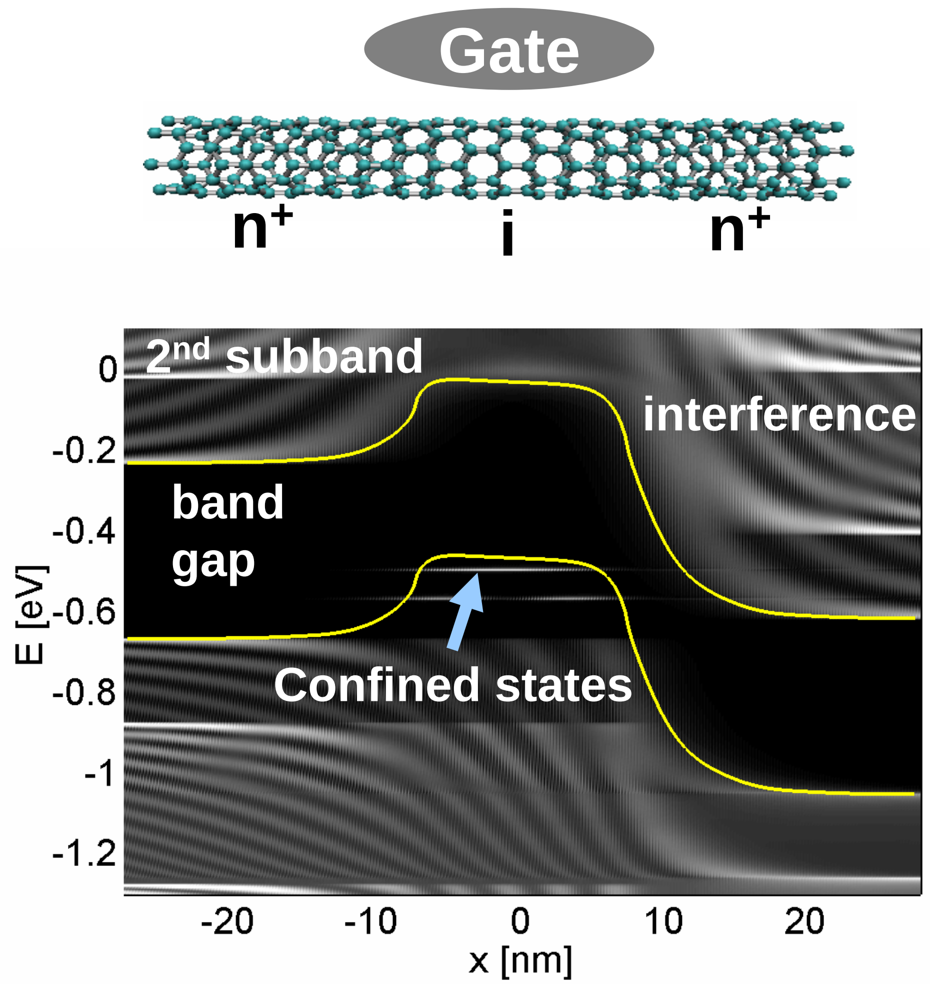
$$\Sigma_S = \begin{bmatrix} [\tau g_S \tau^+] & 0 & 0 & \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & \\ & & & \mathrm{O} \end{bmatrix} \qquad \Sigma_D = \begin{bmatrix} \mathrm{O} & & & \\ & 0 & 0 & 0 \\ & 0 & 0 & 0 \\ & 0 & 0 & [\tau g_D \tau^+] \end{bmatrix}$$

$$G^r = [EI - H - \Sigma_S - \Sigma_D]^{-1}$$

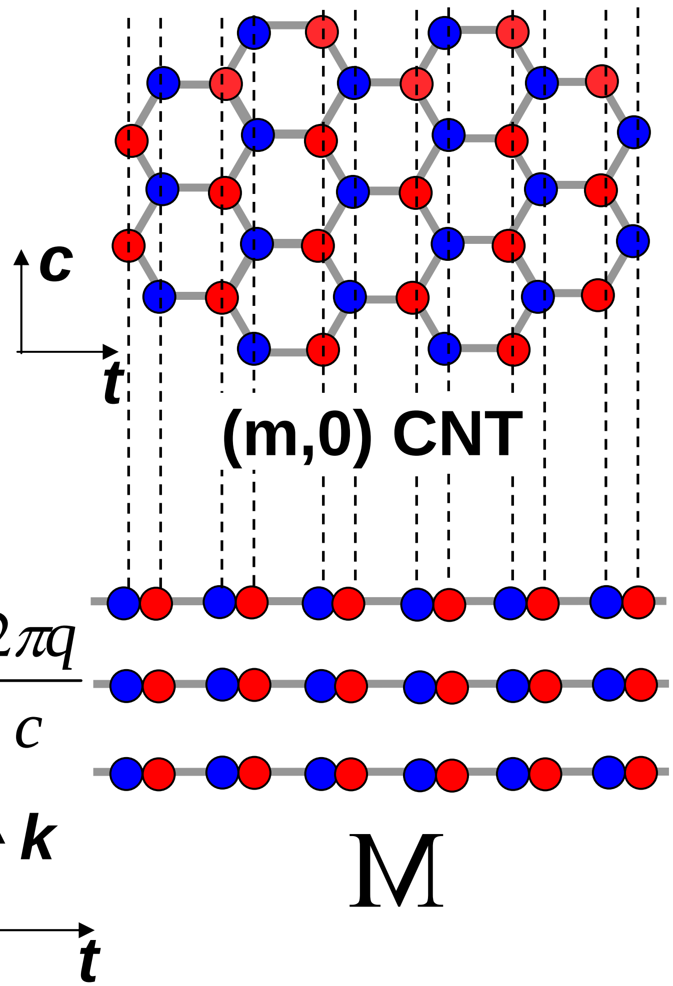
Recursive algorithm for G^r: $O(m^3N)$

Lake et al., JAP, **81**, 7845, 1997

CNTFETs: real-space results



CNTFETs: mode-space approach (ballistic)



$$k_q = \frac{2\pi q}{c}$$

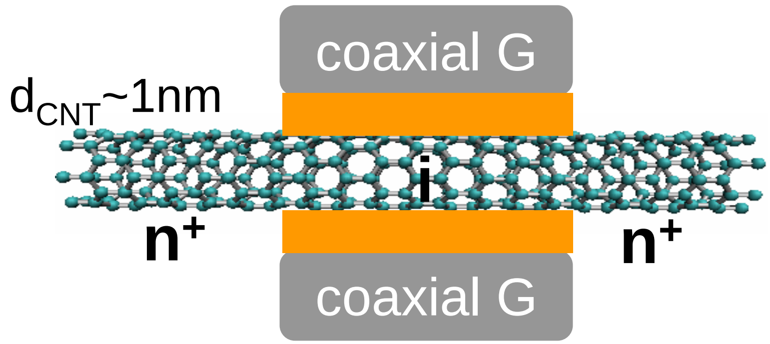
The *q*th mode

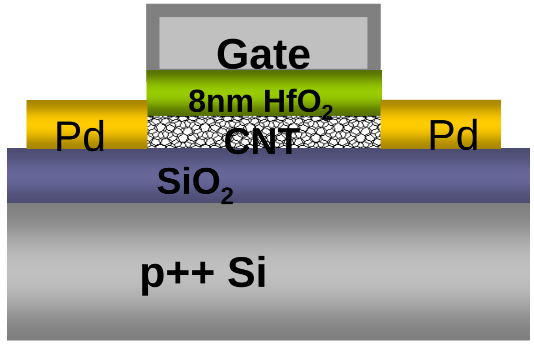
$$H_q = \begin{bmatrix} u_1 & b_q & & & & \\ b_q & u_2 & t & & & \\ & t & u_3 & \mathrm{O} & & \\ & & \mathrm{O} & \mathrm{O} & b_q & \\ & & & b_q & u_N & \end{bmatrix}$$

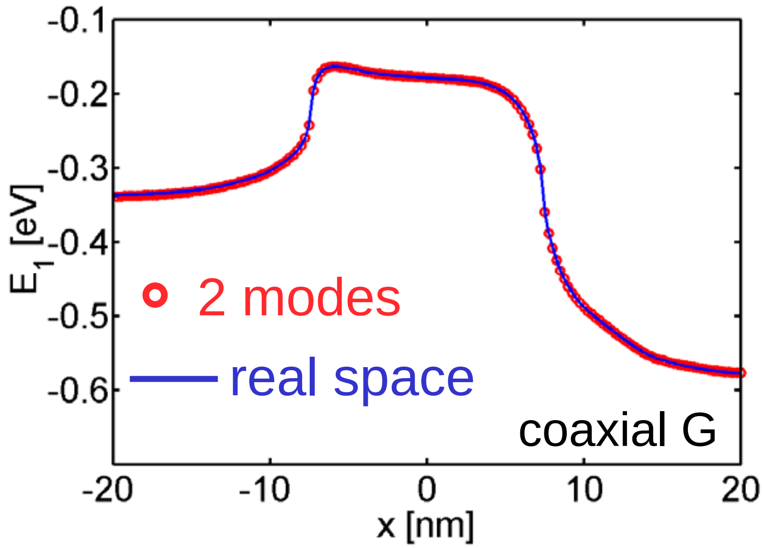
- **Σ_S (1,1) and Σ_D (N,N) analytically computed**
- **Computational cost: O(N)**

real space $O(m^3N)$

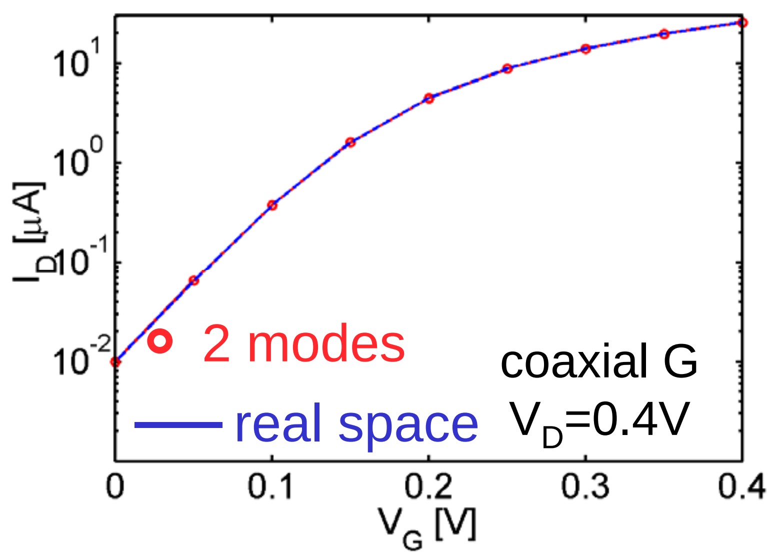
CNTFETs: mode-space results



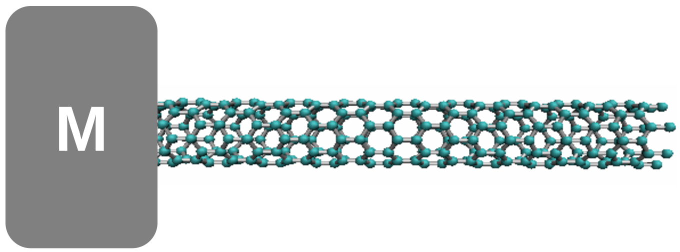


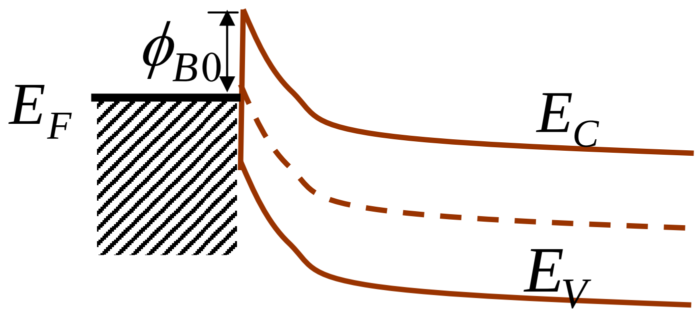


band profile (ON)

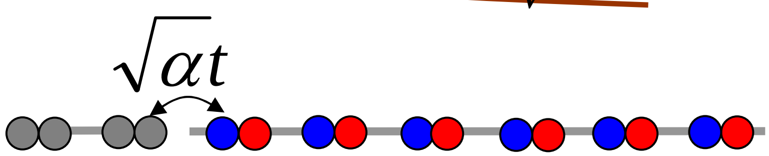


CNTFETs: treatment of M/CNT contacts





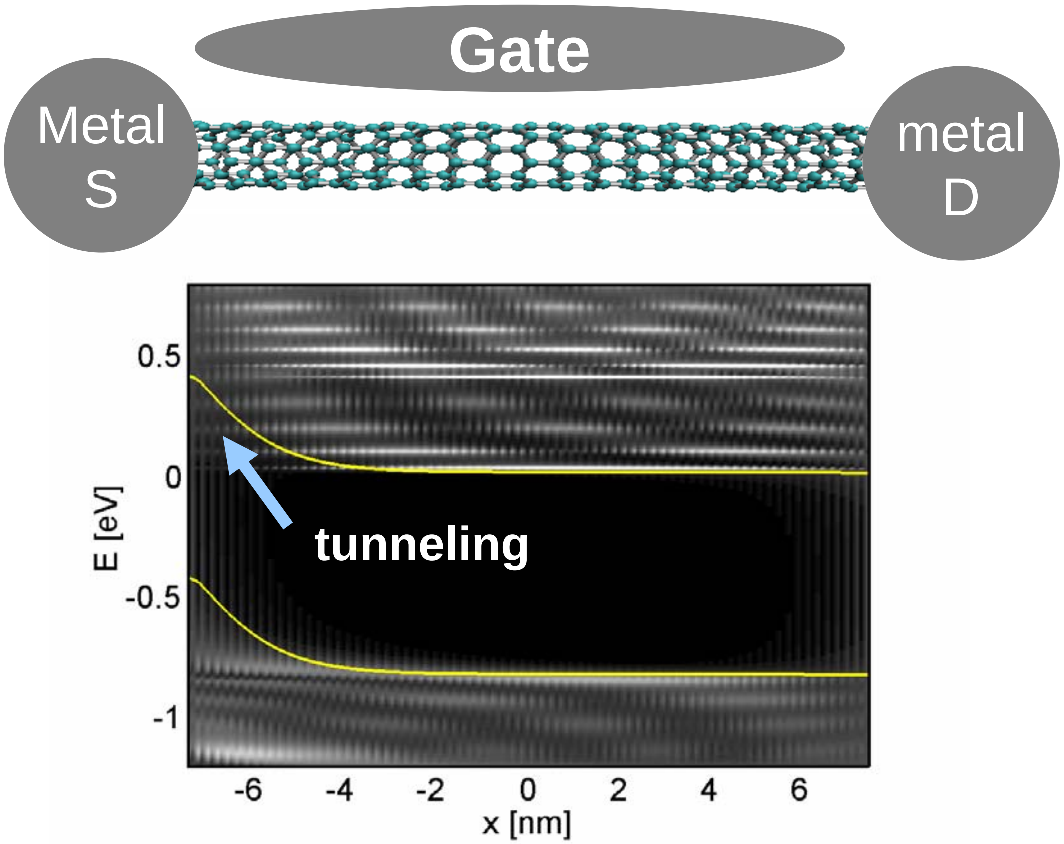
ϕ_{B0} : band discontinuity



$$\Sigma_m \approx \begin{bmatrix} it\alpha & 0 & \\ 0 & 0 & \\ & & \text{O} \end{bmatrix}$$

Kienle et al, *ab initio* study of contacts in progress

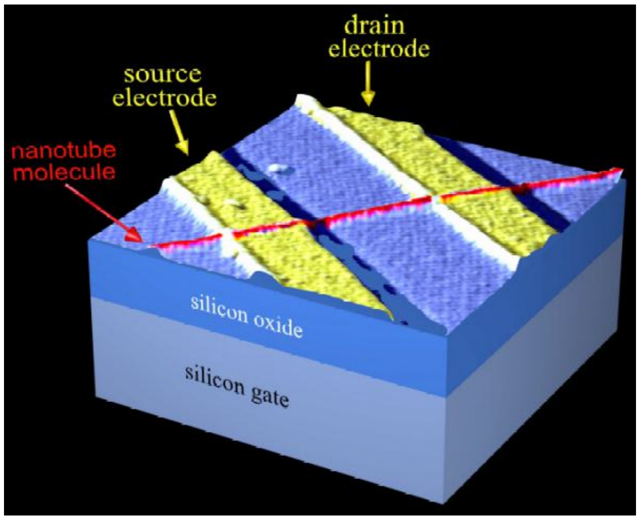
CNTFETs: treatment of M/CNT contacts



$V_D = V_G = 0.4V$

Charge transfer in unit cell: Leonard et al., APL, **81**, 4835, 2002

CNTFETs: 3D Poisson solver



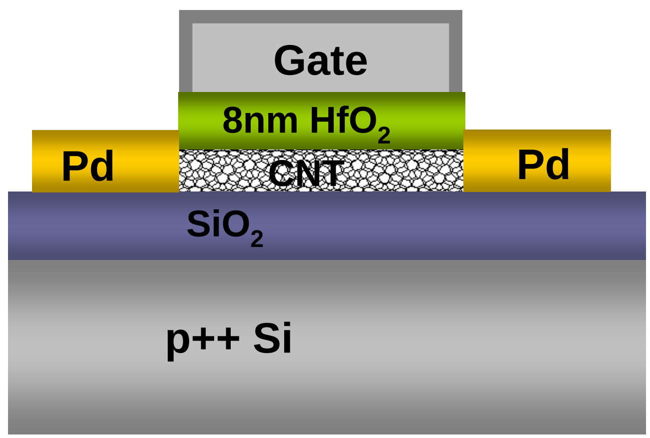
Method of moments:

$$V(\vec{r}) = \int K(\vec{r} - \vec{r}')\rho(\vec{r}')d\vec{r}'$$

Electrostatic kernel:

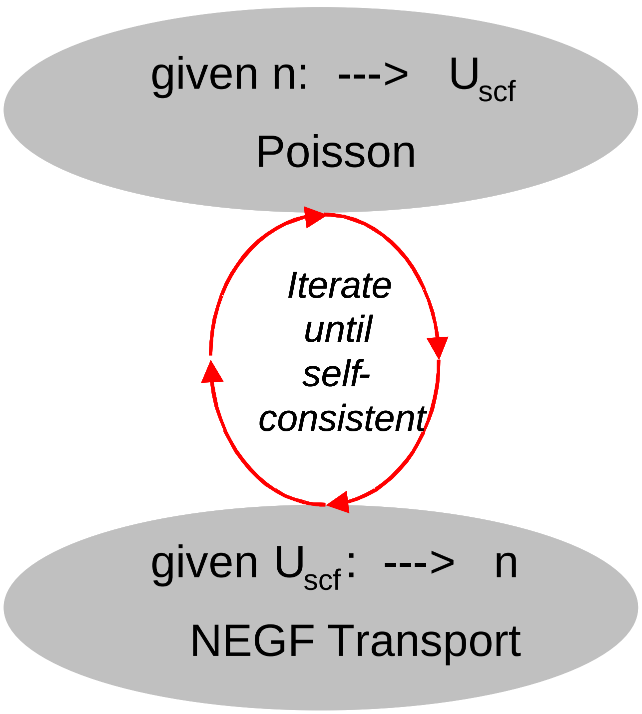
$$K(\vec{r} - \vec{r}')$$

$K(\vec{r} - \vec{r}')$ for 2 types of dielectrics available in Jackson, *Classical Electrodynamics, 1962*



Neophytou, Guo, and Lundstrom, 3D Electrostatics of CNTFETs, IWCE10

CNTFETs: numerical techniques

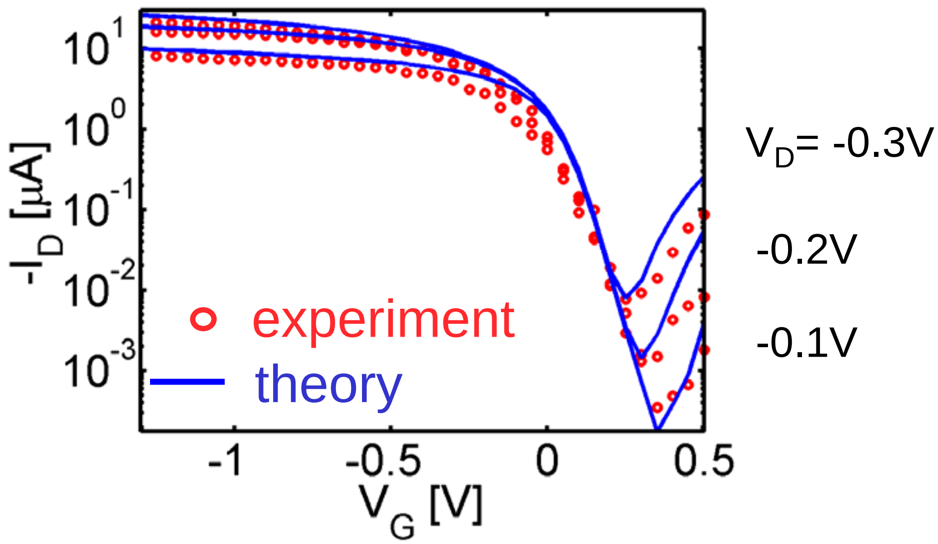


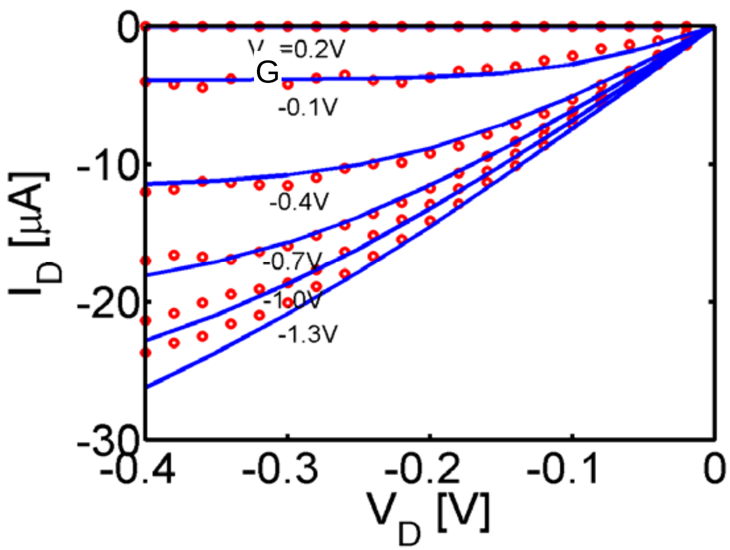
- **Non-linear Poisson**
- **Recursive algorithm for**

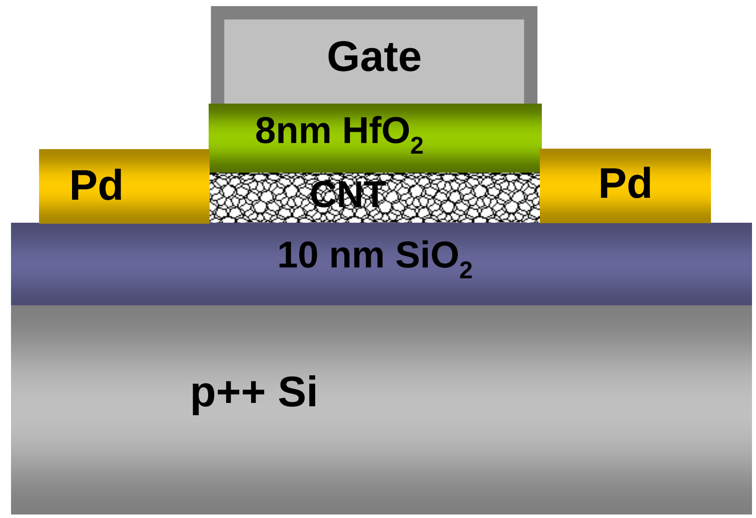
$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1}$$

- **Gaussian quadrature for doing integral**
- **Parallel different bias points**
- **~20min for full I-V of a 50-nm CNTFET**

CNTFETs: theory vs. experiment







Javey, et al., *Nano Letters*, **4**, 1319, 2004

ϕ_{Bp}=0

d_{CNT} ~1.7nm

R_S=R_D~1.7KΩ

Summary

A simulator for ballistic CNTFETs is developed

- atomistic treatment of the CNT
- 3D electrostatics
- phenomenological treatment of M/CNT contacts
- efficient numerical techniques

Theory is calibrated to experiment