Coupling Electrons, Phonons, and Photons – Challenges in Multiphysics Transport Simulation

I. Knezevic
Department of Electrical and Computer Engineering,
University of Wisconsin – Madison, Madison, WI 53706, USA
e-mail: knezevic@engr.wisc.edu

In nanoscale electronic systems, carriers of charge – electrons and holes – interact with the applied electromagnetic fields, lattice vibrations, other charge carries and charged impurities, and various structural defects, such as alloy atoms or rough boundaries and interfaces.

In the low-field regime (i.e. under low applied fields or temperature gradients), we can assume that phonons are near equilibrium, with the lattice temperature equal to that of the surroundings, and we can account for the interaction of charge carriers with phonons accordingly. However, far-from-equilibrium transport yields drastic alterations in the distribution of phonons owing to emission by the hot electrons, and the lattice heating, in turn, affects electronic transport.

At low-frequency optical or electrical excitations, we can assume that the quasistatic approximation holds, so we can introduce the electrostatic potential and solve Poisson's equation together with transport, rather than account for the full electromagnetic wave dynamics. In contrast, high-frequency excitations, with periods shorter than the typical carrier relaxations times, necessitate a full account of the electromagnetic field dynamics, as electrons feel considerably varying fields between two scattering events.

Bottom line is that a general simulation approach to far-from-equilibrium and time-dependent transport must be a multiphysics one: It requires self-consistent coupling of the dynamics of charge carriers, phonons, and electromagnetic fields. Developing such three-pronged simulation tools is, of course, a complex endeavor. In this talk, I will discuss the challenges that arise, and which types of techniques may be best amenable to coupling, having in mind the current state-of-the art in each of the three areas as well as associated computational requirements. I will present our recent work on the (1) self-consistent coupling of electronic and thermal transport in quantum cascade lasers [1,2] and thermoelectrics [3,4] and (2) self-consistent coupling of electromagnetic wave solvers with transport solvers [5,6] for ac transport in supported graphene with charged impurity clusters [7,8].

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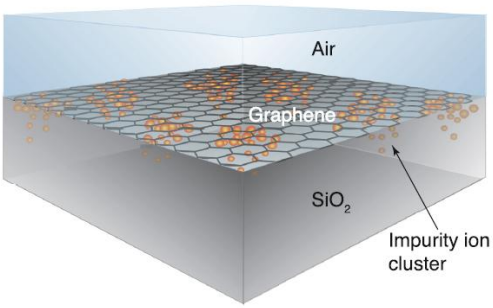

Figure 1: A schematic of the simulated structure, depicting a monolayer of graphene on an SiO_2 substrate, with air on top. Electron and hole ensemble Monte Carlo simulation (EMC) is coupled with the finite-difference time domain (FDTD) solution of Maxwell's curl equations and molecular dynamics (MD) to treat short-range Coulomb interactions to account for high-frequency response of this system. Clusters of substrate impurities near the graphene sheet are also shown. From Ref. [5], Sule, Hagness, and Knezevic, Phys. Rev. B **89**, 165402 (2014).

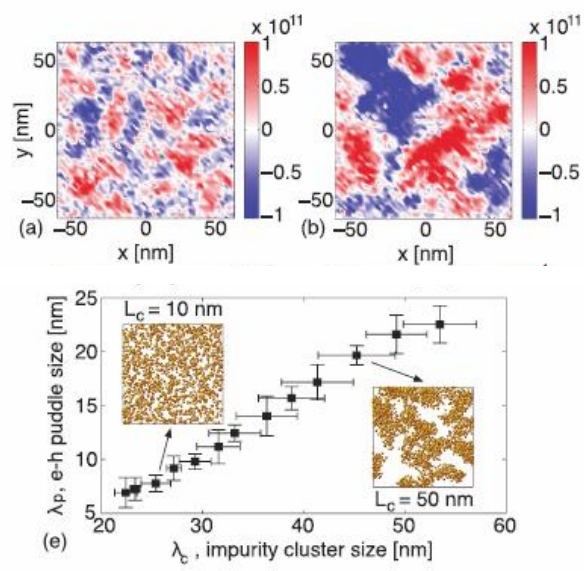

Figure 2: Carrier density distribution (blue, electrons; red, holes) depicting the electron-hole puddles formed in graphene at the Dirac point for (a) uniform random and (b) clustered (cluster size 46 nm) impurity distributions, both with impurity sheet density equal to 5×10^{11}cm^{-2}. Panel (e) represents the relationship between the average puddle size and the underlying cluster size. Adapted from Ref. [5], Sule, Hagness, and Knezevic, Phys. Rev. B **89**, 165402 (2014).

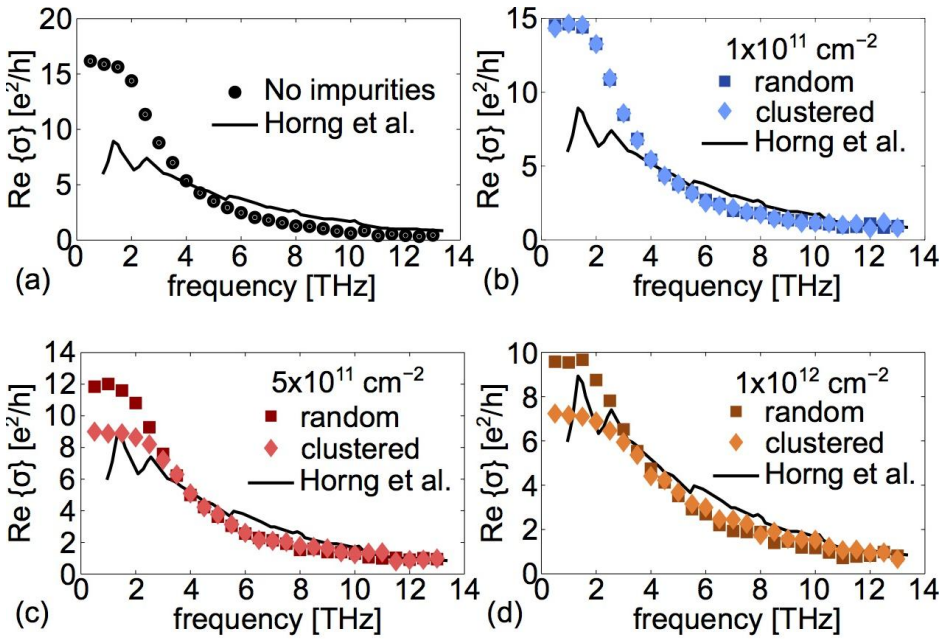

Figure 3: THz-frequency transport in supported graphene based on EMC/FDTD/MD simulation. The 4 panels present the data from [7], J. Horng *et al.*, Phys. Rev. B **83**, 165113 (2011), and numerical fits for different impurity sheet densities with clustered and uniform random impurity distributions. While the high-frequency tail is fairly insensitive to the impurity distribution, the low-frequency range of the curve cannot be reproduced with reasonable impurity densities unless the impurities are assumed to be clustered.