MNPBEM SOP 1.0 (11/4/2024)

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# **Introduction**

Beyond Mie calculations, numerical simulations are often required to ensure our experimental results. We use MATLAB-based MNPBEM library to simulate the optical properties of plasmonic nanoparticles.1, 2

# **MNPBEM Installation**

1. Go to the GitHub repository “MNPBEM\_GUI” (<https://github.com/Nikolaos-Matthaiakakis/MNPBEM_GUI/tree/master>).
2. Press the green button saying “<> Code” and “Download ZIP”.
3. Extract all from “MNPBEM\_GUI-master.zip” in your folder.
4. Rename “MNPBEM\_GUI\_master” to “MNPBEM\_GUI” to avoid pathing errors.
5. You completed installing MNPBEM17 and MNPBEM-GUI (Graphical User Interface), the latest version of MNPBEM as of 10/29/2024.

\*If you want to use MNPBEM-GUI, the user manual is available under the “help” folder.

\*In this SOP, BEM simulations are performed with MATLAB code under MNPBEM17.

You can just copy and paste the following folder to your path.

\\samba.campuscluster.illinois.edu\illinois-flandes\Katsuya Shiratori\04\_codes\MNPBEM\_GUI

You can also download it from our GitHub repository.

https://github.com/LandesLinkLab/MNPBEM\_GUI

# **Simulation Workflow**

Here, I briefly explain the workflow of MNPBEM using the MATLAB code.

For more details, please read the original papers by Hohenester *et. al*.1, 2

## **Material Properties**

## **% set dielectric environment**

## **epstab = {epsconst(1.0), epstable('gold\_olmon.dat')};**

## 

## **Nanoparticle Geometry**

## **Simulation Parameters**

## **Running Simulation**

# **Example 1: Scattering/Absorption Spectra of AuNS and AuNR**

# **Example 2: Electric Fields of AuNS and AuNR**

# **Example 3: Charge Density Distributions of AuNS and AuNR**

# **Post-Processing**

## **Result Visualization**

## **Data Interpretation**

# **FDTD Benchmarking**

For more details, please find the PowerPoint slides titled “FDTD\_benchmark.ppt” in the MNPBEM\_GUI folder.

# **Common Troubleshooting**

## **Import New Dielectric Material**

1. Obtain the tabulated dielectric data in a text file from resources like RefractiveIndex.Info (<https://refractiveindex.info/>).
2. Go to the folder MNPBEM17 > Material.
3. Run “txt2dat.m” to convert to a dat file. For example, the new gold dielectric function by Olmon3 titled as “Au\_dielectric\_function\_olmon\_2012.txt” is converted to “gold\_olmon.dat”. Please pay attention to the output unit (eV).
4. Converted dat file should be in the folder “@epstable”.
5. Check if the output is reasonable with other sources like similar dielectric functions and reported values.

## **Case of Unpolarized Light**

1. Combine the simulated results from two orthogonal polarizations, one polarization and another rotated by 90 degrees, to simulate the interaction with unpolarized light.
2. Go to the folder MNPBEM17 > Examples > unpolarized\_light
3. Run “combine2unpolarized.m” while uploading those two simulated results.
4. Check if the output is reasonable with other sources like similar dielectric functions and reported values.

# **Updates**

Version 1.0 Notes: First iteration of SOP by Katsuya Shiratori ([katsuya2@illinois.edu](mailto:katsuya2@illinois.edu))

# **References and Resources**

(1) Hohenester, U.; Trugler, A. MNPBEM - A Matlab toolbox for the simulation of plasmonic nanoparticles. *Comput. Phys. Commun.* **2012**, *183* (2), 370-381. DOI: 10.1016/j.cpc.2011.09.009.

(2) Waxenegger, J.; Trügler, A.; Hohenester, U. Plasmonics simulations with the MNPBEM toolbox: Consideration of substrates and layer structures. *Comput. Phys. Commun.* **2015**, *193*, 138-150. DOI: 10.1016/j.cpc.2015.03.023 (acccessed 2023-05-09T19:31:28).

(3) Olmon, R. L.; Slovick, B.; Johnson, T. W.; Shelton, D.; Oh, S.-H.; Boreman, G. D.; Raschke, M. B. Optical dielectric function of gold. *Phys. Rev. B* **2012**, *86* (23), 1-14. DOI: 10.1103/physrevb.86.235147 (acccessed 2022-10-06T16:09:03).