NEGF through finite-volume discretization

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As device sizes have been pushed to the nanometers, the need for numerical methods capable of describing the more quantum- mechanical nature of flow at those scales has become pressing. The Non-Equilibrium Green's Function (NEGF) method has filled this need nicely, with its capacity to describe both the ballistic and diffusive transport regimes, as well as all regimes in between.

Most common implementations of the NEGF approach are done using the Finite-Difference Method (FDM) on uniform grids. This discretization scheme allows one to study many types of planar devices, such as MOSFETs, superlattices and planar heterojunctions. Within this paradigm, carrier scattering can be included through the self- energy approach, almost always under the assumption of local interaction, and a number of specialized numerical schemes have been developed, such as the Recursive Green's Function (RGF) method, to solve the resulting linear algebra in an efficient manner.[1]

However, there are a number of important fields of nano-technology where the nano- structures of interest are decidedly non-planar. Examples include: thermoelectrics, where nano-granular systems are of interest; so- called invisible dopant or shell-antishell systems with spherical structures; and systems of nano-inclusions or nano-voids, which have a number of applications. In these systems, a numerical approach capable of handling incoherent and coherent transport on structures of generic shape is required.

In this talk, we will present work on an implementation of the NEGF method using a Finite-Volume Method (FVM) approach, capable of describing: unstructured-grids, carrier scattering at the self-energy level, anisotropic effective masses, and coupling with classical partial differential equations of charge(i.e. Poisson's equation) and heat (i.e. Fourier's law) within the same discretization scheme.

Here we introduce an extension of the Vienna Schroedinger-Poisson (VSP) solver[2] adapted for the NEGF approach, with electron- phonon scattering, within the effective mass model. Discretization is based on an element- based FVM approach, which is ultimately derived from a conservation law formalism and thus guarantees charge conservation at each element. This makes it well suited for the treatment of anisotropic flow. An important aspect of the solver is the treatment of the open-boundary and the derivation of the appropriate form of the contact self-energy, which although well known for FDM and FEM approaches,[3] requires special consideration for FVM.

Furthermore, the use of an FVM approach allows for seamless coupling with not just a Poisson's equation treatment of charge, but a Fourier's law treatment of classical heat flow.

During the talk specific examples, drawn from the field of nano-structured thermoelectrics, demonstrating both: decoherence of flow, with increasing electron- phonon scattering strength, in non-planar structures; as well as the results for a coupled "quantum charge"-"classical heat" transport simulation, indicating self-heating effects. will be explored.

This talk will discuss new results from the extension of the Vienna Schroedinger-Poisson (VSP) solver to include the NEGF model on unstructured-grids within a Finite-Volume discretization approach, with electron-phonon scattering and the ability to seamlessly couple with classical heat flow equations.

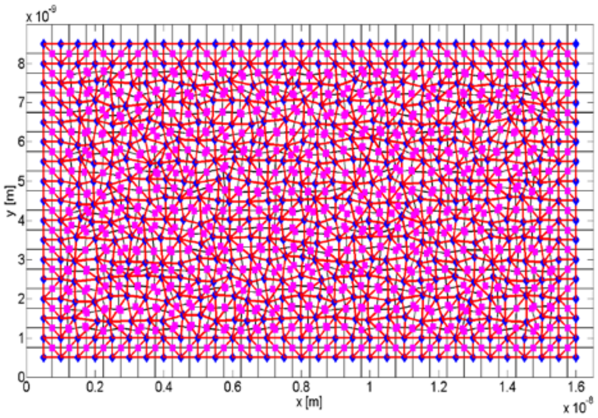

Fig. 1. Sample, random unstructured mesh of arectangular 15 nm by 7.5 nm channel. The blue diamonds represent vertices, or the defined system points. From them Voronoi cells are constructed (black) and divided into triangles (i.e. 2D simplices), which form the base element of the approach. Pink squares represent the circumcenters of these elements. The shown grid is intentionally randomized in order to demonstrate a non-uniform grid.

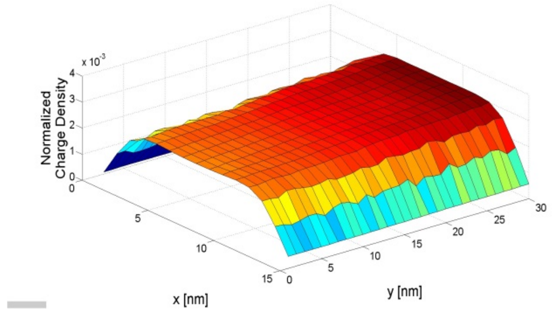

Fig. 2. Normalized charge density for the same grid, showing a flat well behaved distribution of charge in the confined channel.

[1] Lake, R., Klimeck, G., Bowen, R.C. and Jovanovic, D.,1997. Single and multiband modeling of quantum electron transport through layered semiconductor devices. Journal of Applied Physics, 81(12), pp.7845-7869.

[2] Baumgartner, O., Stanojevic, Z., Schnass, K., Karner,M. and Kosina, H., 2013. VSP—a quantum-electronic simulation framework. Journal of Computational Electronics, 12(4), pp.701-721.

[3] Jiang, H., Shao, S., Cai, W. and Zhang, P., 2008.Boundary treatments in non-equilibrium Green's function (NEGF) methods for quantum transport in nano-MOSFETs. Journal of Computational Physics,227(13), pp.6553-6573.