High–Order Perturbation of Surfaces (HOPS) Algorithms for the Simulation of Localized Surface Plasmon Resonances

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Governing Equation

We seek outgoing/bounded, 2π–periodic solutions of

$$\Delta u + (k^u)^2 u = 0, \quad r > \bar{g} + g(\theta), \tag{1a}$$
$$\Delta w + (k^w)^2 w = 0, \quad r < \bar{g} + g(\theta), \tag{1b}$$
$$u - w = \zeta, \quad r = \bar{g} + g(\theta), \tag{1c}$$
$$\partial_N u - \tau^2 \partial_N w = \psi, \quad r = \bar{g} + g(\theta), \tag{1d}$$

where the Dirichlet and Neumann data are

$$\zeta(\theta) := \left[-u^{\text{inc}}\right]_{r=\bar{g}+g(\theta)}$$
$$\psi(\theta) := \left[-\partial_N u^{\text{inc}}\right]_{r=\bar{g}+g(\theta)},$$

and

$$\tau^2 = \begin{cases} 1, & \text{Transverse Electronic (TE),} \\ (k^u/k^w)^2 & \text{Transverse Magnetic (TM).} \end{cases}$$

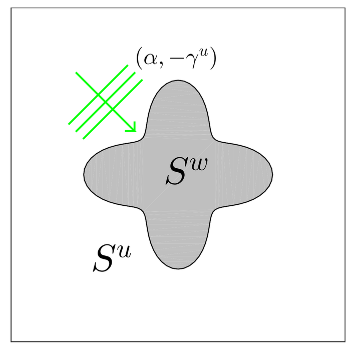


*Figure 1 : **Cross-section of a metallic nanorod***

Regarding the Outgoing Wave Condition (Sommerfeld Radiation Condition) and Boundedness Boundary Condition, the solutions to (1a) and (1b) are equivalent to

$$\begin{cases} \Delta u + (k^u)^2 u = 0, & \bar{g} + g(\theta) < r < R^o, \\ \partial_r u + T^{(u)}[u] = 0, & r = R^o > \bar{g} + |g|_{L^\infty}, \end{cases} \tag{1a'}$$

$$\begin{cases} \Delta w + (k^w)^2 w = 0, & R_i < r < \bar{g} + g(\theta), \\ \partial_r w - T^{(w)}[w] = 0, & r = R_i < \bar{g} - |g|_{L^\infty}, \end{cases} \tag{1b'}$$

with order–one Fourier multipliers $\{T^{(u)}, T^{(w)}\} := \{-k^u \frac{H'_D(k^u R^o)}{H_D(k^u R^o)}, k^w \frac{J'_D(k^w R_i)}{J_D(k^w R_i)}\}$.

1 Boundary Formulation

1.1 Dirichlet–Neumann Operator (DNO)

Let the outer/inner Dirichlet traces and their (outward) Neumann counterparts be

$$U(\theta) := u(\bar{g} + g(\theta), \theta), \quad \tilde{U}(\theta) := -(\partial_N u)(\bar{g} + g(\theta), \theta), \tag{2a}$$
$$W(\theta) := w(\bar{g} + g(\theta), \theta), \quad \tilde{W}(\theta) := (\partial_N w)(\bar{g} + g(\theta), \theta). \tag{2b}$$

Define the Dirichlet–Neumann Operators

$$G^{(u)} : U \to \tilde{U}, \quad G^{(u)}[U] = G^{(u)}(R^o, \bar{g}, g)[U] := \tilde{U},$$
$$G^{(w)} : W \to \tilde{W}, \quad G^{(w)}[W] = G^{(w)}(R_i, \bar{g}, g)[W] := \tilde{W}.$$

The boundary conditions, (1c) and (1d), become

$$U - W = \zeta, \quad -G^{(u)}[U] - \tau^2 G^{(w)}[W] = \psi,$$
$$\Longrightarrow \quad (G^{(u)} + \tau^2 G^{(w)})[U] = -\psi + \tau^2 G^{(w)}[\zeta]. \tag{3}$$

1.2 Impedance–Impedance Operator (IIO)

Let the outer/inner Impedance and their outer/inner counterparts be

$$I^u := -\sigma_u \partial_N u + i\eta u|_{r=\bar{g}+g(\theta)}, \quad \tilde{I}^u := -\sigma_u \partial_N u - i\eta u|_{r=\bar{g}+g(\theta)},$$
$$I^w := \sigma_w \partial_N w + i\eta w|_{r=\bar{g}+g(\theta)}, \quad \tilde{I}^w := \sigma_w \partial_N w - i\eta w|_{r=\bar{g}+g(\theta)},$$

where $\eta \in \mathbb{R}^+$, $\sigma_u = \sigma_w = 1$ (TE) or $\{\sigma_u = 1/n_u^2, \sigma_w = 1/n_w^2\}$ (TM). Define the Impedance–Impedance Operators

$$Q : I^u \to \tilde{I}^u, \quad Q[I^u] = Q(R^o, \bar{g}, g)[I^w] := \tilde{I}^u, \tag{4a}$$
$$S : I^w \to \tilde{I}^w, \quad S[I^w] = S(R_i, \bar{g}, g)[I^w] := \tilde{I}^w. \tag{4b}$$

The boundary conditions, (1c) and (1d), become

$$I^u + S[I^w] = i\eta - \sigma_u \psi, \quad Q[I^u] + I^w = -i\eta - \sigma_u \psi.$$

2 HOPS Methods

2.1 Method of Field Expansions (FE)

We view $g(\theta) = \varepsilon f(\theta)$. For ε sufficiently small and f smooth the operators, $\{G^{(u)}, G^{(w)}\}$, and data, $\{\zeta, \psi\}$, can be shown to be analytic in ε so that the following Taylor series are strongly convergent

$$\{G^{(u)}, G^{(w)}, \zeta, \psi\} = \{G^{(u)}, G^{(w)}, \zeta, \psi\}(\varepsilon f) = \sum_{n=0}^{\infty} \{G_n^{(u)}, G_n^{(w)}, \zeta_n, \psi_n\} \varepsilon^n.$$

Suppose that scattered fields, $\{u, w\}$, depend analytically upon ε. Take the field u in the outer domain, $\{r > \bar{g} + \varepsilon f(\theta)\}$,

$$u = u(r, \theta; \varepsilon) = \sum_{n=0}^{\infty} u_n(r, \theta) \varepsilon^n, \quad \text{or} \quad U = U(\varepsilon f) = \sum_{n=0}^{\infty} U_n \varepsilon^n.$$

Inserting this into (1a') with DNO (2a), finds that the u_n must be 2π–periodic, outward–propagating solutions of the elliptic boundary value problem

$$\Delta u_n + (k^u)^2 u_n = 0, \quad \bar{g} < r < R^o,$$
$$u_n(\bar{g}, \theta) = \delta_{n,0} U - \sum_{\ell=0}^{n-1} \frac{f^{n-\ell}}{(n-\ell)!} \partial_r^{n-\ell} u_\ell(\bar{g}, \theta), \quad r = \bar{g},$$
$$\partial_r u_n + T^{(u)}[u_n] = 0, \quad r = R^o.$$

The exact solutions are

$$u_n(r, \theta) = \sum_{p=-\infty}^{\infty} \hat{u}_{n,p} \frac{H_p(k^u r)}{H_p(k^u \bar{g})} e^{ip\theta}, \tag{5}$$

and the $\hat{u}_{n,p}$ are determined recursively from the boundary conditions, beginning at order zero, with $\hat{u}_{0,p} = \hat{U}_p$.
Rewrite the boundary condition (3), at order $\mathcal{O}(\varepsilon^n)$,

$$(G_0^{(u)} + \tau^2 G_0^{(w)})[U_n] = -\psi_n + \sum_{m=0}^{n} G_{n-m}^{(w)}[\zeta_m] - \sum_{m=0}^{n-1} (G_{n-m}^{(u)} + \tau^2 G_{n-m}^{(w)})[U_m]$$

With the exact solution (5), one can get a recurrence relation

$$G_n^{(u)}(f)[U] = -\frac{f}{\bar{g}} G_{n-1}^{(u)}(f)[U] - k^u \bar{g} \sum_{\ell=0}^{n} \sum_{p=-\infty}^{\infty} \hat{u}_{\ell,p} \frac{(k^u f)^{n-\ell}}{(n-\ell)!} \frac{H_p^{(n+1-\ell)}(k^u \bar{g})}{H_p(k^u \bar{g})} e^{ip\theta} + \cdots$$

Similar considerations hold for the DNO $G^{(w)}$.

2.2 Method of Transformed Field Expansions (TFE)

The method of Transformed Field Expansions proceeds in much the same way as the FE approach, save that a domain–flattening change of variables is effected prior to perturbation expansion. Applied to the interior problem (1b'), with IIO (4b), the change of variables maps the perturbed domain $\{R_i < r < \bar{g} + g(\theta)\}$ to the separable one $\{R_i < r' < \bar{g}\}$. This transformation changes the field w into

$$v(r', \theta') := w\left(\frac{(\bar{g} + g(\theta') - R_i)r' - R_i g(\theta')}{\bar{g} - R_i}, \theta'\right),$$

and modifies the problem to

$$\Delta v + (k^w)^2 v = F(r', \theta'; g), \quad R_i < r' < \bar{g},$$
$$\sigma_w\{A(g, \bar{g}, R_i)\partial_{r'} v + B(g, \bar{g}, R_i)\partial_{\theta'} v\} + i\eta C(g, \bar{g}, R_i) v = \chi(\theta'; g), \quad r' = \bar{g},$$
$$\partial_{r'} v - T^{(w)}[v] = K(\theta'; g), \quad r' = R_i,$$

where

$$-(\bar{g} - R_i)^2 F = g(\bar{g} - R_i)(r' - R_i)\partial_{r'}[r' \partial_{r'} v] + \cdots \quad \text{and} \quad K = \frac{g}{\bar{g} - R_i} T^{(w)}[v].$$

3 Numerical Results

3.1 Convergence Study

Take an exact solution to (1) and compare our numerically simulated solution. For implementation, consider 2π-periodic, outgoing solutions of Helmholtz equation, (1a), and the bounded counterpart for (1b)

$$u^q(r, \theta) = A_u^q H_q(k^u r) e^{iq\theta}, \quad w^q(r, \theta) = A_w^q J_q(k^w r) e^{iq\theta}, \quad q \in \mathbf{Z}, \quad A_u^q, A_w^q \in \mathbf{C}.$$

We approximate $\{u, w\}$ by

$$u^{N_\theta, N}(r, \theta) := \sum_{n=0}^{N} \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{u}_{n,p} e^{ip\theta} \varepsilon^n, \quad w^{N_\theta, N}(r, \theta) := \sum_{n=0}^{N} \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{w}_{n,p} e^{ip\theta} \varepsilon^n.$$

- Select the 2π-periodic and analytic function $f(\theta) = e^{\cos(\theta)}$, and compute the exterior Neumann data, $\tilde{U}(\theta) := [-\partial_N u^q]_{r=a+\varepsilon f(\theta)}$.

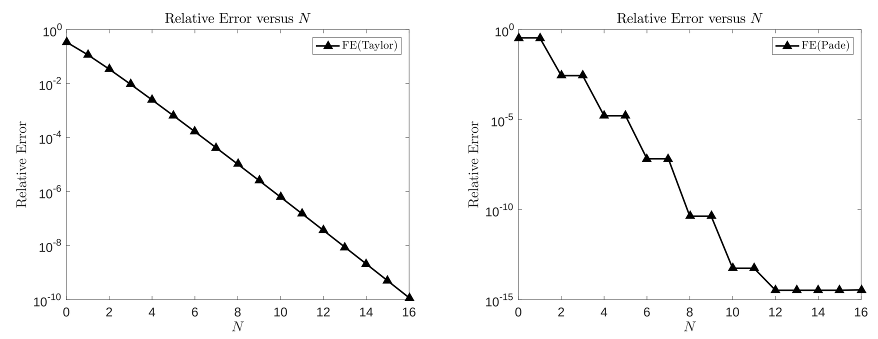


*Figure 2 : **Relative error versus perturbation order (FE)***
$q = 2, \quad A_u^q = 2, \quad A_w^q = 1, \quad \bar{g} = 0.025, \quad \varepsilon = 0.002, \quad N_\theta = 64, \quad N = 16$

- Reprise these calculations with a much larger choices of perturbation parameter, $\varepsilon = 0.01, 0.05$, using both FE and TFE.

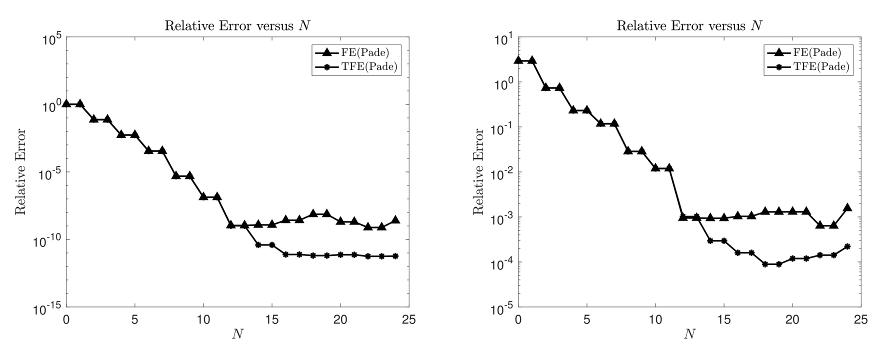
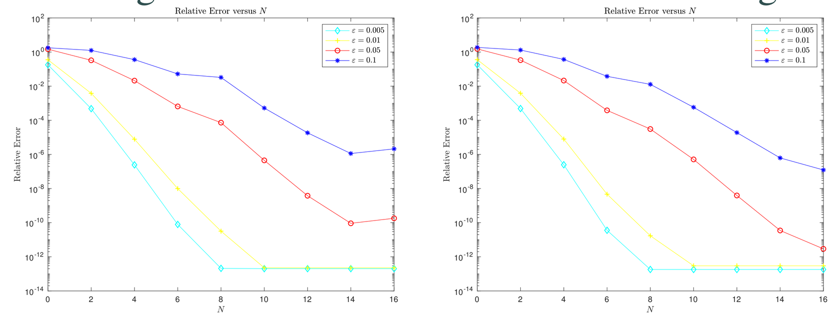


*Figure 3 : **Relative error versus perturbation order (FE)***
$\bar{g} = 0.025, \quad c = \bar{g}/10, \quad b = 10\bar{g}, \quad N_r = 64, \quad N = 24.$

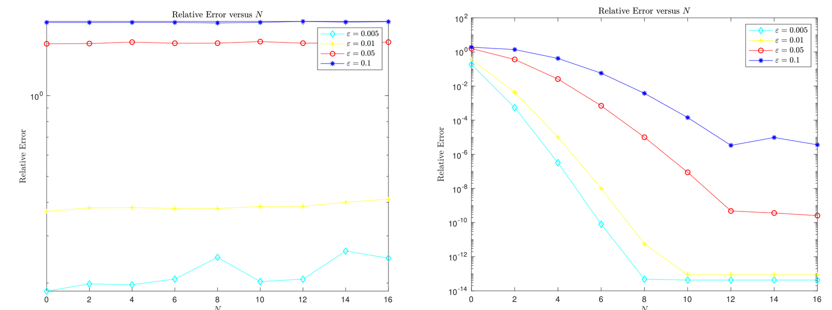
3.2 DNO versus IIO

There exist Dirichlet eigenvalues w.r.t. DNO $G^{(w)}$ such that the solutions explode. However, the IIOs sovle this Problem. Use TFE approach to compute the exterior Neumann data $\tilde{U}$ and impedance data $\tilde{I}^u$ at the interface. Both DNO and IIO converge with choices away from Dirichlet eigenvalue but DNO fails at a Dirichlet eigenvalue.



(a) **DNO** (b) **IIO**

*Figure 4 : **DNO versus IIO***

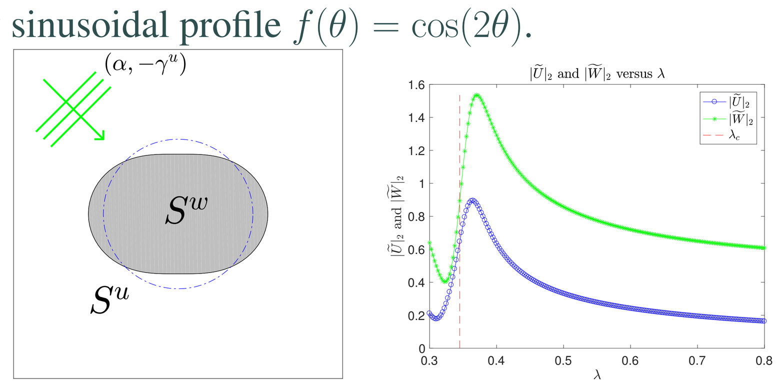


(a) **DNO** (b) **IIO**

*Figure 5 : **DNO versus IIO: a Dirichlet eigenvalue***

3.3 Simulation of Nanorods

Return to the problem of scattering of plane–wave incident radiation $u^{\text{inc}} = \exp(i(\bar{g} + g(\theta))(\alpha\cos(\theta) - \gamma^u \sin(\theta)))$ by a nanorod which demands the Dirichlet (1c) and Neumann conditions (1d). We consider a low–frequency sinusoidal profile $f(\theta) = \cos(2\theta)$.



(a) ***Cross–section of a silver nanorod (S^w) shaped by $r = \bar{g} + \varepsilon\cos(2\theta)$ housed in a vacuum (dielectric) under plane (S^u).***

(b) ***Reflection and Transmission maps at $\varepsilon = \bar{g}/10$, with the Fröhlich value of the LSPR as a dashed red line and $\bar{g} = 0.025$, $N_\theta = 64$, $N = 16$.***

*Figure 6 : **Nanorod Simulation***

The deformation parameter (one tenth of the rod radius) can produce a sizable shift in the LSPR.

4 Forthcoming Research

- The analyticity of Dirichlet–Neumann Operator
- The existence of IIO which guarantees a complete solution scheme
- Extension to Three Dimensional Layered-Media

References

[1] David P. Nicholls and Xin Tong. High-order perturbation of surfaces algorithms for the simulation of localized surface plasmon resonances in two dimensions. *J. Sci. Comput.*, Feb 2018.

[2] David P. Nicholls. Stable, high-order computation of impedance–impedance operators for three-dimensional layered medium simulations. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 474(2212), 2018.