QRing – A scalable parallel software tool for quantum transport simulations in carbon nanoring devices based on NEGF formalism and a parallel C++ / MPI / PETSc algorithm.

The ability of a nanomaterial to conduct charge is essential for many nanodevice applications. While suitable nanomaterials should have acceptable electron transport properties in the absence of disorder, numerous studies have shown that disorder (including phononic or plasmonic effects) can disrupt, or even block, electric current in nanomaterials. On the other hand, some defects in graphene nanoribbons (GNRs), particularly those near the edges, seem to have negligible impact on the current. Phonons for example distort the lattice and appear as scattering centers to electrons. This leads to electrical resistance and heating. Electron-phonon scattering is also key in the understanding of positive magneto-resistance, superconductivity, Peierls instability, Raman scattering and chirality in electronic transport. Additionally, velocity renormalization, carrier lifetime corrections and dramatic reduction of high carrier mobility are known in graphene due to electron-phonon scattering with optical phonons in high fields while in the low-energy limit quasi-elastic scattering of electrons by long-wavelength acoustic phonons will dominate. Another quickly expanding area of nanodevice applications with CNTs and GNRs is nanoplasmonics, where coherent electronic oscillations can be tuned via gate voltage and doping. Graphene THz devices are being created due to the strong plasmon confinement and high electron mobility in a single graphene sheet with fascinating applications in fast sensor technology. Strong exciton-plasmon coupling in semiconducting carbon nanotubes have been theoretically predicted together with scattering of surface plasmons and electrons in general, and corrections have been observed experimentally to the Dirac-like electronic dispersion in graphene. Thus, a theoretically accurate account of both electron-phonon and electron-plasmon coupling in CNT and GNR based structures is of ultimate importance to properly predict the performance of these new nanoplasmonic devices. Thus, this objective aims to understand how disorder, as caused by the inelastic scattering of charge carriers on defects, phonons and plasmons, changes the current pathways, i.e., the routes electrons take while traversing the nanomaterial. The ideas of transmission eigenchannels (scattering states with well-defined transmission probabilities) and local currents (currents between two arbitrary points) will be used together to address several fundamental questions: How is current deflected by disorder, if at all? Over what length scales do phonons or plasmons perturb the current pathways? Conveniently, the non-equilibrium Green's function method described further will easily provide all quantities needed for this analysis.

A curved manifold-based approach is employed in the electronic structure, phonon dispersion, and electron-phonon interaction modeling. In a collaboration with Georgia Tech's M. Leamy and Florida A&M University's M. Encinosa the first two, decoupled models have already been completed using closely-related techniques for carbon nanotubes and nanotoroids. A recently developed multi-scale continuum approach (M. Leamy) forms the basis for reduced-order phonon modeling of carbon nanostructures. Electron-plasmon and exciton-plasmon couplings in carrier transport may be incorporated as well in an effective quasi-particle tightbinding description after appropriate transformation (Boguliobov canonical transformation) and diagonalization of the Hamiltonian containing a free exciton, a free plasmon and an exciton-plasmon interaction term. The device Green's function G_d derived with the NEGF method above will now function as key input to develop the localized descriptions of eigenchannels and

local currents. In the eigenchannels' scheme, the transmission matrix T(E) is diagonalized where eigenvalues describe maximum transition probabilities from the left to the right lead across the device region. With the use of the parallel sparse matrix library PETSc, we can efficiently determine eigenvalues and eigenvectors by diagonalizing the transmission matrix directly. The C++ code has an object-oriented and modular structure using MPI parallelism and sparse matrix software libraries such as PETSc. PETSc includes routines to manipulate large sparse matrices quickly and efficiently using an optimal distribution of the memory allocation for the matrix over multiple cores. The algorithm is setup in such a way that the transmission function T(E) may be calculated at a single energy E by inverting the Hamiltonian matrix to obtain the transport Green's function via the use of PETSc on multiple compute cores. Integrated observables such as the source-drain current I_{SD} for example can then be calculated by integrating over the transmission function values for a pre-defined energy range using a second layer of parallelism using MPI. High-performance computing resources are available via the new Florida-wide HPC network SSERCA.org (Sunshine State Education and Research Computing Alliance), primarily for code development and benchmarking, while large-scale simulation runs using 1000 and more cores are conducted on national computational resources such as National Science Foundation XSEDE's 'Stampede' cluster at the Texas Advanced Computing Center (TACC) and the Department of Energy computational facilities 'Titan' and NICS/Beacon at Oak Ridge National Laboratory (ORNL).