MNPBEM SOP 1.0 (11/11/2024)

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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.

Please carefully read the original papers by Hohenester *et. al*.1, 2 for more details.

## **Dielectric Properties**

MNPBEM manages the dielectric properties of the materials in epstab.

You can define the dielectric properties in three ways: 1) epsconst to define a constant dielectric function such as glass or CTAB3, 2) epsdrude to define a dielectric function using the Drude model, and 3) epstable to define a frequency-dependent dielectric function using tabulated data such as gold dielectric function measured by Olmon.4 Please go to Common Troubleshooting > Import New Dielectric Material for user-defined dielectric materials.

The following example code defines the constant dielectric function of air and tabulated dielectric functions of Au measured by Olmon.

**% set dielectric environment**

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

Note that the order in epstab is important to define the interactions between objects in the section.

## **Nanoparticle Geometry**

MNPBEM has many classes of nanoparticle geometry, but we commonly use trisphere, tripolygon, and tripod to describe spheres, sphere dimer, triangles, and rods.

The following code defines the sphere with a 28 nm diameter using 722 vertices.

**% initialize nanosphere**

**radius = 14.5;**

**p = trisphere(722, 2\*radius); % (number of vertices, diameter)**

In the end, you need to define the interaction of the dielectric materials by setting up a comparticle object as follows:

**% set up COMPARTICLE object**

**p = comparticle(epstab, {p}, [2, 1], 1, op);**

The third argument inout=[2, 1] describes how the particle boundaries and the dielectric functions are related.1 Please look at the examples for more complicated configurations, such as a rod with a CTAB layer on the substrate.

## **Simulation Parameters**

Simulation parameters such as the number of vertices, wavelength range, and plane excitation influence the outcome.

**% plane wave excitation ([x-polarization], [z-direction])**

**exc = planewave([1, 0, 0], [0, 0, 1], op);**

**% wavelength 400 to 1000 nm by 1 nm step**

**enei = 400:1:1000;**

## **Running Simulation**

Simulation time varies depending on how fine you define the vertices of the nanoparticle geometry or wavelength.

Please consider using the SCS cluster (Common Troubleshooting > Use SCS cluster for Faster Simulation) for faster running options.

# **Example: AuNR with CTAB on a Glass Substrate**

## **Far-Field Simulation**

## **Near-Field Simulation**

## **Surface Charge Simulation**

# **Post-Processing**

## **Result Visualization**

## **Data Interpretation**

# **FDTD Benchmarking**

Please find the PowerPoint slides titled “FDTD\_benchmark.ppt” in the MNPBEM\_GUI folder for more details.

# **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 Olmon4 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.

## **Use SCS Cluster for Faster Simulation**

1. Go to the SCS HPC (High-Performance Computing) website (<https://scs.illinois.edu/resources/computing/scs-hpc-high-performance-computing-cluster-lop#kb-toc-anchor0>).
2. Create the SCS cluster account using the form (<https://apps.atlas.illinois.edu/FormBuilderSurvey/Survey/las/SCS/scs_cluster_form/>).
3. Install MobaXterm (<https://mobaxterm.mobatek.net/>) for GUI.
4. Run <>.
5. 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) Ye, X.; Zheng, C.; Chen, J.; Gao, Y.; Murray, C. B. Using binary surfactant mixtures to simultaneously improve the dimensional tunability and monodispersity in the seeded growth of gold nanorods. *Nano Lett* **2013**, *13* (2), 765-771. DOI: 10.1021/nl304478h.

(4) 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).