High-Order Perturbation of Surfaces Algorithms for the Simulation of Localized Surface Plasmon Resonances

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Chicago Area SIAM Student Conference 2018

June 17, 2018

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Collaborators and References

Collaborator on this project:

- David Nicholls: my PhD advisor at UIC

Thanks:

- Youngjoon Hong
- Marieme Ngom

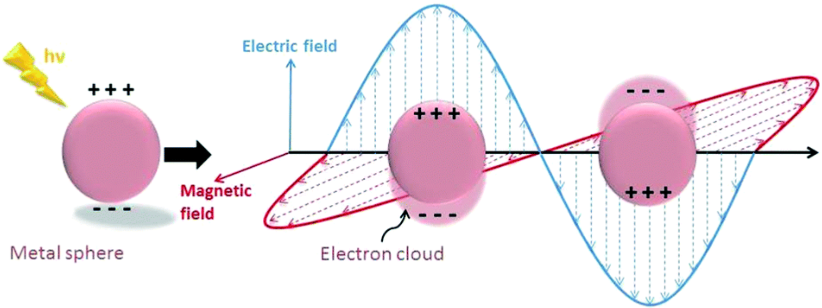
References:

- DPN and XT, "High-Order Perturbation of Surfaces Algorithms for the Simulation of Localized Surface Plasmon Resonances in Two Dimensions", to appear, *Journal of Scientific Computing*

Nanoplasmonics

- Nanoplasmonics: The study of optical phenomena in the nanoscale vicinity of metal surfaces.
- **Question**: Can electromagnetic radiation be concentrated or confined in a region less than half the light's wavelength?
  (Visible light: 400-700 nm)
- **Answer**: Yes, for a conducting metal.
  For instance, for a nanoparticle:
  - **smaller** than the skin depth (roughly 25 nm),
  - **larger** than distance electron moves in one period (roughly 2 nm)
- A plane electromagnetic wave drives the free electrons in the metal generating a charge and restoring force. This electron oscillator has quanta: a surface plasmon (SP).
- We will investigate a surface plasmon resonance (SPR) between a surface plasmon on a grating and the incident radiation.

Nanoplasmonics

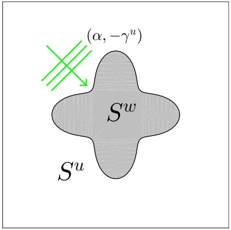


Remark: this figure is from the paper "Metal nanoparticle photocatalysts: emerging processes for green organic synthesis", *Catalysis Science & Technology*

Governing Equation for Doubly-Layered Medium

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

$$\begin{aligned} &\Delta u + (k^u)^2 u = 0, && r > a + g(\theta), && (1a)\\ &\Delta w + (k^w)^2 w = 0, && r < a + g(\theta), && (1b)\\ &u - w = \zeta, && r = a + g(\theta), && (1c)\\ &\partial_{\mathbf{N}} u - \tau^2 \partial_{\mathbf{N}} w = \psi, && r = a + g(\theta), && (1d)\end{aligned}$$



where the Dirichlet and Neumann data are

$$\zeta(\theta) := \left[-u^{\text{inc}}\right]_{r=a+g(\theta)} = -e^{i(a+g(\theta))(\alpha\cos(\theta)-\gamma^u\sin(\theta))}$$

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

and

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

Governing Equation: Exterior Problem

Definition 1: Given a sufficiently smooth deformation $g(\theta)$, the unique periodic solution of

$$\Delta u + (k^u)^2 u = 0, \qquad a + g(\theta) < r < b, \tag{2a}$$
$$u = U := u(a + g(\theta), \theta), \qquad r = a + g(\theta), \tag{2b}$$
$$\partial_r u + T^{(u)}[u] = 0, \qquad r = b, \tag{2c}$$

defines the Dirichlet–Neumann Operator (DNO)

$$G^{(u)}[U] = G^{(u)}(b, a, g)[U] := -(\partial_N u)(a + g(\theta), \theta) = \tilde{U}.$$

We define the order-one Fourier multiplier at the boundary as

$$T^{(u)}[\xi(\theta)] := \sum_{p=-\infty}^{\infty} -k^u \hat{\xi}_p \frac{H_p'(k^u b)}{H_p(k^u b)} e^{ip\theta}$$

Governing Equation: Interior Problem

Definition 2: Given a sufficiently smooth deformation $g(\theta)$, if we are not at a Dirichlet eigenvalue of the Laplacian on $\{c < r < a + g(\theta)\}$, the unique periodic solution of

$$\Delta w + (k^w)^2 w = 0, \qquad c < r < a + g(\theta), \tag{3a}$$

$$w = W := w(a + g(\theta), \theta), \qquad r = a + g(\theta), \tag{3b}$$

$$\partial_r w - T^{(w)}[w] = 0, \qquad r = c, \tag{3c}$$

defines the Dirichlet–Neumann Operator (DNO)

$$G^{(w)}[W] = G^{(w)}(c, a, g)[W] := (\partial_N w)(a + g(\theta), \theta) = \tilde{W}. \tag{4}$$

We define the order-one Fourier multiplier at the boundary as

$$T^{(w)}[\mu(\theta)] := \sum_{p=-\infty}^{\infty} k^w \hat{\mu}_p \frac{J_p'(k^w c)}{J_p(k^w c)} e^{ip\theta}$$

Doubly-Layered Problem, revisit

Rewrite the boundary conditions (1c) and (1d)

$$U - W = \zeta, \qquad r = a + g(\theta), \tag{5a}$$

$$-G^{(u)}[U] - \tau^2 G^{(w)}[W] = \psi, \qquad r = a + g(\theta), \tag{5b}$$

Eliminate W in (5a), the (5b) becomes

$$(G^{(u)} + \tau^2 G^{(w)})[U] = -\psi + \tau^2 G^{(w)}[\zeta]. \tag{6}$$

We use a High-Order Perturbation of Surfaces (HOPS) scheme to simulate scattering returns with $g(\theta) = \varepsilon f(\theta)$. For ε sufficiently small and f smooth the DNOs, $\{G^{(u)}, G^{(w)}\}$, and data, $\{\zeta, \psi\}$, can be shown to be analytic in ε so that the following Taylor series are strongly convergent

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

Doubly-Layered Problem, revisit

The resulting scattered field can be shown to be analytic as well

$$U = U(\varepsilon f) = \sum_{n=0}^{\infty} U_n \varepsilon^n$$

We write (6) as

$$\left(\sum_{n=0}^{\infty} \left(G_n^{(u)} + \tau^2 G_n^{(w)} \right) \varepsilon^n \right) \left[\sum_{m=0}^{\infty} U_m \varepsilon^m \right] = - \sum_{n=0}^{\infty} \psi_n \varepsilon^n + \tau^2 \left(\sum_{n=0}^{\infty} G_n^{(w)} \varepsilon^n \right) \left[\sum_{m=0}^{\infty} \zeta_m \varepsilon^m \right],$$

and at order $O(\varepsilon^n)$

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

The data, $\{\zeta_n, \psi_n\}$, is easy to get by Taylor expansions. All that remains is to specify forms for DNOs, $\{G_n^{(u)}, G_n^{(w)}\}$.

The Method of Field Expansions: Exterior Problem

The method of Field Expansions is based on the supposition that the scattered fields, $\{u, w\}$, depend *analytically* upon ε. Focusing on the field u in the outer domain, this implies

$$u = u(r, \theta; \varepsilon) = \sum_{n=0}^{\infty} u_n(r, \theta)\varepsilon^n.$$

Inserting into (2), one finds that the u_n must be $2\pi-$periodic , outward-propagating solutions of the elliptical boundary value problem:

$$\Delta u_n + (k^u)^2 u_n = 0, \qquad a < r < b, \tag{7a}$$

$$u_n(a, \theta) = \delta_{n,0} U - \sum_{m=0}^{n-1} \frac{f^{n-m}}{(n-m)!} \partial_r^{n-m} u_m(a, \theta), \qquad r = a, \tag{7b}$$

$$\partial_r u_n + T^{(u)}[u_n] = 0, \qquad r = b, \tag{7c}$$

The exact solution to (7a) and (7c) is

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

and the $\hat{u}_{n,p}$ are determined *recursively* from the boundary conditions, (7b), for example, at zero order,

$$\hat{u}_{0,p} = \hat{U}_p.$$

From this the DNO, $G^{(u)}[U]$, can be computed from

$$\begin{aligned} G^{(u)}[U] &= -(\partial_N u)(a + g(\theta), \theta) \\ &= \sum_{n=0}^{\infty} \sum_{p=-\infty}^{\infty} \left\{ -k^u (a + \varepsilon f) \frac{H_p'(k^u(a+\varepsilon f))}{H_p(k^u a)} \right. \\ &\quad \left. + \frac{\varepsilon f'}{(a+\varepsilon f)} (ip) \frac{H_p(k^u(a+\varepsilon f))}{H_p(k^u a)} \right\} \hat{u}_{n,p} e^{ip\theta} \varepsilon^n. \end{aligned}$$

Expanding the Hankel functions $H_p'(k^u(a+\varepsilon f))$ and $H_p(k^u(a+\varepsilon f))$ in ε one can get the operators $\{G_n^{(u)}(f)\}$.

The Method of Transformed Field Expansions

The method of Transformed Field Expansions proceeds a domain-flattening change of variables prior to perturbation expansion. We consider the TFE method applied to the interior problem (3). The change of variable is

$$r' = \frac{(a-c)r + cg(\theta)}{a + g(\theta) - c}, \quad \theta' = \theta,$$

which maps the perturbed domain $\{c < r < a + g(\theta)\}$ to the separable one $\{c < r' < a\}$. This transformation changes the field w into

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

and modifies (3) to (dropped the primed notation)

$$\begin{aligned} &\Delta v + (k^w)^2 v = F(r, \theta; g), && c < r < a, \\ &v = W, && r = a, \\ &\partial_r v - T^{(w)}[v] = K(\theta; g), && r = c. \end{aligned}$$

TFE: Interior Problem

It is not difficult to see that

$$-(a-c)^2 F = g(a-c)(r-c)\partial_r[r\partial_r v] + g\partial_\theta[g\partial_\theta v] + \cdots + \sum_{j=1}^{4} C_j(g)(k^w)^2 v$$

with

$$\begin{aligned} C_1(g) &= g[2(a-c)r^2 + 2g(a-c)(r-c)r], \\ C_2(g) &= g^2[r^2 + 4(r-c)r + (r-c)^2], \\ C_3(g) &= g^3[2(r-c)r/(a-c) + 2(r-c)^2/(a-c)], \\ C_4(g) &= g^4(r-c)^2/(a-c)^2, \end{aligned}$$

and

$$K = g/(a-c)\,T^{(w)}[v].$$

In addition, the (4) changes when we proceed the change of variables.

$$G^{(w)}[W] = \frac{a-c}{a-c+g}\left[(a+g) + \frac{(g')^2}{a+g}\right]\partial_r v - \frac{g'}{a+g}\partial_\theta v.$$

TFE: Interior Problem

Setting $g = \varepsilon f$ and expanding

$$v(r,\theta,\varepsilon) = \sum_{n=0}^{\infty} v_n(r,\theta)\varepsilon^n,$$

the interior problem (8) results to find solutions v_n of

$$\begin{aligned} \Delta v_n + (k^w)^2 v_n &= F_n, && c < r < a, \\ v_n &= \delta_{n,0} W, && r = a, \\ \partial_r v_n - T^{(w)}[v_n] &= K_n, && r = c, \end{aligned}$$

where

$$-(a-c)^2 F_n = f(a-c)(r-c)\partial_r[r\partial_r v_{n-1}] + f\partial_\theta[f\partial_\theta v_{n-2}] + \cdots + \sum_{j=1}^{4} C_j(f)(k^w)^2 v_{n-j}$$

and

$$K_n = g/(a-c)\,T^{(w)}[v_{n-1}].$$

TFE: Interior Problem

Provided with the $\{v_n\}$, the opertors $\{G_n^{(w)}(f)\}$ can be computed by

$$G_n^{(w)}[W] = -f\left(\frac{1}{a} + \frac{1}{a-c}\right) G_{n-1}^{(w)}[W] - \frac{f^2}{a(a-c)} G_{n-2}^{(w)}[W] + a\partial_r v_n + 2f\partial_r v_{n-1} + \frac{f^2 + (f')^2}{a}\partial_r v_{n-2} - \frac{f'}{a}\partial_\theta v_{n-1} - \frac{f(f')}{a(a-c)}\partial_\theta v_{n-2}.$$

Remark: The TFE approach to compute DNOs requires an additional discretization in the vertical direction (r direction) which we achieve by a Chebyshev collocation approach.

Validation by the Method of Manufactured Solutions

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

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

For a given choice of $f = f(\theta)$ we compute, e.g., the exact exterior Neumann data

$$\nu^{\text{ex}}(\theta) := [-\partial_N u^q]_{r=a+\varepsilon f(\theta)} = \tilde{U}(\theta).$$

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

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

Convergence Study

We select the 2π-periodic and analytic function

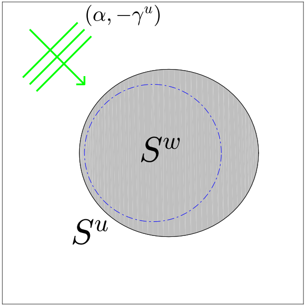
$$f(\theta) = e^{\cos(\theta)},$$

and compute the exact surface current, ν^{ex}. We make the physical parameters choices

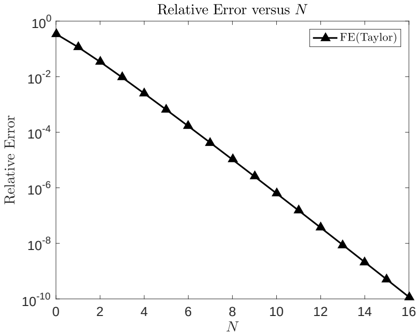
$$q = 2, \quad A_u^q = 2, \quad A_w^q = 1,$$
$$a = 0.025, \quad \varepsilon = 0.002,$$

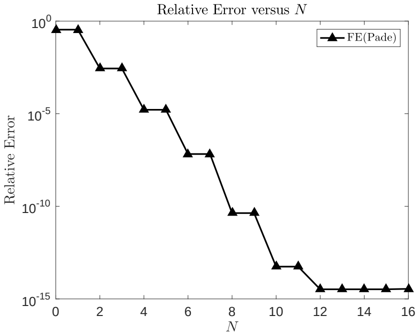
and numerical parameter choices

$$N_\theta = 64, \quad N = 16.$$



Convergence Study

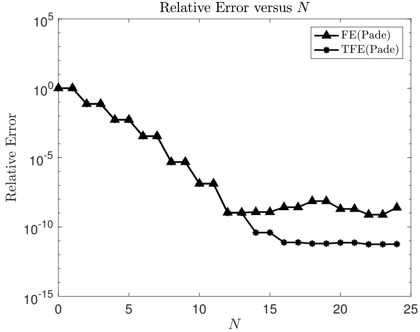


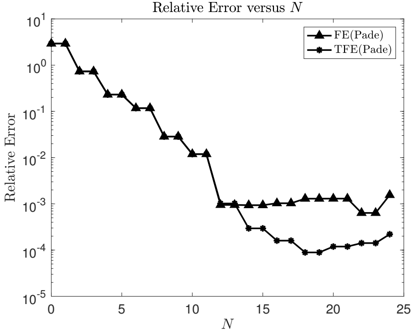


Convergence Study

We then reprise these calculations with a much larger choices of perturbation parameter, $\varepsilon = 0.01, 0.05$. We use both FE and TFE with the same choice of $f(\theta)$. The physical and numerical parameters are

$$a = 0.025, \quad c = a/10, \quad b = 10a, \quad N_r = 64, \quad N = 24.$$





Simulation of Nanorods

Return to the problem of scattering of plane-wave incident radiation which demands the Dirichlet (1c) and Neumann conditions (1d). We consider metallic nanorods housed in a dielectric with outer interface shaped by

$$r = a + g(\theta) = a + \varepsilon f(\theta).$$

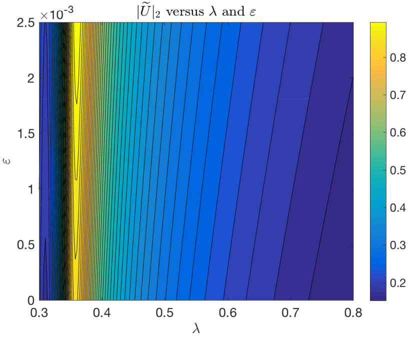
We illuminate this structure over a range of incident wavelengths $\lambda_{min} \leq \lambda \leq \lambda_{max}$ and perturbation sizes $\varepsilon_{min} \leq \varepsilon \leq \varepsilon_{max}$, and compute the magnitudes of the reflected and transmitted surface currents, $\tilde{U}$ and $\tilde{W}$, using FE approach.

An Analytic Deformation

Analytic profile: $f(\theta) = e^{\cos(\theta)}$
Numerical parameters: $N_\lambda = 201, \quad N_\varepsilon = 201, \quad N_\theta = 64, \quad N = 16.$
Physical configuration:

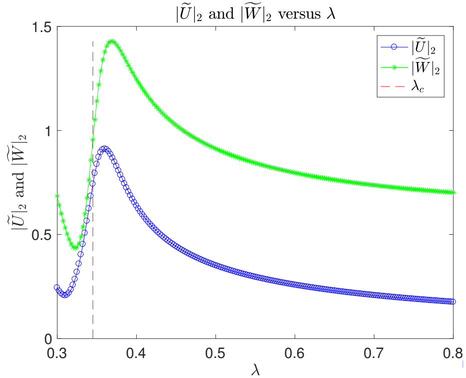
$$a = 0.025, \quad \lambda_{min} = 0.300, \quad \lambda_{max} = 0.800$$

$$\varepsilon_{min} = 0, \quad \varepsilon_{max} = a/10, \quad \text{inner} = \text{silver}, \quad \text{outer} = \text{vacuum}$$



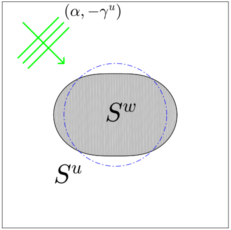
An Analytic Deformation

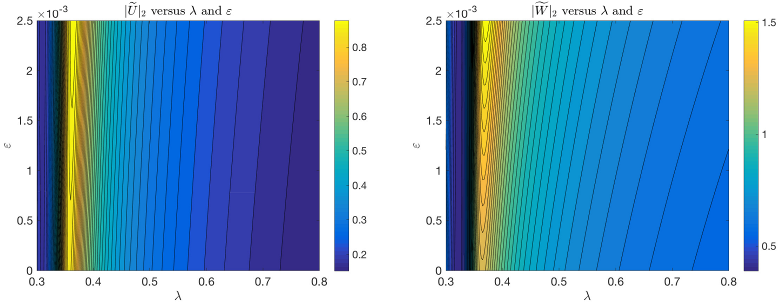
In the case of a nanorod with a perfectly circular cross–section we computed the value as the λ_F satisfying the Fröhlich condition and in subsequent plots this is depicted by a dashed red line. We display the final Slice $\varepsilon = \varepsilon_{max}$ for a silver nanorod shaped by the analytic profile, in vacuum.



A Low-Frequency Cosine Deformation

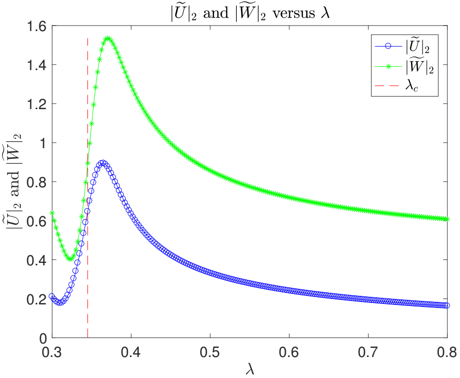
Low-frequency sinusoidal profile:
$f(\theta) = \cos(2\theta)$





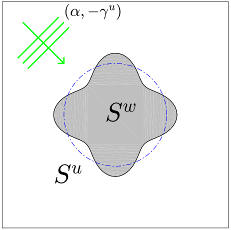
A Low-Frequency Cosine Deformation

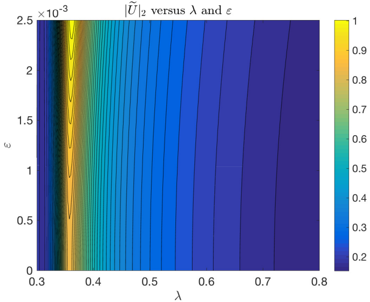
We display the final Slice $\varepsilon = \varepsilon_{max}$ for a silver nanorod shaped by the sinusoidal profile, in vacuum.

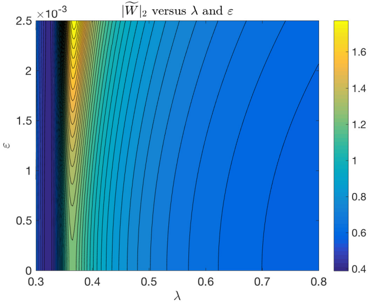


A Higher Frequency Cosine Deformation

Higher frequency sinusoidal profile:
$f(\theta) = \cos(4\theta)$

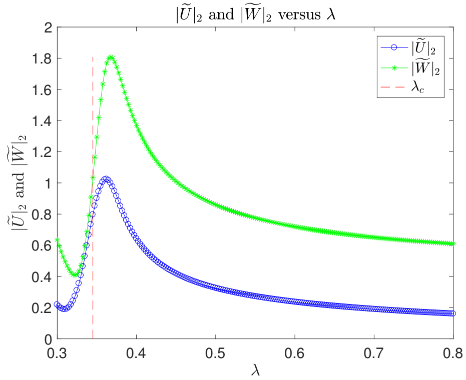






A Higher Frequency Cosine Deformation

We display the final Slice $\varepsilon = \varepsilon_{max}$ for a silver nanorod shaped by the sinusoidal profile, in vacuum.



Future Work

- Consider the problem enforced by Impedance-to-Impedance Operator e.g.

$$U := [-\partial_N u + i\eta u]_{r=a+g}$$
$$I^u[U] := [-\partial_N u - i\eta u]_{r=a+g}$$

- The existence of IIO which guarantees a complete solution scheme

Thank you!

Comments and Questions!

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