ERROR ANALYSIS OF BOUNDARY CONDITION APPROXIMATIONS IN THE MODELING OF COAXIALLY-GATED CARBON NANOTUBE FIELD-EFFECT TRANSISTORS

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The modeling of carbon nanotube field-effect transistors (CNFETs) is an active area of research driven by the goal of evaluating the performance limits of the devices in terms of charge transport and scaling [1-3]. It has been proposed that the optimal device is coaxially gated, offering the best control over the charge distribution in the channel [3]. Therefore, the majority of modeling research has focused on this structure, and groups have established the framework for the fabrication of vertically aligned, coaxially gated structures at high density [4]. The *de facto* simulation standard exploits the axial symmetry of the device and involves numerically solving Schrödinger's equation, using either non-equilibrium Green's functions (NEGF) or the effective mass approximation, and Poisson's equation until self-consistency is obtained [1-3].

Two choices of boundary conditions can be used to solve the two dimensional axially symmetric problem that trade off between simulation space and accuracy. As presented in Ref. [5], a conformal transformation can be used to "mirror" the infinite space beyond the device into a finite semicircular space. While the simulation space is increased by 70%, no error is incurred by enforcing a non-physical boundary condition. Alternately, Neumann boundary conditions may be employed in the gap between the gate and source/drain contacts, reducing the size of the simulation space, but limiting the range of topologies that can be accurately simulated without significant errors. An example is shown in Fig. 1: the simulation space for this topology may be significantly reduced by enforcing Neumann boundary conditions between contacts (dashed lines). In this situation, it is valid to approximate the field lines as normal to the plane, introducing an error of less than 1%.

The purpose of this research is to evaluate the impact of assumed boundary conditions on the error introduced in the potential distribution along the surface of the carbon nanotube in a variety of common topologies. The non-equilibrium case will be evaluated using the finite element method (FEM) and the standard self-consistent Schrödinger-Poisson technique, extending the work of [5] beyond the quasi-Fermi level method and equilibrium case. Key cases of interest will be evaluated (e.g. needle contacts). It will be shown that by a judicious choice of boundary, Neumann boundary conditions may be employed, reducing the size of the simulation space while maintaining an acceptable level of accuracy. This will be of critical importance when simulating non-symmetric devices in three dimensions, where no conformal transform exists.

References:

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Figures:

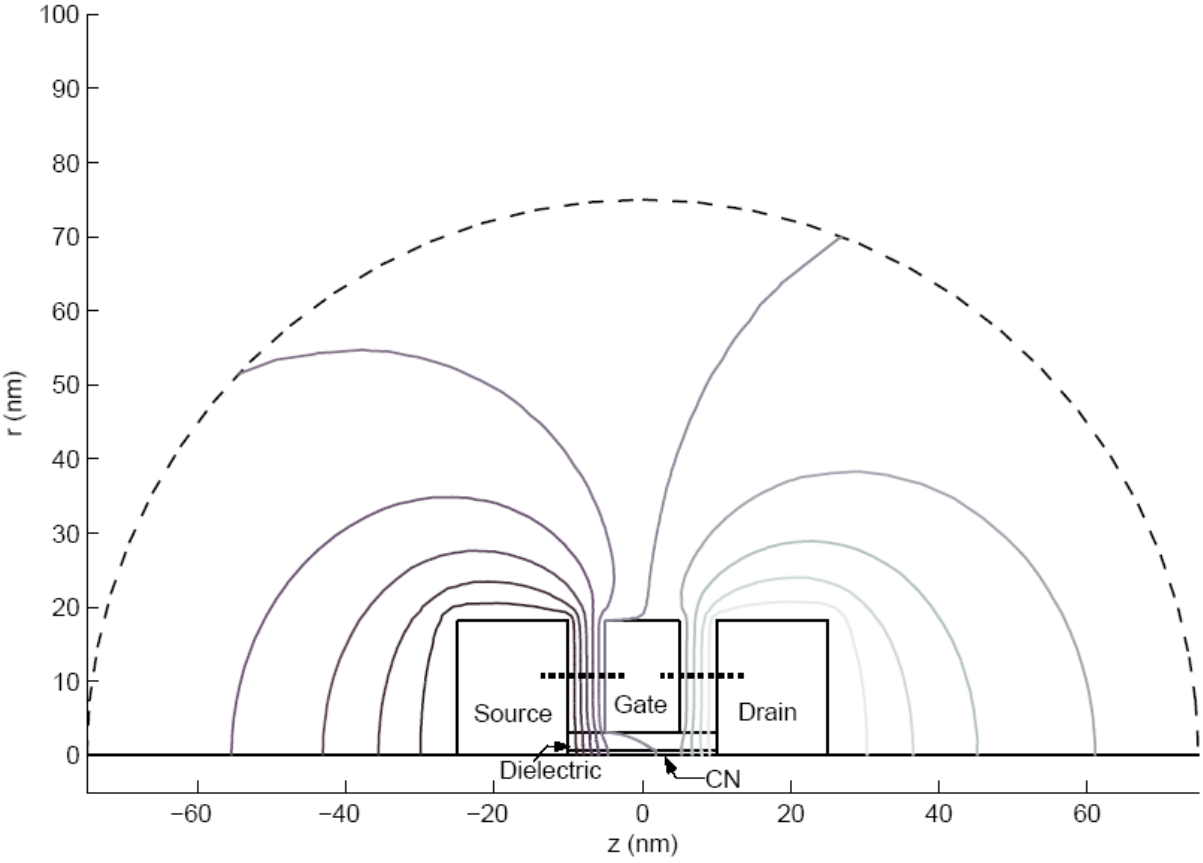

Figure 1: Complete space potential field distribution. Vgs = 0.6V, Vsd = 0.4V. Outer dashed line denotes near-space simulation boundary, dotted lines indicate valid Neumann boundaries. Axis of symmetry located at r=0.