An ADHIE-TDDFT Method for the EM/QM Co-simulation of Coupled 1-D Nanowires

M. Torreele, P. Decler, and D. Vande Ginste
Quest Lab, Ghent University/imec, Belgium

Abstract— Over the past years, the rapid increase in device functionality has stimulated the demand for novel topologies and materials. One such development is the emergence of quantum structures in nanoelectronic components. A new trend consists of using 1-D materials, characterized by small dimensions along the transversal directions. For example, research interest is devoted to gallium arsenide (GaAs) nanowires for the creation of solar cell arrays. Due to the embryonic stage of this research domain, combined with its quantum mechanical nature, physical experiments with the aforementioned structures turn out to be costly. Hence, adequate modeling tools should be leveraged to make prior assessments of the device’s functionality. To capture the complete physics of the problem, the charge carriers’ dynamics dictated by quantum mechanics (QM) should be solved in conjunction with the time evolution of the electromagnetic (EM) fields. However, as these phenomena occur at vastly different spatial and temporal scales, the co-simulation of those systems is challenging.

In this work, we improve upon existing modeling techniques by invoking an alternating-direction hybrid implicit-explicit (ADHIE) scheme. This method allows for strong grid refinement in the directions of interest, i.e., the regions containing the quantum material. It constitutes a compromise between the numerical efficiency of explicit time-stepping and the favorable stability properties of implicit solvers. In that respect, the ADHIE method provides an accurate way of simultaneously solving the EM and QM parts of the multiphysics problem, without being extensively constrained by small time steps. To put our method to the test, we consider two nanowires located in the vicinity of one another. After being excited with an initial current boost, the first nanowire generates an EM field, which affects the current in the second wire by means of near-field coupling. This non-negligible crosstalk might distort the device’s overall performance. The dynamics of the charge carriers in the nanowire are described through the time-dependent density functional theory (TDDFT) formalism, discretized on the real-space grid. TDDFT has proven to yield accurate results in systems with many-electron interactions. The ADHIE method is compared to the traditional Yee-FDTD algorithm and demonstrates a significant reduction in computation time while guaranteeing a comparable level of accuracy.