Accuracy Study of Low- and High-Order Numerical Techniques for Analysis of Scattering on Plasmonic Nanosphere at THz Frequencies

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Outline

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  - PMCHWT and RWG Method of Moments
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Motivation

- Plasmonic nano-particles as transmission lines at THz:
  - Waveguiding at nano-scale level
  - Sub-wavelength confinement*
  - Low attenuation (in theory)
  - High attenuation (in practice)

(*) A. Alu and N. Engheta, *Theory of linear chains of metamaterial/plasmonic particles as subdiffraction optical nanotransmission lines*, Physical Review B. Vol 74, November, 2006
Perturbed case: Statistical disorder has been introduced in the longitudinal position ($z$ direction) of the spheres.

Results by J. Ochoa, X. Ma, A. Cangellaris (Univ. of Illinois at U-C) from IEEE APS/URSI’2013

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Volume E-Field Integral Equation (VIE):

\[
\frac{j(r)}{i\omega \left[ \varepsilon_a(r) - \varepsilon_0 \right]} + \int_V \overline{G}_{e_0}(r, r') \cdot j(r') \, dv' = E^{inc}(r), \quad r \in V
\]

E-Field dyadic Green’s function:

\[
\overline{G}_{e_0}(r, r') = -i\omega \mu_a (1 + 1/k^2\nabla\nabla)G(r, r')
\]

Volume -> Shaubert-Wilton-Glisson (SWG):

\[
j(r) \equiv \sum_{n=1}^{N_V} j_n f_n (r) \quad \rightarrow \quad \left[ Z_{VV}^{Ej} \right] \cdot \left[ j \right] = \left[ v^{inc} \right]
\]
RWG MoM solution of PMCHWT

**PMCHWT Integral Equation:**

\[
\begin{align*}
\hat{t} \cdot \int_{S} [\vec{G}_{e0}(r,r') + \vec{G}_{e1}(r,r')] \cdot J(r') dS' + \hat{t} \cdot \int_{S} [\vec{G}_{m0}(r,r') + \vec{G}_{m1}(r,r')] \cdot K(r') dS' &= \hat{t} \cdot E^{inc}(r), \quad r \in S \\
\hat{t} \cdot \int_{S} [\vec{G}_{m0}(r,r') + \vec{G}_{m1}(r,r')] \cdot J(r') dS' + \hat{t} \cdot \int_{S} [\vec{G}_{e0}(r,r') + \vec{G}_{e1}(r,r')] \cdot K(r') dS' &= \hat{t} \cdot H^{inc}(r), \quad r \in S
\end{align*}
\]

E-Field dyadic Green’s function:

\[
\vec{G}_{e0}(r,r') = -i \omega \mu_a \left(1 + 1/k^2 \nabla \nabla\right) G(r,r')
\]

H-Field dyadic Green’s function:

\[
\vec{G}_{m0}(r,r') = \nabla G(r,r') \times \vec{I}
\]

Surface -> Rao-Wilton-Glisson (RWG) MoM:

\[
J(r') \approx \sum_{n=1}^{N_S} J_n F_n(r)
\]

\[
\begin{bmatrix}
Z_{0}^{EJ} & Z_{1}^{EJ} & Z_{0}^{EK} & Z_{1}^{EK} \\
Z_{0}^{HJ} & Z_{1}^{HJ} & Z_{0}^{HK} & Z_{1}^{HK}
\end{bmatrix}
\begin{bmatrix}
J \\
K
\end{bmatrix}
= 
\begin{bmatrix}
E^{inc} \\
H^{inc}
\end{bmatrix}
\]

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Surface Electric Field Integral Equation:

\[
\begin{align*}
\frac{-K(r)}{2} - \hat{t} \cdot \int_S G_{e0}(r, r') \cdot J(r') dS' + \hat{t} \cdot \int_S \tilde{G}_{m0}(r, r') \cdot K(r') dS' &= \hat{t} \cdot E^{\text{inc}}(r), \quad r \in S \\
\frac{K(r)}{2} - \hat{t} \cdot \int_S G_{e1}(r, r') \cdot J(r') dS' + \hat{t} \cdot \int_S \tilde{G}_{m1}(r, r') \cdot K(r') dS' &= 0, \quad r \in S
\end{align*}
\]

Locally Corrected Nystrom discretization = point sampling on Bezier patches:

\[
\tilde{J}(\vec{r}) = \sum_{q=1}^{Q} w_q J^1_q \hat{a}^1_q \delta(\vec{r} - \vec{r}_q) + \sum_{q=1}^{Q} w_q J^2_q \hat{a}^2_q \delta(\vec{r} - \vec{r}_q)
\]

\[
\tilde{K}(\vec{r}) = \sum_{q=1}^{Q} w_q K^1_q \hat{a}^1_q \delta(\vec{r} - \vec{r}_q) + \sum_{q=1}^{Q} w_q K^2_q \hat{a}^2_q \delta(\vec{r} - \vec{r}_q)
\]

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Radial dipole excitation: $|E(r, t=0)|$

VIE with 2594 tets:

Mie over 2594 tets:

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Radial dipole excitation: $|\mathbf{E}(\mathbf{r}, t=0)|$

790THz, \( R=10\text{nm} \), \( r'=22\text{nm} \)

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Radial dipole excitation: $|E(r, t=0)|$

$\varepsilon = -3.8 + j0.19$, 790THz, $R=10\text{nm}$, $r'=22\text{nm}$

Slice over y axis

Slice over z axis

Local artifacts in SWG MoM solution (especially near surface)

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Radial dipole excitation: $|\mathbf{E}(r,t=0)|$

790THz, R=10nm, r'=22nm, SWG-VIE

- 1 sphere case
- Only 2 digits of precision can be obtained by mesh refinement, typical for LO Methods
Radial dipole excitation: $|E(r,t=0)|$

- 1 sphere case
- Only 2 digits of precision can be obtained by mesh refinement, typical for LO Methods

$790\text{THz}, R=10\text{nm}, r'=22\text{nm}, \text{RWG-PMCHWT}$
Radial dipole excitation: $|\mathbf{E}(\mathbf{r}, t=0)|$

- 1 sphere case
- HO behavior can be achieved for dielectric and plasmonic cases
- Up to 9 digits of precision

790THz, R=10nm, r’=22nm, HO-LCN
15 Exact Spheres

Sphere #

Mag J (Average on 1 sphere)
Mag J (Only 1 point on 1 sphere)

Flux of J

Magnitude of X-directed Flux of J
15 Deformed Spheres

15 Plasmonic 27 Element Deformed Spheres at Order 5

15 Plasmonic 24 Element Deformed Spheres at Order 5
Conclusions

- Integral equation (IE) methods for plasmonics at THz:
  - Schaubert-Wilton-Glisson Moment Method for Volume IE:
    - Applicable numerical scheme
    - Slow error convergence
    - Poor conditioning of matrix equation
    - Produces notably higher error in case of plasmonic structures
    - Too heavy without fast algorithm
    - Can handle general anisotropy
  - Rao-Wilton-Glisson Moment Method for PMCHWT IE:
    - Applicable numerical scheme
    - Slow (low-order) error convergence
    - Adequate conditioning of matrix equation
    - Cannot handle general anisotropy
  - Locally-Corrected Nystrom solution of EFIE:
    - Applicable numerical scheme
    - Fast error convergence
    - Adequate conditioning of the matrix equation
    - Cannot handle general anisotropy