MNPBEM SOP 1.0 (11/11/2024)

Contents

[**Introduction** 1](#_Toc182226189)

[**MNPBEM Installation** 1](#_Toc182226190)

[**Simulation Workflow** 2](#_Toc182226191)

[**Dielectric Properties** 2](#_Toc182226192)

[**Initialization** 2](#_Toc182226193)

[**Simulation Parameters** 3](#_Toc182226194)

[**Nanoparticle Geometry** 3](#_Toc182226195)

[**Running Simulation** 4](#_Toc182226196)

[**Example: AuNR with CTAB on a Glass Substrate** 4](#_Toc182226197)

[**Simulation Workflow** 4](#_Toc182226198)

[**Far-Field Simulation** 5](#_Toc182226199)

[**Near-Field Simulation** 5](#_Toc182226200)

[**Surface Charge Simulation** 6](#_Toc182226201)

[**FDTD Benchmarking** 6](#_Toc182226202)

[**Common Troubleshooting** 6](#_Toc182226203)

[**Import New Dielectric Material** 6](#_Toc182226204)

[**Case of Unpolarized Light (at work)** 7](#_Toc182226205)

[**Use SCS Cluster for Faster Simulation (at work)** 7](#_Toc182226206)

[**Apply Mirror Symmetry** 7](#_Toc182226207)

[**Updates** 7](#_Toc182226208)

[**References and Resources** 8](#_Toc182226209)

# **Introduction**

Beyond analytical simulations like Mie calculations, numerical simulations are often required to simulate the optical properties of arbitrarily shaped nanoparticles under complicated dielectric environments.1-3 In the past decade, we have been using finite-difference time-domain (FDTD) simulations because the simulated spectra often matched our experimental data.4-10 However, the commercial software package Ansys Lumerical FDTD Solutions is not available for free. Moreover, Dieperink et. al. reported that boundary element method (BEM) achieved more fast and accurate results than FDTD.11 For these reasons, we decided to use the open-source MATLAB toolbox, what is called MNPBEM, to simulate the optical properties of plasmonic nanoparticles.12, 13 In this SOP, we will walk through how to simulate the optical properties (scattering/absorption cross-section, electric field, and surface charge) of plasmonic nanoparticles (sphere, sphere dimer, and rod) using substrate and/or ligand layer (CTAB).

# **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 11/11/2024.
6. Set up the help pages by running the program makemnpbemhelp after adding the path of the main directory. You should be able to search “MNPBEM Toolbox Documentation” from MATLAB help.

\*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, you will understand the workflow of MNPBEM using the MATLAB code. Please carefully read the original papers or MNPBEM Toolbox Documentation by Hohenester *et. al*.12, 13 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 CTAB14, 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.15 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.

## **Initialization**

BEM solvers compute the surface charges for given external excitations, which can be used to compute scattering/absorption cross sections and electric field maps.

**% option for BEM simulation**

**op = bemoption(‘sim’, ‘stat’);**

**‘sim’** selects between quasistatic (**‘stat’**) or retarded (**‘ret’**) solvers. Please visit MNPBEM Toolbox Documentation > MNPBEM User Guide > BEM solvers for more options.

Quasistatic simulations usually work well and fast for small metallic nanoparticles (dimensions below 100 nm), while retarded simulations solve the full Maxwell equations and are usually much slower than the quasistatic ones.

Please use a quasi-static solver for testing and getting a feeling of how the results will look approximately, at least for structures that are significantly smaller than the light wavelength. However, the MNPBEM developer recommended to compare from time to time with the results of the retarded solver.12

After setting the nanoparticle geometry, set up BEM solver as follows:

**% set up BEM solver with COMPARTICLE object p**

**bem = bemsolver(p, op);**

## **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;**

## **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.12 If the code successfully runs but the outcome is not unexpected, this argument often has something wrong. Please look at examples for more complicated configurations, such as a rod with a ligand layer on the substrate.

## **Running Simulation**

Simulation time varies depending on the type of BEM simulations (quasistatic or retarded) and how fine you define the vertices of the nanoparticle geometry or wavelength.

If you need retarded simulations, please consider using the mirror system (Common Troubleshooting > Apply Symmetry) or the SCS cluster (Common Troubleshooting > Use SCS cluster for Faster Simulation) for faster running options.

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

In this example, you will learn the MATLAB codes to simulate the optical properties of AuNR with a CTAB layer (n=1.44) on a glass substrate (n=1.52).

Please open “Rod\_CTAB\_Sub.m” under Examples folder.

## **Simulation Workflow**

**%% dielectric properties**

**epstab = {epsconst(1^2), epstable('gold\_olmon.dat'), epsconst(1.52^2), epsconst(1.33^2), epsconst(1.44^2)};**

**%% initialization for BEM options and layer**

**ztab = 0;**

**op = layerstructure.options;**

**layer = layerstructure(epstab, [1, 3], ztab, op);**

**op = bemoptions('sim', 'stat', 'interp', 'curv', 'waitbar', 0, 'layer', layer);**

**%% simulation parameters**

**% plane wave excitation**

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

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

**%% nanoparticle geometry**

**% initialize nanorod**

**width\_rod = 20;**

**length\_rod = 60;**

**nphi = 3;**

**ntheta = 3;**

**nz = 3;**

**core = trirod(width\_rod, length\_rod, [(width\_rod+1)\*(pi/nphi), (width\_rod+1)/ntheta, (length\_rod-width\_rod+1)/nz], 'triangles');**

**% initialize shell**

**shellthickness = 3.5;**

**shell = trirod(width\_rod+shellthickness\*2, length\_rod+shellthickness\*2, [(width\_rod+1)\*(pi/nphi), (width\_rod+1)/ntheta, (length\_rod-width\_rod+1)/nz], 'triangles');**

**p = comparticle(epstab, {core, shell}, [2, 5; 5, 1], 1, 2, op);**

**p = rot(p, 90, [0, 1, 0]);**

**p = shift(p, [0, 0, -min(p.pos(:, 3)) + 1]);**

**% initialize layer structure**

**if ~exist( 'greentab', 'var' ) || ~greentab.ismember( layer, enei, p )**

**% automatic grid for tabulation**

**tab = tabspace( layer, p, 'nz', 5 );**

**% Green function table**

**greentab = compgreentablayer( layer, tab );**

**% precompute Green function table**

**greentab = set( greentab, enei, op, 'waitbar', 0 );**

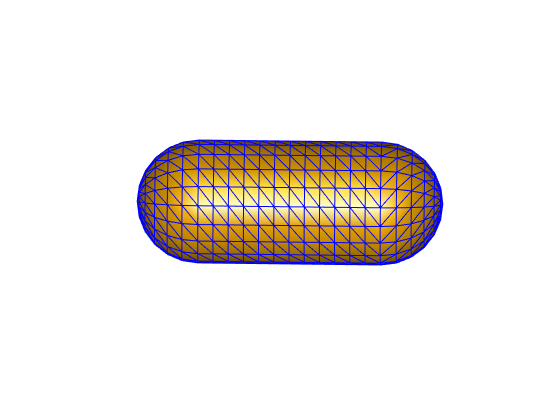
**end**

**op.greentab = greentab;**

**%% initialization for BEM solver**

**bem = bemsolver(p, op);**

When you visualize the nanoparticle geometry, you should be able to see the following.



## **Far-Field Simulation**

**%% far-field simulaiton**

**sca = zeros(length(enei), 2);**

**ext = zeros(length(enei), 2);**

**multiWaitbar('BEM solver', 0, 'Color', 'g', 'CanCancel', 'on');**

**% loop over wavelengths**

**for ien = 1 : length(enei)**

**% surface charge**

**sig = bem \ exc(p, enei(ien));**

**% scattering and extinction cross sections**

**sca(ien, :) = exc.sca(sig);**

**ext(ien, :) = exc.ext(sig);**

**multiWaitbar('BEM solver', ien / numel(enei));**

**end**

**multiWaitbar('CloseAll');**

**fig1 = figure('visible','on');**

**abs = ext - sca;**

**plot(enei, sum(abs, 2), '-','LineWidth', 1);**

**xlabel('Wavelength (nm)', 'FontSize', 20);**

**ylabel('Absorption cross section (nm^2)', 'FontSize', 20);**

**fig2 = figure('visible','on');**

**plot(enei, sum(sca, 2), '-', 'LineWidth', 1);**

**xlabel('Wavelength (nm)', 'FontSize', 20);**

**ylabel('Scattering cross section (nm^2)', 'FontSize', 20);**

## **Near-Field Simulation**

**%% near-field simulation**

**% wavelength of interest**

**enei = 600;**

**% surface charge**

**sig = bem \ exc(p, enei);**

**% scattering and extinction cross sections**

**sca(1, :) = exc.sca(sig);**

**ext(1, :) = exc.ext(sig);**

**[x, y] = meshgrid(linspace(-70, 70, 284), linspace(-35, 35, 142));**

**% particle boundary at z = 10 nm**

**emesh = meshfield(p, x, y, 10, op, 'mindist', 0.15, 'nmax', 2000);**

**% induced and incoming electric field**

**e = emesh(sig) + emesh(exc.field(emesh.pt, enei));**

**% norm of electric field**

**ee = sqrt(dot(e, e, 3));**

**% plot electric field**

**figure(2)**

**imagesc(x(:), y(:), ee);**

**% clim([1 15]);**

**colormap('whitejet'); % need to install the colormap**

**colorbar;**

**xlabel('x (nm)');**

**ylabel('y (nm)');**

**set(gca,'YDir','norm');**

**axis equal tight**

## **Surface Charge Simulation**

**%% surface charge simulation**

**% plot surface charge SIG at particle outside**

**figure(3);**

**plot(p, sig.sig);**

**colormap('whitejet');**

**clim([-0.1 0.1])**

**colorbar**

You will see the simulation outcomes in the next section.

# **FDTD Benchmarking (at work)**

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 Olmon15 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 (at work)**

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 (at work)**

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. <Under testing>
5. Check if the output is reasonable with other sources like similar dielectric functions and reported values.

## **Apply Mirror Symmetry**

1. You want to apply the mirror system when the particle can be flipped at the x- or y-axis or both and transforms into itself, and the excitation preserves the symmetry.
2. You can apply the mirror system by adding BEM options ‘sym’ and defining a specific symmetry in the particle geometry function.
3. Please run “demospecstat14.m” for an example.
4. Check if the output is reasonable with simulations without the mirror system at least once.

Please visit MNPBEM Toolbox Documentation > MNPBEM User Guide > Layer structure > Mirror symmetry for more details.

# **Updates**

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

# **References and Resources**

(1) Kelly, K. L.; Coronado, E.; Zhao, L. L.; Schatz, G. C. The optical properties of metal nanoparticles: The influence of size, shape, and dielectric environment. *J. Phys. Chem. B* **2003**, *107* (3), 668-677. DOI: 10.1021/jp026731y.

(2) Zhao, J.; Pinchuk, A. O.; McMahon, J. M.; Li, S.; Ausman, L. K.; Atkinson, A. L.; Schatz, G. C. Methods for Describing the Electromagnetic Properties of Silver and Gold Nanoparticles. *Acc. Chem. Res.* **2008**, *41* (12), 1710-1720. DOI: 10.1021/ar800028j.

(3) Myroshnychenko, V.; Rodriguez-Fernandez, J.; Pastoriza-Santos, I.; Funston, A. M.; Novo, C.; Mulvaney, P.; Liz-Marzan, L. M.; de Abajo, F. J. G. Modelling the optical response of gold nanoparticles. *Chem. Soc. Rev.* **2008**, *37* (9), 1792-1805. DOI: 10.1039/b711486a.

(4) Hoggard, A.; Wang, L.-Y.; Ma, L.; Fang, Y.; You, G.; Olson, J.; Liu, Z.; Chang, W.-S.; Ajayan, P. M.; Link, S. Using the Plasmon Linewidth To Calculate the Time and Efficiency of Electron Transfer between Gold Nanorods and Graphene. *ACS Nano* **2013**, *7* (12), 11209-11217. DOI: 10.1021/nn404985h (acccessed 2022-06-15T20:08:07).

(5) Yorulmaz, M.; Nizzero, S.; Hoggard, A.; Wang, L. Y.; Cai, Y. Y.; Su, M. N.; Chang, W. S.; Link, S. Single-particle absorption spectroscopy by photothermal contrast. *Nano Lett* **2015**, *15* (5), 3041-3047. DOI: 10.1021/nl504992h.

(6) Smith, K. W.; Zhao, H.; Zhang, H.; Sánchez-Iglesias, A.; Grzelczak, M.; Wang, Y.; Chang, W.-S.; Nordlander, P.; Liz-Marzán, L. M.; Link, S. Chiral and Achiral Nanodumbbell Dimers: The Effect of Geometry on Plasmonic Properties. *ACS Nano* **2016**, *10* (6), 6180-6188. DOI: 10.1021/acsnano.6b02194 (acccessed 2022-06-14T22:41:23).

(7) Joplin, A.; Hosseini Jebeli, S. A.; Sung, E.; Diemler, N.; Straney, P. J.; Yorulmaz, M.; Chang, W. S.; Millstone, J. E.; Link, S. Correlated Absorption and Scattering Spectroscopy of Individual Platinum-Decorated Gold Nanorods Reveals Strong Excitation Enhancement in the Nonplasmonic Metal. *ACS Nano* **2017**, *11* (12), 12346-12357. DOI: 10.1021/acsnano.7b06239.

(8) Cai, Y. Y.; Liu, J. G.; Tauzin, L. J.; Huang, D.; Sung, E.; Zhang, H.; Joplin, A.; Chang, W. S.; Nordlander, P.; Link, S. Photoluminescence of Gold Nanorods: Purcell Effect Enhanced Emission from Hot Carriers. *ACS Nano* **2018**, *12* (2), 976-985. DOI: 10.1021/acsnano.7b07402.

(9) Ostovar, B.; Cai, Y. Y.; Tauzin, L. J.; Lee, S. A.; Ahmadivand, A.; Zhang, R.; Nordlander, P.; Link, S. Increased Intraband Transitions in Smaller Gold Nanorods Enhance Light Emission. *ACS Nano* **2020**, *14* (11), 15757-15765. DOI: 10.1021/acsnano.0c06771.

(10) Lee, S. A.; Ostovar, B.; Landes, C. F.; Link, S. Spectroscopic signatures of plasmon-induced charge transfer in gold nanorods. *J. Chem. Phys.* **2022**, *156* (064702), 1-10. DOI: 10.1063/5.0078621 (acccessed 2022-04-12T20:19:49).

(11) Mees Dieperink, A. S., Nathalie Claes, Sara Bals, Wiebke Albrecht. Considerations for Electromagnetic Simulations for a Quantitative Correlation of Optical Spectroscopy and Electron Tomography of Plasmonic Nanoparticles. *arXiv* **2024**. (acccessed 2024-10-15T02:58:01).

(12) 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.

(13) 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).

(14) 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.

(15) 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).