Analysis of Transient Electromagnetic Interactions on Nanodevices Using a Quantum-corrected Integral Equation Approach

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PROBLEM DESCRIPTION
Simulation of transient fields on plasmonic nanostructures with sub-nanometer gaps. Quantum tunneling is accounted for using an auxiliary tunnel[1].

PROPOSED SOLUTION
Formulate and implement a time domain Poggio-Miller-Chan-Harrington-Wu-Tsai (PMCHWT) [2] integral equation solver

Advantages:
• Time domain, broad band analysis
• Requires only surface discretization (instead of the volumetric discretization of the whole computation domain)
• Implicitly satisfies the radiation condition

Challenges:
• Computation of the Green function of dispersive media
• Temporal convolutions due to Green function of dispersive media

IMPACT
Potential to replace low-order accurate finite difference time domain (FDTD) methods

PMCHWT FORMULATION
Consider the generic problem

\[ \mathbf{H}_{\text{inc}} (\mathbf{r}, t) = \mathbf{J}_{\text{inc}} (\mathbf{r}, t) \]

\[ \mathbf{E}_{\text{inc}} (\mathbf{r}, t) = \mathbf{M}_{\text{inc}} (\mathbf{r}, t) \]

\[ \mathbf{V}_m : \text{Volume} \]
\[ \varepsilon_0 : \text{Permittivity} \]
\[ \mu_0 : \text{Permeability} \]
\[ \gamma_i : \text{Surface} \]
\[ \hat{n}_{\gamma_i} : \text{Unit normal vector} \]
\[ \mathbf{J}_i : \text{Electric current density} \]
\[ \mathbf{M}_i : \text{Magnetic current density} \]

Scattered and incident fields are related to each other by boundary conditions to yield PMCHWT equation

\[ \hat{n}_{\gamma_i} \times \left( \nabla \mathbf{E}_{\text{inc}} - \nabla \mathbf{E}_{\text{sca}} \right)_j = - \hat{n}_{\gamma_i} \times \left( \nabla \mathbf{H}_{\text{inc}} - \nabla \mathbf{H}_{\text{sca}} \right)_k \]

Scattered fields are written in terms of equivalent surface current densities

\[ \mathbf{E}_{\text{sca}} (\mathbf{r}, t) = \sum_j \left[ \mu_0 \mathbf{M}_j (\mathbf{r}, t) + \nabla \mathbf{J}_j (\mathbf{r}, t) \right] \]

\[ \mathbf{H}_{\text{sca}} (\mathbf{r}, t) = \sum_k \left[ \varepsilon_0 \mathbf{J}_k (\mathbf{r}, t) + \nabla \mathbf{M}_k (\mathbf{r}, t) \right] \]

Green function of the dispersive medium is obtained by fast relaxed vector fitting (FRVF) algorithm [3]

\[ G_\gamma (\mathbf{R}, t) = \frac{1}{4\pi} \int_0^{\infty} \frac{e^{-\gamma l}}{\mathbf{R}} \mathbf{R} \left[ \delta (\mathbf{R}) + \frac{\partial}{\partial t} \delta (\mathbf{R}) \right] (t_0) + \sum_{\gamma_i} G_\gamma (\mathbf{R}, t_0) e^{-\gamma_i l} \]

\[ \mathbf{R} = \frac{t - R}{c_0} \text{is the retarded time and} \quad \mathbf{R} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \text{is the speed of light} \]

\[ e_{\text{sca}} (t) = F^{-1} \left[ r_0 \delta (\mathbf{R}) + \sum_{\gamma_i} r_0 \delta (\mathbf{R}) e^{-\gamma_i l} \right] \]

MARCHING ON-IN-TIME (MOT) SCHEME
Equivalent surface current densities are approximated by an expansion in terms of temporal and spatial basis functions

\[ \mathbf{J}_i (r, t) = \sum_{j=1}^N e_{\text{sca}}^j (t) \mathbf{J}_j (r) \quad \mathbf{M}_i (r, t) = \sum_{k=1}^N e_{\text{sca}}^k (t) \mathbf{M}_k (r) \]

Substituting the expanded currents in scattered fields and testing the resulting equation with Galerkin procedure in space at time step \( t = i\Delta t \) yields MOT matrix system:

\[ \mathbf{Z}_i \mathbf{J}_i = \mathbf{V}_i - \sum_{i=1}^{i-1} \mathbf{Z}_i \mathbf{J}_j \]

DOUBLE TEMPORAL CONVOLUTION
After discretization, double convolution is written as

\[ F_{\gamma} (t) = \gamma (t) + T (t - j\Delta t) \]

\[ F_{\gamma} (t) = Q (t) + T (t - j\Delta t) \]

Expand the first convolution with some interpolation functions

\[ \mathbf{F}_{\gamma} (t) = \gamma (t) + T (t - j\Delta t) \]

\[ \mathbf{F}_{\gamma} (t) = Q (t) + T (t - j\Delta t) \]

Double convolution is discretized as

\[ \gamma (t) + T (t - j\Delta t) \]

\[ \gamma (t) + T (t - j\Delta t) \]

NUMERICAL EXAMPLE
Sodium dimer with a cylindrical tunnel. Radius of one sphere is 2.17 nm and radius and length of tunnel are 0.25 nm and 2.65 nm. Permittivity values are taken from [1].

\[ \mathbf{E}_{\text{inc}} (\mathbf{r}, t) = \mathbf{E}_{\text{sca}} (\mathbf{r}, t) \quad \text{g} (t) = \cos (2\pi f_0 t) \exp (-t^2 / 2\tau^2) \]

\[ f_0 = f_{\text{inc}} = 500 \text{ THz} \quad \tau = 3 / (2\pi f_{\text{inc}}) \quad \Delta t = 0.0063 s \quad N = 4000 \quad N_{\text{eq}} = 608 \]

REFERENCES