Analysis of Transient Electromagnetic Interactions on Nanodevices using a Quantum Corrected Integral Equation Approach

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Analysis of electromagnetic interactions on nanodevices can oftentimes be carried out accurately using “traditional” electromagnetic solvers. However, if a gap of sub-nanometer scale exists between any two surfaces of the device, quantum-mechanical effects including tunneling should be taken into account for an accurate characterization of the device’s response. Since the first-principle quantum simulators can not be used efficiently to fully characterize a typical-size nanodevice, a quantum corrected electromagnetic model has been proposed as an efficient and accurate alternative (R. Esteban et al., Nat. Commun., 3(825), 2012). The quantum correction is achieved through an effective layered medium introduced into the gap between the surfaces. The dielectric constant of each layer is obtained using a first-principle quantum characterization of the gap with a different dimension.

In this work, this quantum correction scheme is incorporated into a surface integral equation solver for accurately analyzing transient electromagnetic interactions on nanodevices. More specifically, a marching on in time (MOT) scheme is developed to solve the Poggio-Miller-Chan-Harrington-Wu-Tsai surface integral equation (PMCHWT-SIE) (L. N. Medgyesi-Mitschang et al., J. Opt. Soc. Am. A, 11, 1383-1398, 1994) that is enforced on interfaces between different dielectric volumes. The dielectric constants of the layers introduced in the gap are represented using a Drude model, where parameters are computed from the results of a quantum characterization of the gap. Equivalent electric and magnetic currents introduced on the interfaces of the dielectric volumes and layers in the gap are expanded in terms of Rao-Wilton-Glisson (RWG) basis functions in space and polynomial interpolants in time. Inserting this expansion into the PMCHWT-SIE and Galerkin testing the resulting equation at discrete times yield a system of equations. This system is solved for the unknown expansion coefficients of the currents using an MOT scheme. This scheme calls for computation of the time domain samples of the Green functions of the unbounded media with the material properties of each volume and their (dispersive) dielectric constants. These samples are obtained by inverse Fourier transforming the rational functions fitted to the frequency domain samples using a fast relaxed vector fitting (FRVF) algorithm (B. Gustavsen, IEEE Trans. Power Del. 21, 1587-1592, 2006). Computation of the double temporal convolutions involving these time samples, which are called for by the MOT scheme, is carried out using the technique described in (I. Uysal et. al., IEEE Antennas Wireless Propag. Lett., 2015).

Numerical results, which demonstrate the effect of the quantum correction on the transient electromagnetic interactions, will be presented.