A Non-Overlapping Domain Decomposition Method for Simulating Localized Surface Plasmon Resonances: High Accuracy Numerical Simulation

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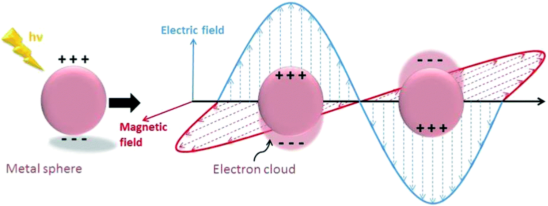
SIAM Conference on Computational Science and Engineering (CSE19)

March 1, 2019

Localized Surface Plasmon Resonance

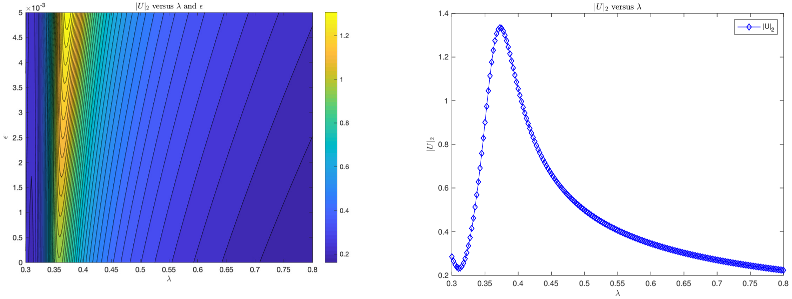
- The (surface) plasmon field in the metal is about 5 nm meaning that the surface plasmon does not penetrate deep into the metal.
- When light strikes the surface of a metal nanoparticle, if the electron cloud is excited at the resonance frequency, the light is absorbed more strongly. This case is called 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.



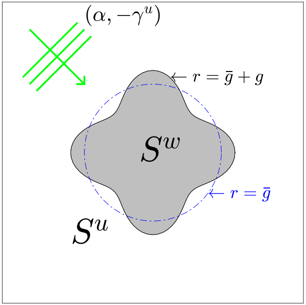
The figure is from *Metal nanoparticle photocatalysts: emerging processes for green organic synthesis*.

Localized Surface Plasmon Resonance

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

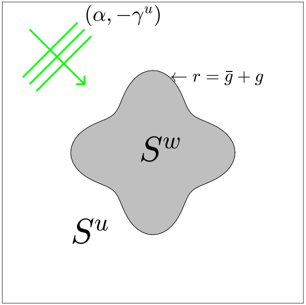


The Geometry



- 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

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

- 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

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

where u^{inc} is the incident radiation, and $\tau^2 = \begin{cases} 1, & \text{TE} \\ (k^u/k^w)^2 & \text{TM.} \end{cases}$

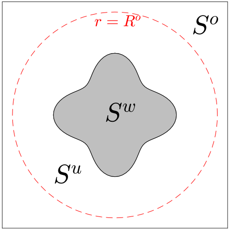
Transparent Boundary Conditions

- 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 $u(R^o, \theta) = \xi(\theta)$, is

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

where H_p is the pth Hankel function of first kind.



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

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

- 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 $S_i := \{r < R_i\}$.
- The order-one Fourier multiplier $T^{(w)}$ is

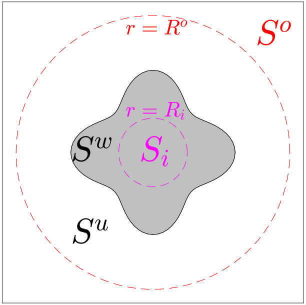
$$\partial_r w(R_i, \theta) = \sum_{p=-\infty}^{\infty} k^w \hat{\mu}_p \frac{J_p'(k^w R_i)}{J_p(k^w R_i)} e^{ip\theta} =: T^{(w)}\,[\mu(\theta)]\,,$$

where J_p is the pth Bessel function of first kind.

A summary

The Penetrable obstacle scattering problem is equivalent to solve

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



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

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

- At the interface, we have

$$\begin{cases} u - w = -u^{\text{inc}} \\ \partial_{\mathbf{N}} u - \tau^2 \partial_{\mathbf{N}} w = -\partial_N u^{\text{inc}} \end{cases} \Rightarrow \begin{cases} U - W = \zeta, \\ -\tilde{U} - \tau^2 \tilde{W} = \psi. \end{cases}$$

- Define the Dirichlet–Neumann Operators

$$G^{(u)} : U \to \tilde{U}, \quad G^{(w)} : W \to \tilde{W}. \left(\Rightarrow \begin{cases} U - W = \zeta, \\ -G^{(u)}[U] - \tau^2 G^{(w)}[W] = \psi. \end{cases} \right)$$

Impedance–Impedance Operator (IIO)

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

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

  where $\tau^u = \tau^w = 1$ (TE) or $\{\tau^u = 1/\epsilon^{(u)}, \tau^w = 1/\epsilon^{(w)}\}$ (TM).
- 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.
- Define the Impedance–Impedance Operators

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

- The boundary conditions at the interface

$$\begin{cases} u - w = -u^{\text{inc}} \\ \partial_{\mathbf{N}} u - \tau^2 \partial_{\mathbf{N}} w = -\partial_N u^{\text{inc}} \end{cases} \Rightarrow \begin{cases} I^u + \tilde{I}^w = \xi \\ \tilde{I}^u + I^w = \chi \end{cases} \Rightarrow \begin{pmatrix} \mathbb{1} & S \\ Q & \mathbb{1} \end{pmatrix} \begin{pmatrix} I^u \\ I^w \end{pmatrix} = \begin{pmatrix} \xi \\ \chi \end{pmatrix}.$$

  ,
- Why IIO?

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

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

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

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

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, $\{\nu, \chi\}$, can be shown to be analytic in ε so that the following Taylor series are strongly convergent

$$\{Q, S, \nu, \chi, I^u, I^w\} = \{Q, S, \nu, \chi, I^u, I^w\}(\varepsilon) = \sum_{n=0}^{\infty} \{Q_n, S_n, \nu_n, \chi_n, I_n^u, I_n^w\} \varepsilon^n.$$

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

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

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

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 to 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 $\{Q_m, S_m\}$, $m = 1, \ldots n-1$.
- Recall that

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

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

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

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

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

- 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

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

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

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

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

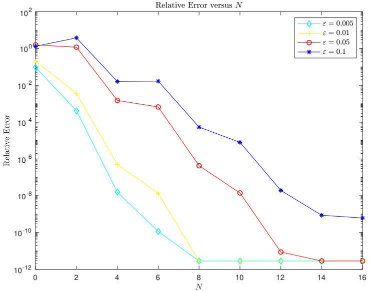
$$u^{N_\theta,N}(r,\theta) := \sum_{n=0}^{N} \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{u}_{n,p} e^{ip\theta} \varepsilon^n, \quad w^{N_\theta,N}(r,\theta) := \sum_{n=0}^{N} \sum_{p=-N_\theta/2}^{N_\theta/2-1} \hat{w}_{n,p} e^{ip\theta} \varepsilon^n.$$

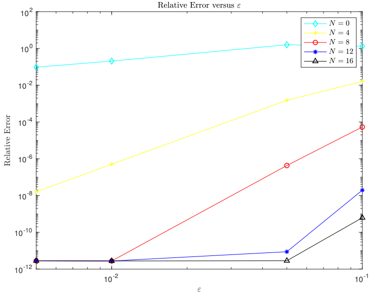
DNO versus IIO

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

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

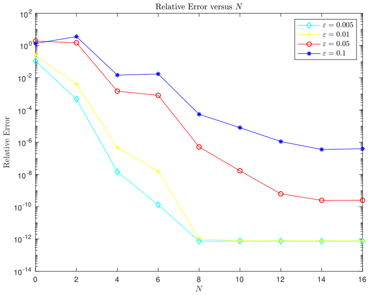
- The operators are $Y = 3.4i, Z = -3.4i$.
- To begin with our study, with the choice $\bar{g} = 0.5$, we carry out simulations with IIO formulation.

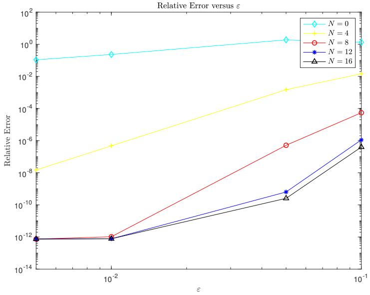




DNO versus IIO

- We repeat this with our DNO approch,

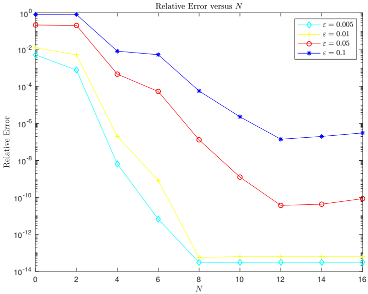


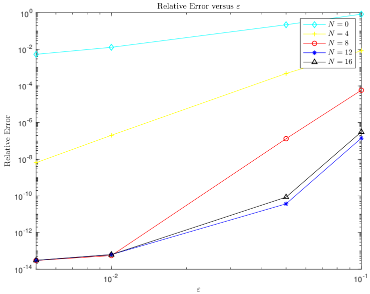


- In this non-resonant configuration ($\bar{g} = 0.5$), both algorithms display a spectral rate of convergence as N is refined (improving as ε is decreased).

DNO versus IIO: a nearly-resonant configuration

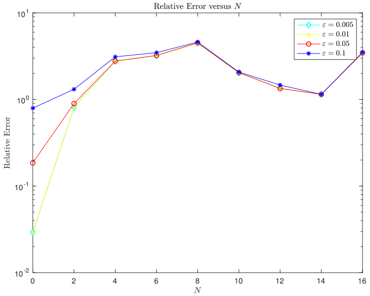
- We note that the choice of $\bar{g} = 1$ will induce a singularity in the interior DNO $G^{(w)}$.
- To test the performance, we select $\bar{g} = 1 - 10^{-12}$.
- The IIO algorithm shows

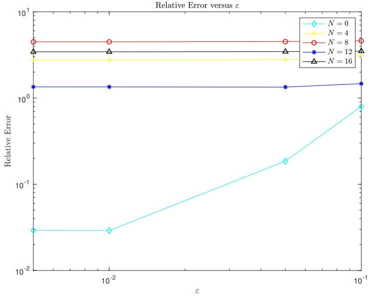




DNO versus IIO: a nearly-resonant configuration

- The DNO algorithm shows

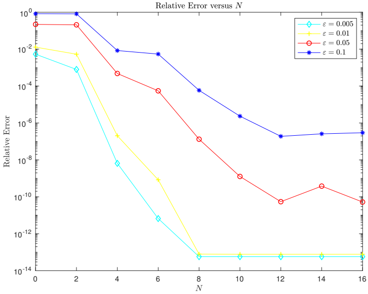


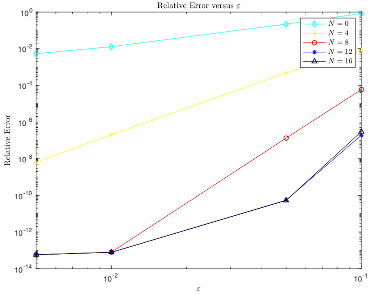


- In this nearly resonant configuration, while IIO algorithm displays a spectral rate of convergence as N is refined, the DNO approach does not provide results of the same quality.

DNO versus IIO: a resonant configuration

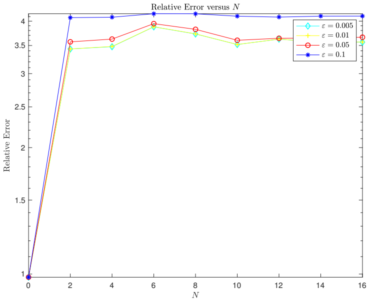
- Last, we select $\bar{g} = 1 - 10^{-16}$ (to machine precision).
- The IIO algorithm shows

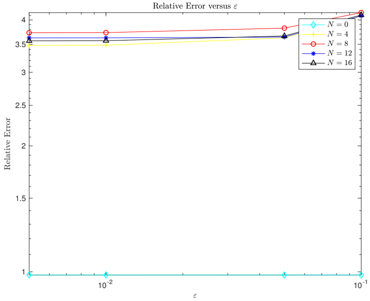




DNO versus IIO: a resonant configuration

- 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.

Thank you!

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Comments and Questions!