Coupling length-scales from drift-diffusion to non equilibrium Green's functions

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MANUSCRIPT LAYOUT

Non equilibrium Green's functions (NEGF) have become a standard tool to analyze transport in nanodevices when quantum coherence plays a relevant role [1]. Yet, the evaluation of NEGF is numerically expensive, especially when scattering is included. On the other hand the need to solve quantum transport equations is only necessary on selected subregions of an electronic device. A multiscale/multiphysics approach is therefore necessary in order to efficiently compute transport. To this end we have developed a coupling scheme between drift-diffusion (DD) and NEGF transport models which are solved on different subdomains. The simulations are coupled by imposing potential boundary conditions and current continuity. We give details of how this is done in the finite-element based TiberCAD transport tool [2] and present the efficient implementation of an iterative GF algorithm. Applications to Si nanowire MOSFETs are shown.

DISCUSSION

Finite element (FEM) representations of continuous media equations and atomistic tight binding (TB) approaches [3] share an identical underlining mathematical formalism: the weak form solution of a differential equation using a finite set of localized basis functions. From the point of view of a single particle quantum mechanical problem this produces structurally similar matrix representations of the Hamiltonian. Furthermore, quantities that can be derived from a Green's function approach to transport, such as charge densities and current, have an analogous meaning. This allows a formal unification between FEM and TB quantum transport calculations which is at the basis of our multiscale approach. Towards this end we have developed a general purpose NEGF library working with any sparse Hamiltonian and Overlap matrices relaying on an efficient block-iterative algorithm. Recent developments using a more advanced Knitting algorithm will also be presented.

Boundary conditions are specified on *N*-1 dimensional contacts from which the mesh needs to be extruded as shown in Fig. 2, in order to construct the surface Green's functions with usual iterative schemes. Mesh reordering and partitioning strategies suitable for the block-iterative scheme have also been developed. For this we set an auxiliary Laplace problem whose solution is used to reorder the degree of freedom. The sparsity map of the reordered Hamiltonian is shown in Fig. 3.

Fig. 4 shows the band profile of the SiNW obtained from the DD simulation. It is possible to appreciate the potential drops in the NW leads depending on the applied drain and gate potentials. This, in turns, imposes corresponding boundary conditions to the ballistic sub-region. Tunneling calculations are shown in Fig. 5. The code is easily generalized to 8x8 k.p Hamiltonians and with similar approaches can be adapted to a tight-binding/FEM coupling.

CONCLUSION

We have developed a multiscale scheme coupling drift-diffusion transport with quantum transport based on NEGF. This approach opens new possibilities in studying nanoscale devices coupled to macroscopic contacts.

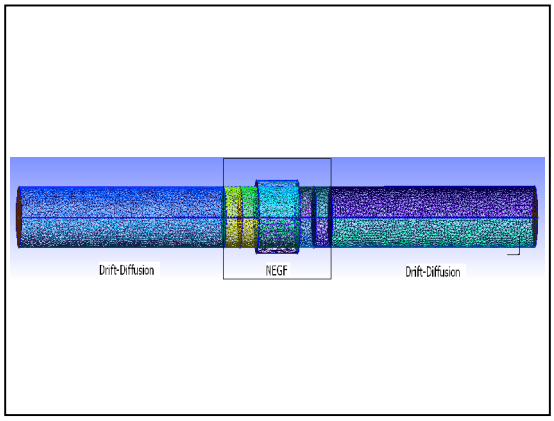

Fig. 1. Finite Element Mesh of a SiNW MOSFET of 126nm.

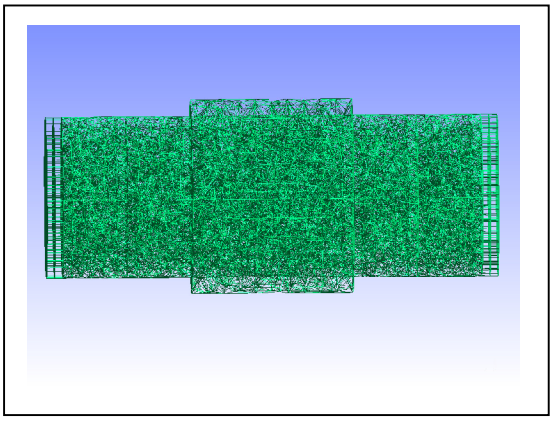

Fig. 2. Detail of the mesh extrusion for the constructuion of the surface Green's functions.

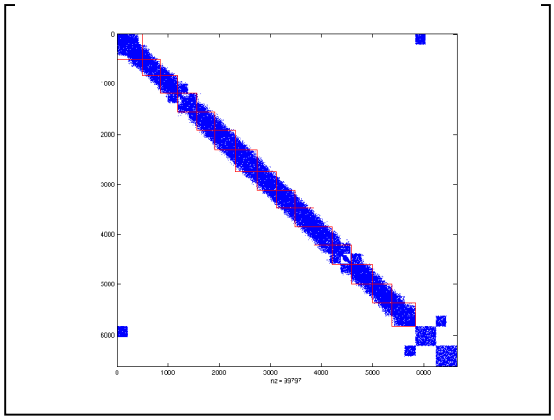

Fig. 3. Patritioning of the device that preserve proper ordering in the contact regions

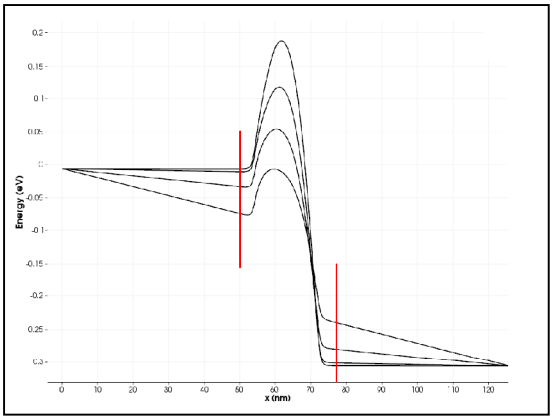

Fig. 4. Conduction band-edge profile for increasing Vg =0.0, 0.1, 0.2, 0.3 V. Red lines mark the NEGF region.

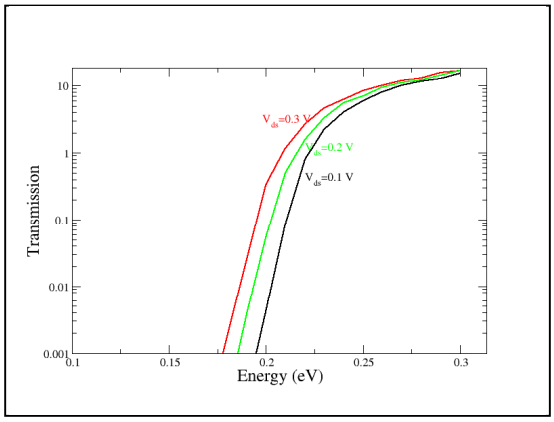

Fig. 5. Transmission as a function of energy at Vgs=0.0 V.

REFERENCES

[1] A.Pecchia and A. Di Carlo, *Transport in nanoscale and molecular devices,* Rep. Prog. Phys. **67**, 1497 (2004).

[2] M. Auf der Maur et al. *The multiscale paradigm in electronic device simulation.,*IEEE Trans. Elect. Dev. 58, 1425 (2011)

[3] With TB we mean any local orbital representation of the Hamiltonian that can be ab-initio, semi-empirical or even empirical, as explained in [1].