

Simulation of Localized Surface Plasmon Resonances via Dirichlet–Neumann Operators and Impedance–Impedance Operators

Xin Tong

Joint work with Professor David Nicholls

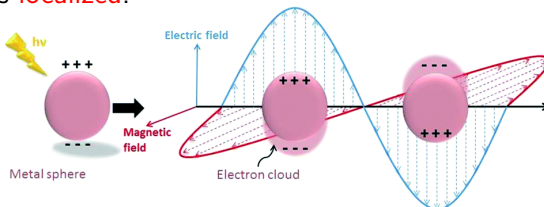
Department of Mathematics, Statistics and Computer Science
University of Illinois at Chicago

The Mathematics of Finite Elements and Applications 2019 (MAFELAP 2019)

July 7, 2019

Localized Surface Plasmon Resonance (LSPR)

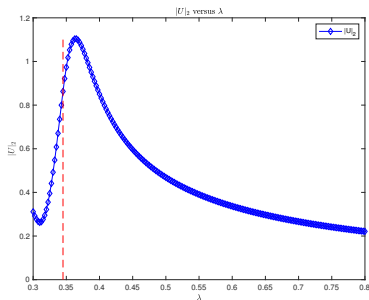
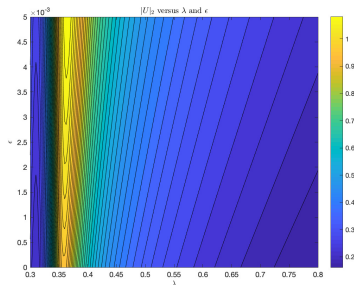
- The plasmon field is generated by the oscillation of electrons. This field in the metal is about 5 nm meaning that the surface plasmon does not penetrate deep into the metal.
- When light strikes the surface of a metal nanoparticle, if the electron cloud is excited at the resonance frequency, the light is absorbed more strongly. This case is called a **resonance**.
- When the dimension of the interface is much less than the surface plasmon propagation length (measured in μm or mm), the surface plasmon is **localized**.



The figure is from *Metal nanoparticle photocatalysts: emerging processes for green organic synthesis*.

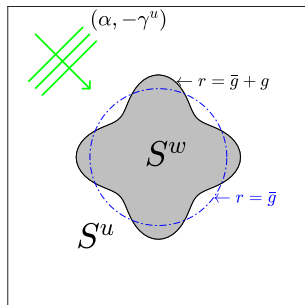
Localized Surface Plasmon Resonance

- There is an example showing that the resonance can be induced by selecting the appropriate light wavelength (frequency).



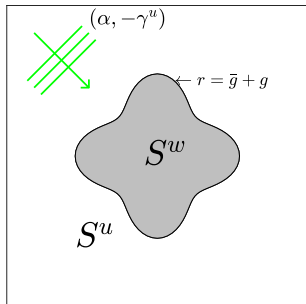
- The dashed red line represents the Fröhlich value of LSPR.

The Geometry



- We consider a y-invariant, doubly layered structure.
- Dielectrics occupy the unbounded exterior; a metal fills the bounded interior.
- The interface is described in polar coordinates by $r = \bar{g} + g(\theta)$.
- exterior domain $S^u := \{r > \bar{g} + g(\theta)\}$
interior domain $S^w := \{r < \bar{g} + g(\theta)\}$

Incident Radiation



- The structure is illuminated by **monochromatic** plane-wave incident radiation of frequency ω .
- Consider the **reduced** electric and magnetic fields

$$\mathbf{E}(r, \theta) = e^{i\omega t} \underline{\mathbf{E}}, \quad \mathbf{H}(r, \theta) = e^{i\omega t} \underline{\mathbf{H}}.$$

- Incident, scattered, total fields are all 2π -periodic in θ .
- The scattered radiation is “outgoing” in S^u and bounded in S^w .

The Penetrable obstacle scattering problem

- In this 2D setting the time-harmonic Maxwell equations decouple into two scalar Helmholtz problems: Transverse electric (TE) and transverse magnetic (TM) polarizations.
- We define the invariant (y) directions of the scattered (electric or magnetic) fields by $\{u(r, \theta), w(r, \theta)\}$ in S^u and S^w , respectively.

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

$$\begin{aligned}
 \Delta u + (k^u)^2 u &= 0, & r > \bar{g} + g(\theta), \\
 \Delta w + (k^w)^2 w &= 0, & r < \bar{g} + g(\theta), \\
 u - w &= -u^{\text{inc}} := \xi, & r = \bar{g} + g(\theta), \\
 \tau^u \partial_{\mathbf{N}} u - \tau^w \partial_{\mathbf{N}} w &= \tau^u (-\partial_{\mathbf{N}} u^{\text{inc}}) := \tau^u \nu, & r = \bar{g} + g(\theta),
 \end{aligned}$$

where u^{inc} is the incident radiation, and $\tau^u = \tau^w = 1$ (TE) or $\{\tau^u = 1/\epsilon^{(u)}, \tau^w = 1/\epsilon^{(w)}\}$ (TM).

Transparent Boundary Conditions

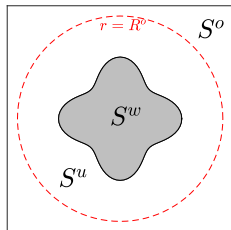
- Regarding the **Outgoing Wave Condition (Sommerfeld Radiation Condition)**, we introduce an artificial boundary — $\{r = R^o, \quad R^o > \bar{g} + |g|_{L^\infty}\}$ and define the domain $S^o := \{r > R^o\}$.
- The solution of Helmholtz problem on S^o with Dirichlet boundary data, say $u(R^o, \theta) = \underline{u}(\theta)$, is

$$u(r, \theta) = \sum_{p=-\infty}^{\infty} \hat{u}_p \frac{H_p(k^u r)}{H_p(k^u R^o)} e^{ip\theta},$$

where H_p is the p th Hankel function of first kind.

- We compute the *outward-pointing* Neumann data at the artificial boundaries, and define the order-one Fourier multipliers $T^{(u)}$,

$$-\partial_r u(R^o, \theta) = \sum_{p=-\infty}^{\infty} -k^u \hat{u}_p \frac{H'_p(k^u R^o)}{H_p(k^u R^o)} e^{ip\theta} =: T^{(u)}[\underline{u}(\theta)].$$



- Then the periodic, outward propagating solutions to

$$\Delta u + (k^u)^2 u = 0, \quad r > \bar{g} + g(\theta),$$

equivalently solve

$$\begin{aligned} \Delta u + (k^u)^2 u &= 0, & \bar{g} + g(\theta) < r < R^o, \\ \partial_r u + T_u[u] &= 0, & r = R^o. \end{aligned}$$

- Similarly, we choose another artificial boundary — $\{r = R_i, \quad 0 < R_i < \bar{g} - |g|_{L^\infty}\}$ which defines the domain $S_i := \{r < R_i\}$ and the Dirichlet data $\underline{w}(\theta)$.
- The order-one Fourier multiplier $T^{(w)}$ is

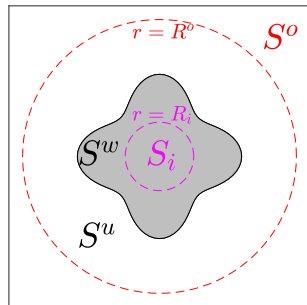
$$\partial_r w(R_i, \theta) = \sum_{p=-\infty}^{\infty} k^w \hat{w}_p \frac{J'_p(k^w R_i)}{J_p(k^w R_i)} e^{ip\theta} =: T^{(w)}[\underline{w}(\theta)],$$

where J_p is the p th Bessel function of first kind.

A summary

The penetrable obstacle scattering problem is equivalent to solve

$$\begin{aligned}
 \Delta u + (k^u)^2 u &= 0, & r > \bar{g} + g(\theta), \\
 \Delta w + (k^w)^2 w &= 0, & r < \bar{g} + g(\theta), \\
 u - w &= \xi, & r = \bar{g} + g(\theta), \\
 \tau^u \partial_{\mathbf{N}} u - \tau^w \partial_{\mathbf{N}} w &= \tau^u \nu, & r = \bar{g} + g(\theta), \\
 \partial_r u + T^{(u)}[u] &= 0, & r = R^o, \\
 \partial_r w - T^{(w)}[w] &= 0, & r = R_i.
 \end{aligned}$$



Non-Overlapping Domain Decomposition Method

- The idea is thinking the solution layer by layer. What about the interface?
- Let the outer/inner Dirichlet traces and their (outward) Neumann counterparts be

$$\begin{aligned} U(\theta) &:= u(\bar{g} + g(\theta), \theta), & \tilde{U}(\theta) &:= -(\partial_N u)(\bar{g} + g(\theta), \theta), \\ W(\theta) &:= w(\bar{g} + g(\theta), \theta), & \tilde{W}(\theta) &:= (\partial_N w)(\bar{g} + g(\theta), \theta). \end{aligned}$$

- At the interface, we have

$$\begin{cases} u - w = \xi, \\ \tau^u \partial_N u - \tau^w \partial_N w = \tau^u \nu, \end{cases} \Rightarrow \begin{cases} U - W = \xi, \\ -\tau^u \tilde{U} - \tau^w \tilde{W} = \tau^u \nu. \end{cases}$$

- Define the Dirichlet-Neumann Operators

$$G^{(u)} : U \rightarrow \tilde{U}, \quad G^{(w)} : W \rightarrow \tilde{W}. \quad \left(\Rightarrow \begin{cases} U - W = \xi, \\ -\tau^u G^{(u)}[U] - \tau^w G^{(w)}[W] = \tau^u \nu. \end{cases} \right)$$

Impedance–Impedance Operator (IIO)

- Motivation: apply the linear operator $P = \begin{pmatrix} Y & -\mathbb{1} \\ Z & -\mathbb{1} \end{pmatrix}$ to the BCs

$$\begin{cases} u - w = \xi, \\ \tau^u \partial_{\mathbf{N}} u - \tau^w \partial_{\mathbf{N}} w = \tau^u \nu, \end{cases}$$

resulting
$$\begin{aligned} [-\tau^u \partial_N u + Yu] + [\tau^w \partial_N w - Yw] &= [-\tau^u \nu + Y\xi] := \zeta, \\ [-\tau^u \partial_N u + Zu] + [\tau^w \partial_N w - Zw] &= [-\tau^u \nu + Z\xi] := \psi. \end{aligned}$$

- The Y and Z are unequal operators to be specified. We choose $\pm i\eta$ for a constant $\eta \in \mathbb{R}^+$ later for numerical experiment.
- Let the outer/inner Impedance and their outer/inner counterparts be

$$I^u := [-\tau^u \partial_N u + Yu]_{r=\bar{g}+g}, \quad I^w := [\tau^w \partial_N w - Zw]_{r=\bar{g}+g},$$

$$\tilde{I}^u := [-\tau^u \partial_N u + Zu]_{r=\bar{g}+g}, \quad \tilde{I}^w := [\tau^w \partial_N w - Yw]_{r=\bar{g}+g}.$$

- Define the Impedance–Impedance Operators

$$Q : I^u \rightarrow \tilde{I}^u, \quad S : I^w \rightarrow \tilde{I}^w,$$

then write
$$\begin{cases} I^u + \tilde{I}^w = \zeta \\ \tilde{I}^u + I^w = \psi \end{cases} \Rightarrow \begin{pmatrix} \mathbb{1} & S \\ Q & \mathbb{1} \end{pmatrix} \begin{pmatrix} I^u \\ I^w \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix}.$$

Definition 1 [Exterior Problem with DNO]: Given a sufficiently smooth deformation $g(\theta)$, the unique periodic solution of

$$\begin{aligned}\Delta u + (k^u)^2 u &= 0, & \bar{g} + g(\theta) < r < R^o, \\ u(\bar{g} + g(\theta), \theta) &= U, & r = \bar{g} + g(\theta), \\ \partial_r u + T^{(u)}[u] &= 0, & r = R^o,\end{aligned}$$

defines the DNO

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

Definition 2 [Interior Problem with DNO]: Given a sufficiently smooth deformation $g(\theta)$, if we are not at a Dirichlet eigenvalue of the Laplacian on $\{R_i < r < \bar{g} + g(\theta)\}$, the unique periodic solution of

$$\begin{aligned}\Delta w + (k^w)^2 w &= 0, & R_i < r < \bar{g} + g(\theta), \\ w(\bar{g} + g(\theta), \theta) &= W, & r = \bar{g} + g(\theta), \\ \partial_r w - T^{(w)}[w] &= 0, & r = R_i,\end{aligned}$$

defines the DNO

$$G^{(w)}[W] = G^{(w)}(R_i, \bar{g}, g)[W] := (\partial_N w)(\bar{g} + g(\theta), \theta) = \tilde{W}.$$

Definition 3 [Exterior Problem with IIO]: Given a sufficiently smooth deformation $g(\theta)$, the unique periodic solution of

$$\begin{aligned} \Delta u + (k^u)^2 u &= 0, & \bar{g} + g(\theta) < r < R^o, \\ -\tau^u \partial_{\mathbf{N}} u + Yu &= I^u, & r = \bar{g} + g(\theta), \\ \partial_r u + T^{(u)}[u] &= 0, & r = R^o, \end{aligned}$$

defines the IIO

$$Q[I^u] = Q(R^o, \bar{g}, g)[I^u] := -\tau^u \partial_{\mathbf{N}} u + Zu := \tilde{I}^u.$$

Definition 4 [Interior Problem with IIO]: Given a sufficiently smooth deformation $g(\theta)$, the unique periodic solution of

$$\begin{aligned} \Delta w + (k^w)^2 w &= 0, & R_i < r < \bar{g} + g(\theta), \\ \tau^w \partial_{\mathbf{N}} w - Zw &= I^w, & r = \bar{g} + g(\theta), \\ \partial_r w - T^{(w)}[w] &= 0, & r = R_i, \end{aligned}$$

defines the IIO

$$S[I^w] = S(R_i, \bar{g}, g)[I^w] := \tau^w \partial_{\mathbf{N}} w - Yw := \tilde{I}^w.$$

Numerical Methods

- Many numerical algorithms have been devised for the simulation of these problems, for instance, Finite Differences, Finite Elements, Spectral Elements.
- These methods suffer from the requirement that they discretize the **full volume** of the problem domain.
- Surface Methods, especially the **High-Order Perturbation of Surfaces (HOPS)** methods:
 - provide the solution at interface (we want)
 - only discretize the layer interfaces;
 - deliver high-accuracy simulations with greatly reduced operation counts.
- Foundational contributions:
 - ① Field Expansions: Bruno & Reitich (1993),
 - ② Transformed Field Expansions: Nicholls & Reitich (1999).

Perturbation Expansions

- As with all HOPS schemes, the Method of Field Expansions (FE) begins with the $g(\theta) = \varepsilon f(\theta)$.
- Provided that f is sufficiently smooth, $\{Q, S\}$, and data, $\{\zeta, \psi\}$, can be shown to be analytic in ε so that the following Taylor series are strongly convergent

$$\{Q, S, \zeta, \psi, I^u, I^w\} = \{Q, S, \zeta, \psi, I^u, I^w\}(\varepsilon) = \sum_{n=0}^{\infty} \{Q_n, S_n, \zeta_n, \psi_n, I_n^u, I_n^w\} \varepsilon^n.$$

- It is straightforward to identify a recursive formula for $\{I_n^u, I_n^w\}$

$$\begin{pmatrix} \mathbb{1} & S_0 \\ Q_0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} I_n^u \\ I_n^w \end{pmatrix} = \begin{pmatrix} \zeta_n \\ \psi_n \end{pmatrix} - \sum_{m=0}^{n-1} \begin{pmatrix} 0 & S_{n-m} \\ Q_{n-m} & 0 \end{pmatrix} \begin{pmatrix} I_m^u \\ I_m^w \end{pmatrix}, \quad \mathcal{O}(\varepsilon^n).$$

- We need $\{Q_0, S_0\}$ and $\{Q_m, S_m\}$, $m = 1, \dots, n-1$.

Method of Field Expansions

- Focusing upon the field u (outer domain), with $u = \sum_{n=0}^{\infty} u_n(r, \theta) \varepsilon^n$.
- Insert it into the **Exterior Problem with IIO**

$$\begin{aligned} \Delta u + (k^u)^2 u &= 0, & \bar{g} + g(\theta) < r < R^o, \\ -\tau^u \partial_{\mathbf{N}} u + Yu &= I^u, & r = \bar{g} + g(\theta), \\ \partial_r u + T^{(u)}[u] &= 0, & r = R^o, \end{aligned}$$

- The u_n must be 2π -periodic, outward-propagating solutions of the elliptic boundary value problem

$$\begin{aligned} \Delta u_n + (k^u)^2 u_n &= 0, & \bar{g} < r < R^o, \\ -\tau^u \partial_{\mathbf{N}} u_n + Yu_n &= I_n^u + L_{n-1}, & r = \bar{g}, \\ \partial_r u_n + T^{(u)}[u_n] &= 0, & r = R^o, \end{aligned}$$

- The exact solution is, with $\hat{u}_{n,p}$ determined by **given data** $I_n^u + L_{n-1}$

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

Method of Field Expansions

- Looking for $\{Q_0, S_0\}$ and $\{Q_m, S_m\}$, $m = 1, \dots, n-1$.
- Recall that

$$\sum_{n=0}^{\infty} Q_n \varepsilon^n = Q[I^u] := -\tau^u(\partial_{\mathbf{N}} u)(\bar{g} + g(\theta), \theta) + (Zu)(\bar{g} + g(\theta), \theta)$$

$$u = \sum_{n=0}^{\infty} u_n(r, \theta) \varepsilon^n \quad \text{and} \quad u_n(r, \theta) = \sum_{p=-\infty}^{\infty} \hat{u}_{n,p} \frac{H_p(k^u r)}{H_p(k^u \bar{g})} e^{ip\theta}.$$

- The calculation involves expanding Hankel functions in power series in ε , equating like power of ε , and etc, which results in

$$Q_0[I^u] = \sum_{p=-\infty}^{\infty} \hat{I}_p^u \frac{-(k^u \bar{g}) \tau^u H'_p(k^u \bar{g}) + Z_p H_p(k^u \bar{g})}{-(k^u \bar{g}) \tau^u H'_p(k^u \bar{g}) + Y_p H_p(k^u \bar{g})} e^{ip\theta}$$

$$Q_n[I^u] = -\frac{f}{\bar{g}} Q_{n-1}(f)[I^u] + \text{Terms}(u_n, u_{n-1}, \dots, u_0, f)$$

- Similarly, S_0 and S_m are computed by **Interior Problem with IIO**.

Method of Transformed Field Expansions

- The method of Transformed Field Expansions (TFE) proceeds a domain-flattening change of variables prior to perturbation expansion. We consider the **Interior Problem with IIO**.
- The change of variable is

$$r' = \frac{(\bar{g} - R_i)r + R_i g(\theta)}{\bar{g} + g(\theta) - R_i}, \quad \theta' = \theta,$$

which 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 (denoted by v) and modifies the problem to

$$\begin{aligned} \Delta v + (k^w)^2 v &= F(r, \theta; g), & R_i < r < \bar{g}, \\ \tau^w \partial_{\mathbf{N}} v - Zv &= I^w, & r = \bar{g}, \\ \partial_r v - T^{(w)}[v] &= K(\theta; g), & r = R_i. \end{aligned}$$

- The Gerlakin methods is applied to solve the non-homogeneous BVP.

Validation by the Method of Manufactured Solutions

- We consider 2π -periodic, outgoing solutions of the Helmholtz equation, and the bounded counterpart

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

- For a given choice of $f = f(\theta)$ we compute, the exact interior Neumann data and the exact interior Impedance data

$$\begin{aligned} \rho^{\text{in}}(\theta) &:= [\partial_N w^q]_{r=\bar{g}+\varepsilon f(\theta)} = \tilde{W}(\theta), \\ \phi^{\text{in}}(\theta) &:= [\tau^u \partial_N w^q - Y w^q]_{r=\bar{g}+\varepsilon f(\theta)} = \tilde{I}^w(\theta). \end{aligned}$$

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

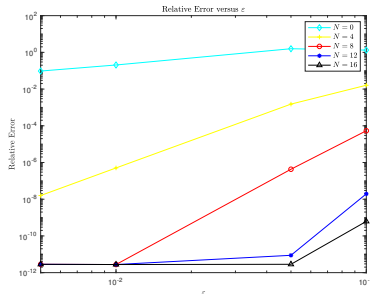
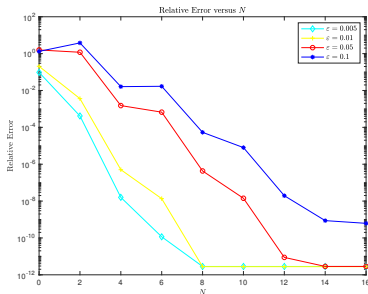
$$u^{N_\theta, N}(r, \theta) := \sum_{n=0}^N \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{u}_{n,p} e^{ip\theta} \varepsilon^n, \quad w^{N_\theta, N}(r, \theta) := \sum_{n=0}^N \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{w}_{n,p} e^{ip\theta} \varepsilon^n.$$

DNO versus IIO

- We select the 2π -periodic and analytic function $f(\theta) = e^{\cos(\theta)}$
- Set the parameters:

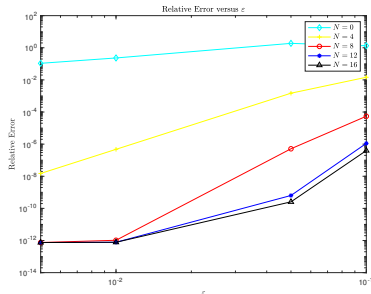
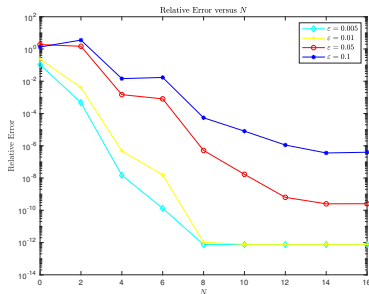
$$q = 2, \quad A_u^q = 2, \quad A_w^q = 1, \quad N_\theta = 64, \quad N = 16.$$

- The operators are $Y = 3.4i, Z = -3.4i$.
- To begin with our study, with the choice $\bar{g} = 0.5$, we carry out simulations with IIO formulation.



DNO versus IIO

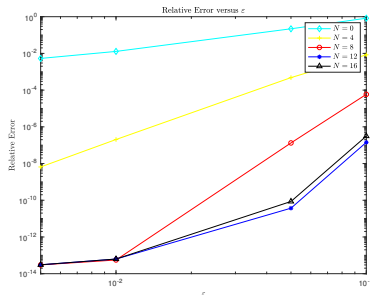
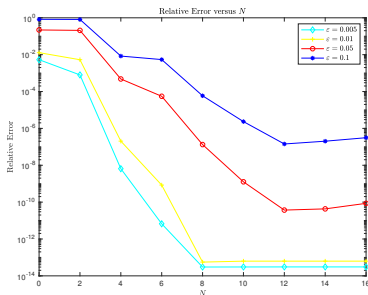
- We repeat this with our DNO approach,



- In this non-resonant configuration ($\bar{g} = 0.5$), both algorithms display a spectral rate of convergence as N is refined (improving as ε is decreased).

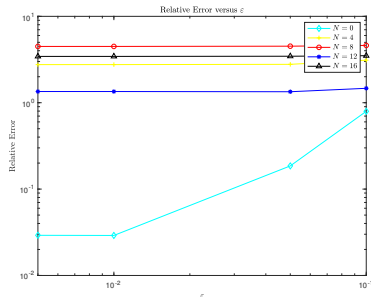
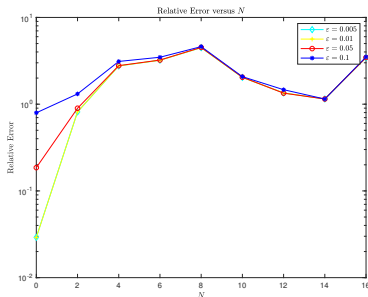
DNO versus IIO: a nearly-resonant configuration

- We note that the choice of $\bar{g} = 1$ will induce a singularity in the interior DNO $G^{(w)}$.
- To test the performance, we select $\bar{g} = 1 - 10^{-12}$.
- The IIO algorithm shows



DNO versus IIO: a nearly-resonant configuration

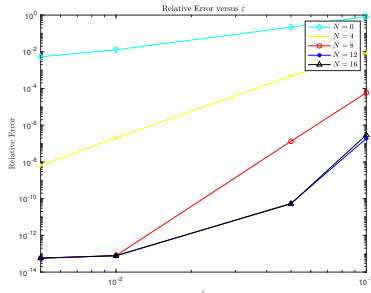
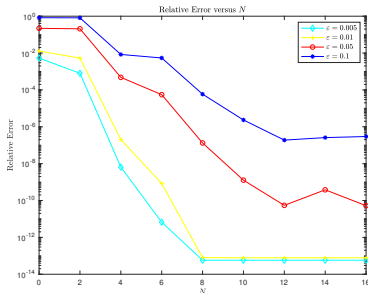
- The DNO algorithm shows



- In this nearly resonant configuration, while IIO algorithm displays a spectral rate of convergence as N is refined, the DNO approach does **not** provide results of the same quality.

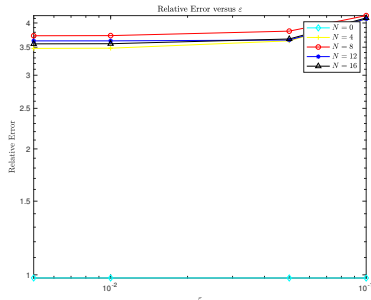
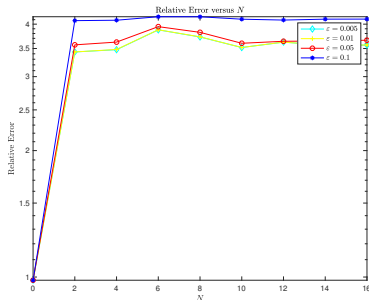
DNO versus IIO: a resonant configuration

- Last, we select $\bar{g} = 1 - 10^{-16}$ (to machine precision).
- The IIO algorithm shows



DNO versus IIO: a resonant configuration

- The DNO algorithm shows



- In this resonant configuration, the IIO algorithm again displays a spectral rate of convergence as N is refined, while the DNO approach delivers completely unacceptable results.

Analyticity of Solutions via IIOs

Rewrite the boundary conditions compactly as $\mathbf{AV} = \mathbf{R}$

$$\underbrace{\begin{pmatrix} \mathbb{1} & S \\ Q & \mathbb{1} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} I^\mu \\ I^w \end{pmatrix}}_{\mathbf{V}} = \underbrace{\begin{pmatrix} \zeta \\ \psi \end{pmatrix}}_{\mathbf{R}}.$$

- We can show, the IIOs, Q and S , are analytic in the perturbation parameter ε so that the following expansions are strongly convergent in an appropriate Sobolev space

$$Q(\varepsilon f) = \sum_{n=0}^{\infty} Q_n(f) \varepsilon^n, \quad S(\varepsilon f) = \sum_{n=0}^{\infty} S_n(f) \varepsilon^n.$$

- Next we can show the operator \mathbf{A} , the data \mathbf{R} , and solution \mathbf{V} , are analytic under certain conditions

$$\{\mathbf{A}(\varepsilon f), \mathbf{V}(\varepsilon f), \mathbf{R}(\varepsilon f)\} = \sum_{n=0}^{\infty} \{\mathbf{A}_n(f), \mathbf{V}_n(f), \mathbf{R}_n(f)\} \varepsilon^n.$$

- Furthermore, the \mathbf{V}_n must satisfy

$$\mathbf{V}_n = \mathbf{A}_0^{-1} \left\{ \mathbf{R}_0 - \sum_{\ell=0}^{n-1} \mathbf{A}_{n-\ell} \mathbf{V}_\ell \right\},$$

Analyticity: the Main Theorem [Nicholls17]

Given two Banach spaces $X = Y = H^{-1/2} \times H^{-1/2}$, suppose that:

H1 $\mathbf{R}_n \in Y$ for all $n \geq 0$, and there exist $C_R > 0$, $B_R > 0$ such that

$$\|\mathbf{R}_n\|_Y \leq C_R B_R^n, \quad n \geq 0.$$

H2 $\mathbf{A}_n : X \rightarrow Y$ for all $n \geq 0$, and there exist $C_A > 0$, $B_A > 0$ such that

$$\|\mathbf{A}_n\|_{X \rightarrow Y} \leq C_A B_A^n, \quad n \geq 0.$$

H3 $\mathbf{A}_0^{-1} : Y \rightarrow X$, and there exists a constant $C_e > 0$ such that

$$\|\mathbf{A}_0^{-1}\|_{Y \rightarrow X} \leq C_e.$$

Then the equation $\mathbf{A}\mathbf{V} = \mathbf{R}$ has a unique solution, and there exist constants $C_V > 0$ and $B_V > 0$ such that

$$\|\mathbf{V}_n\|_X \leq C_V B_V^n, \quad n \geq 0,$$

for any $C_V \geq 2C_e C_R$, $B_V \geq \max\{B_R, 2B_A, 4C_e C_A B_A\}$,

which implies that, $\sum \mathbf{V}_n \varepsilon^n$ converges for all ε such that $0 \leq B_V \varepsilon < 1$.

Sketch of the proof

Hypothesis H1: the \mathbf{R} is estimated using the given data (incident radiation)

$$\mathbf{R}_n = \begin{pmatrix} \zeta_n \\ \psi_n \end{pmatrix} = \begin{pmatrix} \tau^u \nu_n + Y \xi_n \\ -\tau^u \nu_n + Z \xi_n \end{pmatrix}.$$

Hypothesis H3: the existence and invertibility properties of the operator \mathbf{A}_0 are equivalent to the existence and uniqueness properties of the solution to

$$\begin{pmatrix} \mathbb{1} & S_0 \\ Q_0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} I^u \\ I^w \end{pmatrix} = \begin{pmatrix} \zeta \\ \psi \end{pmatrix},$$

where

$$\mathbf{A}_0 = \begin{pmatrix} \mathbb{1} & S_0 \\ Q_0 & \mathbb{1} \end{pmatrix}.$$

Sketch of the proof

Hypothesis H2: the estimates for $\mathbf{A}_n = \begin{pmatrix} 0 & S_n \\ Q_n & 0 \end{pmatrix}$ are equivalent to the analyticity of the IIOs, i.e.

$$\|Q_n[I^u]\|_{H^{-1/2}} \leq C_Q B_Q^n, \quad \|S_n[I^w]\|_{H^{-1/2}} \leq C_S B_S^n.$$

For instance, the analyticity of S is stated in the following.

- 1 Applying TFE to the interior problem results in an elliptic BVP

$$\begin{aligned} \Delta v_n + (k^w)^2 v_n &= F_n, & R_i < r < \bar{g}, \\ \partial_r v_n - \frac{Z}{\tau^w \bar{g}} v_n &= \frac{\delta_{n,0} I^w}{\tau^w \bar{g}} + l_n, & r = \bar{g}, \\ \partial_r v_n - T^{(w)}[v_n] &= h_n, & r = R_i. \end{aligned}$$

- 2 Elliptic estimate shows that

$$\|v_n\|_{H^1} \leq \|F_n\|_{(H^1)'} + \|\delta_{n,0} I^w\|_{H^{-1/2}} + \|l_n\|_{H^{-1/2}} + \|h_n\|_{H^{-1/2}}.$$

- 3 Estimate the non-homogeneous terms $F_n, \delta_{n,0} I^w, l_n, h_n$.
- 4 Estimate S_n by $S_n[I^w] \approx S_{n-1}[I^w] + S_{n-2}[I^w] + \text{Terms}(v_n, v_{n-1}, v_{n-2})$.

Conclusion

We seek outgoing/bounded, 2π -periodic solutions of the penetrable obstacle scattering problem

$$\Delta u + (k^u)^2 u = 0, \quad r > \bar{g} + g(\theta),$$

$$\Delta w + (k^w)^2 w = 0, \quad r < \bar{g} + g(\theta),$$

$$u - w = -u^{\text{inc}}, \quad r = \bar{g} + g(\theta),$$

$$\tau^u \partial_{\mathbf{N}} u - \tau^w \partial_{\mathbf{N}} w = \tau^u (-\partial_N u^{\text{inc}}), \quad r = \bar{g} + g(\theta),$$

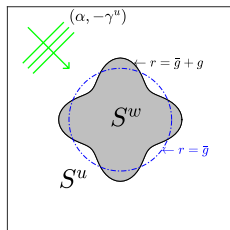
1 The algorithms

- via DNO using FE and TFE
- via IIO using FE and TFE

2 The numerical experiments

- convergence study
- comparison between DNO and IIO
- simulation of nanorods (LSPRs)

3 The analyticity via IIO



Thank you!

and

Comments and Questions!