Green's Function Approach to Efficient 3D Electrostatics of Multi-Scale Problems

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Abstract

We present an efficient method to compute efficiently the general solution (Green's Function) of the Poisson Equation in 3D. The method proves its effectiveness when dealing with multi-scale problems in which lower dimensional objects, such as nanotubes or nanowires (1D), are embedded in 3D. Our case-study is a field effect device with a carbon nanotube channel having diameter around 2 nm and length around 2 μm, integrated onto metallic electrodes having dimensions in the 10 μm range. Since the target is to simulate transport through such a structure, accurate electrostatics down to the 0.1 nm scale is required. Thus, the length scales involved span 5 orders of magnitude (0.1 nm to 10 μm) which in 3D makes it a relatively hard problem.

To solve the Poisson's Equation in this challenging scenario, we opted for an adaptive Finite Element Method as implemented in COMSOL Multiphysics®. We use the following two observations in order to make our simulation very efficient. First, our Poisson Equation involves a linear (1D) charge density along the carbon nanotube (which is a 1D object). Second, we are only interested in the electrostatic potential along the nanotube and not the surroundings. These observations allowed us to utilize a Gaussian charge probe with a radius of 0.1 nm and parameterized position together with the powerful Adaptive Mesh Refinement in COMSOL Multiphysics®. Local refinements were made possible by a properly defined Functional error estimation that concentrates refinements in the surrounding region around the carbon nanotube axis, where accuracy is needed.

With the described approach, the efficiency boost is dramatic. Compared to global mesh refinement, a factor of 10x reduction in the number of degrees of freedom was obtained. Compared to the full simulation of a linear charge profile along the nanotube—by employing an interpolation strategy—we were able to show that our Green's Function approach pays off with an acceleration factor of about 350x. These results open the way towards simulation of realistic carbon nanotube-based sensors including additional multiphysics aspects in the future, deploying other COMSOL Multiphysics® modules to model the relevant sensor physics.

Figures used in the abstract

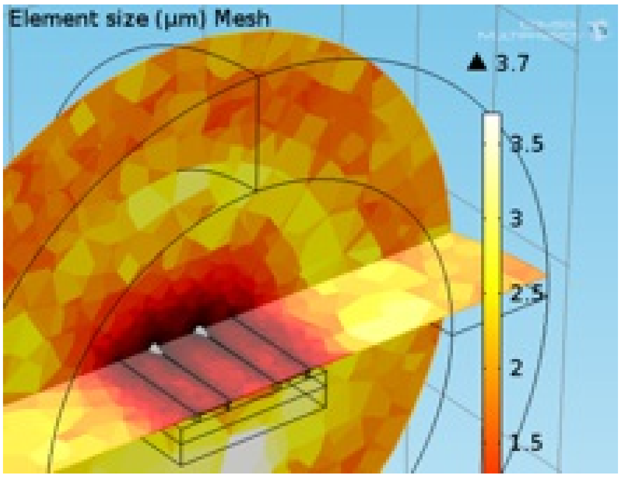

Figure 1: Mesh focusing in 3D electrostatics ar relevant points.