

Mie scattering off plasmonic nanoparticle

Model documentation © COMSOL 2009

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Contents

- I. Model Overview
- II. Model Navigator
- III. Options and settings
- IV. Geometry modeling
- V. Physics settings
- VI. Mesh generation
- VII. Computing the solution
- VIII. Postprocessing and visualization



I. Model Overview

- This model is a tutorial for calculations of differential and total cross-sections (CS), including absorption, scattering, extinction and radar cross-sections.
- It also illustrates the use of symmetry planes in electromagnetic simulations.
- Illustration of COMSOL's Scattered-field Formulation, Perfectly Matched Layers, Swept Meshing and Far-Field integrals.
- User-defined frequency-dependent optical properties of metals.
- Benchmarking against the exact Mie scattering theory.
- Applications: Plasmonics, Nano-Photonics, general Electromagnetic theory.





II. Modeling in the Graphical User Interface: Model Navigator

Model Navigator			
Multiphysics Con	nponent Library User Components		
Space dimension	3D Modes L Multiphysics Module Is Module Ingineering Module Lience Module ansfer Module Iodule		Add Remove Geom1 (3D) Electromagnetic Waves (rfw)
€€ Elec	Tromagnetic waves Harmonic propagation Eigenfrequency analysis Transient analysis Scattered harmonic propagation Indary Mode Analysis tro-Thermal Interaction	(((Dependent variables: tscEx tscEy tscE Application Mode Properties Add Geometry Add Frame
Dependent varia Application mode Element:	bles: scEx2 scEy2 scEz2 psi2 rname: rfw2 Vector - Quadratic		ing application mode: ectromagnetic Waves (rfw)
		\langle	OK Cancel Help





III. Options and settings: Constants

In Options, open Constants menu, and define constant-valued expressions as shown below. Take advantage of COMSOL's automatic unit conversion when entering radius in nanometers:

-	🖗 Constants				×
	Name	Expression	Value	Description	
	lambda0	1 [um]	(1e-6)[m]	Vacuum wavelength	~
	EO	1 [V/m]	1[V/m]	Amplitude of incident E-field	
	R_particle	100 [nm]	(1e-7)[m]	Radius of the particle	
	sigma_geom	pi*R_particle^2	(3.141593e-14)[m ²]	Geometric cross-section	
				•	
					–
	`				
	i 🛱 🔒		OK Can	cel Apply Help	



Options and settings: Application Mode Properties

Make sure you are solving for **Scattered electric field**, and that **Free space wavelength** is the input parameter:

Application Mode Properties 🛛 🗙				
Properties				
Default element type:	Vector - Quadratic	*		
Analysis type:	Harmonic propagation	*		
Solve for:	Scattered electric field			
Specify wave using:	Free space wavelength	>		
Specify eigenvalues using:	Eigenfrequency	~		
Divergence condition:	Off	~		
Weak constraints:	Off	~		
Constraint type:	Ideal	*		
OK Cancel Help				



Options and settings: Application Scalar Variables

- Use lambda0 for the Free space wavelength.
- Define the incident electric field as E0*exp(-j*k0_rfw*z). This creates a linearly x-polarized plane wave propagating in the positive z direction.

Application S	icalar Variables			×		
Name	Expression	Unit	Description			
epsilon0_rfw	8.854187817e-12	F/m	Permittivity of vacuum			
mu0_rfw	4*pi*1e-7	H/m	Permeability of vacuum			
lambda0_rfw	lambda0	m	Free space wavelength			
E0ix_rfw	EO*exp(-j*k0_rfw*z)	V/m	Incident electric field, x component			
E0iy_rfw		V/m	Incident electric field, y component			
E0iz_rfw	0	V/m	Incident electric field, z component			
psi0_rfw	psi0_guess_rfw	V/m ²	Gauge fixing variable scaling			
Synchronize	Synchronize equivalent variables					
OK Cancel Apply Help						



Options and settings: Materials Library

Materials/Coefficients Library		
Materials Material properties (31) Material Properties (33) Electric (AC/DC) Material Properties (33) Electric (AC/DC) Material Properties (33) Ma	bperties Id Electric Fluid Piezoelectric Thernal All ty Value/Expression Description jcEpsReal(nu_rfw)-j*jcEpsImag(nu_rfw) Relative per 0 Electric cond	
User Defined Materials (1) Gold (Johnson and Christy) (1) Gold New Delete Copy Paste Add Library Search Search for: Name Search string:	 Open C Library Click A Browse Check All tab, defined 	Options>Materials/Coefficients dd Library to the file gold_lib.xml, click OK "Hide undefined properties", go to verify that Relative permittivity is I for this material.
Go To	OK Cancel Apply	Unctions Plot Help





IV. Geometry modeling

- Create four spheres centered at the origin (x=0,y=0,z=0), with radii 1e-7, 2e-7, 2.5e-7, and 3e-7. All dimensions must be given in meters (base unit of length in SI system). These four spheres will represent, respectively:
 - 1. the metallic object ("scatterer") of radius 100 nm = 1e-7 m,
 - 2. auxiliary closed surface for additional postprocessing,
 - 3. air/PML boundary, and
 - 4. exterior PML boundary.

Sphere	
Style Solid Face	Axis base point x: 0 y: 0 z: 0 Axis base point a: 0 (degrees)
Sphere parameters Radius: 1e-7 Name: SPH1	Axis direction vector • Cartesian coordinates x: • 0
(OK Cancel Apply Help



Geometry modeling: create symmetry planes

• In Work-Plane Settings: create an x-y plane at z=0. Click OK.

Work-Plane Settings	
Quick Face Parallel Edge Angle Vertices Advanced Plane • ¥-Y z: • Y-Z X: • Y-Z Y:	OK Cancel Apply Help Preview
Workplane (2D geometry): Geom2 💙 🛛 Add	





Symmetry planes, cont'd

 In the 2D geometry tab that appeared, create a square of size 1e-6, centered at the origin:





Symmetry planes, cont'd

- Make sure the square object is selected. Click Embed from the Draw menu. This transfers the flat square object into the 3D geometry tab. This creates a symmetry plane at z=0.
- Open Work-Plane Settings again and create a y-z plane at x=0. This takes you to the 2D geometry tab. Embed the square back into 3D again. This creates a symmetry plane at x=0.
- Open Work-Plane Settings again and create a z-x plane at y=0. This takes you to the 2D geometry tab. Embed the square back into 3D again. This creates a symmetry plane at y=0.
- In 3D geometry tab, select all objects including the symmetry planes, and click Coerce to...Solid from the Draw menu. This converts the flat square objects into interior boundaries inside the spheres, thus splitting them into sectors. These steps will enable us to utilize the symmetry of the problem, and also to use the swept meshing technique.





V. Physics settings

- Subdomain settings
- Boundary settings
- Global expressions
- Integration variables



Subdomain Settings: Taking advantage of the symmetry planes

- Select subdomains 1-24, deselect the checkbox "Active in this domain".
- This disables equations on three quarters of the simulation domain, allowing you to use x=0 and y=0 symmetry planes later on.
- Note that z=0 is not a valid symmetry plane for Mie scattering: wave propagation direction (k=kz) breaks down that geometric symmetry.

Subdomain Settings - Electromagnet	c Waves (rfw)	×
Equation $\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k_0^{-2} (\varepsilon_r - j\sigma/\omega\varepsilon_0) \mathbf{E} = 0, \ \varepsilon_r = 0$	= n ²	
Subdomains Groups Physics Ph	AL Init Element Color	
Subdomain selection Element se	ettings	
21 (air_disabled) Predefine 22 (air_disabled) shape 23 (scatterer_disable) gporder 24 (scatterer_disable) cporder 25 (PML) v 26 (air) v	d elements: Vector - Quadratic v shcurl(2,{'scEx','scEy','scEz'}) shlag(2,'psi') Shape functions 4 4 4 4 2 2 2 2 Constraint order	
Group: PML_disa Select by group Active in this gomain	For your convenience, subdoma group names (air, PML, scattere file; naming groups is not necess	ins are assigned r, etc.) in this model sary for calculations
	OK Cancel Apply Help	



Subdomain Settings: PMLs

• Select subdomains 25,32, activate **PML** of **Spherical** type on them.

Subdomain Settings - Elect	tromagnetic Waves (rfw)		
Equation $\nabla \times (\mu_r^{-1} \nabla \times E) - k_0^2 (\varepsilon_r - j\sigma/\omega e^{-1})$ Subdomains Groups Subdomain selection 27 (air) 28 (scatterer) 29 (scatterer) 30 (air) 31 (air) 32 (PML) Croup: PML Select by group	ϵ_0) E = 0 , $\epsilon_r = n^2$ Physics PML Init Element Type of PML: Absorbing in r direction r_{inner} \times_0 , Y_0 , z_0	t Color Spherical Value/Expression dr_guess_rfw R0_guess_rfw 0 0 0	Unit] m] m] m	Description Width in r direction Inner radius Center point
		ОК Са	ancel	Apply Help





COMSOL

Subdomain Settings: metal domains

• Select subdomains 28,29, click "Load...", load Gold material and apply to these subdomains.

Subdomain Settings - Electromagnetic Waves (rfw)		
Equation		
$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k_0^{-2} (\epsilon_r - j\sigma/\omega\epsilon_0) \mathbf{E} = 0, \ \epsilon_r = n^2$		
Subdomains Groups Physics PML Init Element Color		
Subdomain selection Material properties		
27 (air) Library material: Gold Load		
28 (scatterer) 29 (scatterer) Quantity Value/Expression	Unit	Description
30 (air) O Specify material properties in terms of refractive ind	lex	
31 (air) n 1		Refractive index
Specify material properties in terms of ε_{μ} μ_{μ} and σ		
Group: scatterer 😪 ε _r jcEpsReal(nu_rfw[s])-j*jcEpsImag(n	u_rfw	Relative permittivity
Select by group σ Ο	S/m	Electric conductivity
Active in this domain μ_r 1		Relative permeability
ОК	Cancel	Apply Help

Boundary Settings: symmetry planes

Boundary Settings - Electromagne	etic Waves (rfw)		×		
Equation					
$\mathbf{n} \times \mathbf{E} = 0$					
Boundaries Groups Conditio	ns Material Properties Port F.	ar-Field Color			
Boundary selection Bound	lary sources and constraints				
62 (PEC) A	Boundary condition. Perfect ele	ctric conductor 🛛 👻			
64 (continuity) 65 (PEC)					
66 (PMC) 67 (continuity)	Boundary Settings - Electi	romagnetic Waves	rfw)		
68 (PEC)	Equation				
69 (PMC) 70 (continuity)	n × H = 0				
71 (PEC) 72 (PMC)	Boundaries Groups	Conditions Material P	operties Port Far-Field Color		
73 (Efar) 74 (PEC)	Boundary selection	Boundary sources an	d constraints		
75 (PMC)	55 (outerPML)	Boundary con	Perfect magnetic conductor		
77 (outerPML)	56 (PEC) 57 (PMC)				
Group: PEC	58 (innerPML) 59 (PEC)		Select bour	daries 53, 56,	59, 62, 65, 68, 71, 74,
Select by group	60 (PMC) 61 (Efar)		and apply F	oundary condi	tion: Perfect electric
Interior boundaries	62 (PEC) 63 (PMC)		conductor.	These boundar	ries are perpendicular to
	64 (continuity)		the electric	field	
	66 (PMC)		Soloot bour	darias 51 57	60 62 66 60 72 75
	68 (PEC)			dony condition	Dorfoot magnetic
	69 (PMC)		apply boun	uary conullion. Those houndar	rice are orthogonal to the
	Group: PMC 💌		mognotic fi		nes are unnuyunar tu the
	Select by group		magnetic lie	HU.	
	Interior boundaries				
			ОК	Cancel Apply Help	COMSOL

Boundary Settings: exterior boundaries

• Select boundaries 55,77, apply Scattering Boundary condition, Wave type: Spherical wave.

Boundary Settings - Elect	romagnetic Waves (rfw)	X
Equation		
$\mathbf{n} \times (\nabla \times \mathbf{scE}) \cdot (\mathbf{jk} + 1/\mathbf{r})\mathbf{n} \times \mathbf{scE}$	$(\mathbf{scE} \times \mathbf{n}) = 0$	
Boundaries Groups	Conditions Material Properties Port Far-Field Color	
Boundary selection	Boundary sources and constraints	
53 (PEC)	Boundary condition: Scattering boundary condition	
54 (PMC)	Wave type:	
55 (outerPML) 56 (PEC)	Spherical Wave	
57 (PMC)		
58 (innerPML)		
59 (PEC)		
61 (Efar)		
62 (PEC)		
63 (PMC)		
64 (continuity)		
66 (PMC)		
67 (continuity)		
68 (PEC)		
Group: OuterPML 🚩		
Select by group		
Interior boundaries		
	OK Cancel Apply Hel	2



Boundary Settings: Far-Field variables

• Select boundaries 61,73, select "Interior boundaries", go to Far-Field tab, type "Efar" in the Name column. Check x=0 and y=0 boxes below.

Boundary Settings - E	Electromagnetic Waves (rfw)	×
Equation		
	×/F = F) = 0	
$n \wedge (n_1 - n_2) = 0, n \wedge (n_1 - n_2)$	$(c_1 - c_2) = 0$	
Boundaries Groups	Conditions Material Properties Port Far-Field Color	
Boundary selection	Far-field settings	
59 (PEC)	Name Field Normal derivative	
60 (PMC)		
61 (Efar)		
62 (PEC)		
63 (PMC)		
64 (continuity)		
66 (PEC)		
67 (continuity)		
68 (PEC)		
69 (PMC)	Symmetry planes:	
70 (continuity)		
71 (PEC)	Symmetric H field (PEC)	
72 (PMC)	y=0 Symmetric E field (PMC)	
73 (Efar)		
74 (PEC) 💌	Y Z=0 Symmetric E field (PMC) Y	
	For each name above, COMSOL Multiphysics generates three	
Group: Efar 🛛 🗸	 variables for the vector components of the far electric Sidd. For Contraction derivation accordance the variables 	
Select by group	are generally called 'pamex', 'pamey', and 'pamez'.	
C Soloce S) group	and for axisymmetric geometries 'namer', 'namephi',	
Interior boundaries	and 'namez'.	
		ieih



Global Expressions

In options, open Expressions, Global Expressions, and fill out the following table:

Name	Expression	Unit	Description	
ofact	if(nx*x+ny*y+nz*z>=0,1,-1)		Sign factor for outward normals on interior boundaries	~
onx	nx*ofact	1	Outward normal on interior boundaries, x-component	
ony	ny*ofact	1	Outward normal on interior boundaries, y-component	
onz	nz*ofact	1	Outward normal on interior boundaries, z-component	
PO	0.5*E0^2*c0_rfw*epsilon0_rfw	W/m ²	Incident flux	
scPoxav	0.5*real(scEy*conj(scHz)-scEz*conj(scHy))	W/m ²	Scattered flux, x-component	
scPoyav	0.5*real(scEz*conj(scHx)-scEx*conj(scHz))	W/m ²	Scattered flux, y-component	
scPozav	0.5*real(scEx*conj(scHy)-scEy*conj(scHx))	W/m ²	Scattered flux, z-component	=
nscPoav	onx*scPoxav+ony*scPoyav+onz*scPozav	W/m ²	Scattered normal flux	
nPoav	onx*Poxav_rfw+ony*Poyav_rfw+onz*Pozav_rfw	W/m ²	Total normal flux on interior boundaries	
	sqrt(x^2+y^2+z^2)	m	Radius-vector	
dsigma_near	nscPoav/P0*r^2	m ²	Differential scattering cross-section, near-field definition	
dsigma_far	(normEfar^2/(r/1[m])^2)/abs(E0)^2*r^2	m ²	Differential scattering cross-section, far-field definition	
sigma_ext_near	sigma_near+sigma_abs	[]	Total extinction cross-section, near-field calculation	
sigma_scat_OT	sigma_ext_OT-sigma_abs	[]	Total scattering cross-section, Optical Theorem calculation	
			OK Cancel Apply Help	

You should also **Export Variables To File**, so that you can load these definitions in your next model of radiation scattering.



Subdomain Integration Variables

On subdomains 28,29 define the following integration variable:

s	ubdomain Integrati	ion Va	ariables			$\overline{\mathbf{X}}$
	Source Destination					
	Subdomain selection		Name	Expression	Integration order	Global destination
	23		sigma_abs	4*Qav_rfw/P0	2	
	24					
	25					
	27					
	28					
	29					
	30	Ξ				
	31					
	32					
	Select by group					
					OK Cancel	Apply Help



Boundary Integration Variables

On boundaries 61,73 define the following integration variables:

i	Boundary Integration Va	riables]		
	Source Destination								
	Boundary selection	Name	•	Expression	Integration order	Global destii			
	61	sigma_	near	4*nscPoav/P0	4	A A A A A			
	62	sigma_	far	4*normEfar^2/E0^2	4				
	63	sigma_	_abs_flux	-4*nPoav/P0	4				
	64								
	65								
	66		aiama	noor: Total	anottoring CC	from no	or fic		
	67		sigma	_near. rotai	scallening US	nom nea	ar ne	las	
	68		siama	far. Total se	cattering CS fr	om far fi	shle		
	69 💻		- Sigina						
	70 71		sigma	_abs_flux: A	bsorption CS	from ene	rgy o	conservation	ן ר
	Select by group								
	OK Cancel Apply Help								

Note: variable sigma_far involves surface integration of a far-field variable, normEfar, which itself requires taking a surface integral every time it is evaluated. Calculating the total scattering cross-section in this way is extremely inefficient; see the next slide for a more efficient technique.

Point Integration Variables

On point 16, define the following variables:

Point Integration Va	riables			
Source Destination				
Point selection 9 10 11 12 13 14 15 16	Name sigma_ext_OT f_forward sigma_forward	Expression -4*pi/k0_rfw*imag(Efarx*1[m])/E0 Efarx*1[m]/E0 dsigma_far	Global destination	
17 18 Select by group		OK Cancel		▼ Help

* The variable sigma_ext_OT represents the total extinction cross-section,

calculated through the imaginary part of forward-scattering CS using the Optical Theorem (OT).

* Note: Far-Field variables such as Efarx are measured in units V/m*m=V

and they actually represent the scattering amplitude rather than physical electric field.





Point Integration Variables, cont'd

On point 10, define the variable sigma_back for back-scattering cross-section, i.e. differential scattering cross-section in the direction opposite to wave incidence.

Note: the standard Radar Cross Section is related to this variable as follows: RCS=(4*pi)*sigma_back.

Point Integration Variables					
Source Destination					
Point selection					
	Name	Expression	Global destination		
6	sigma_ext_OT			<u>~</u>	
7	f_forward				
8	sigma_forward				
9	sigma_back	dsigma_far			
10					
12					
13					
14					
15					
Select by group					
				✓	
OK Cancel Apply Help					





VI. Mesh generation

• To facilitate mesh visualization, suppress subdomains 1-24 (use menu Options, Suppress). Equations on these subdomains are not active, and meshing them is unnecessary.







Mesh generation, cont'd

• In Free Mesh Parameters, constrain mesh element size to 0.2e-6/5.

Free Mesh Parameters	
Global Subdomain Boundary Edge Point Advanced Predefined mesh sizes: Normal Custom mesh size Maximum element size: 0.2e-6/5 Maximum element size scaling factor: Element growth rate: 1.5 Mesh curvature factor: 0.6 Mesh curvature cutoff: 0.03 Resolution of narrow regions: 0.5 Coptimize quality Refinement method: Longest	OK Cancel Apply Help
Reset to Defaults Remesh Mesh Selected	



Mesh generation, cont'd

• On Subdomain tab, select subdomains 26-31. Click Mesh Selected.

Free Mesh Parameters		
Free Mesh Parameters	y Edge Point Advanced Subdomain mesh parameters Maximum element size: Element growth rate:	OK Cancel Apply Help
Select Remaining Select Meshed		
Reset to Defaults	Remesh Mesh Selected	J







Mesh generation, PMLs

• In Swept Mesh parameters, select subdomains 25,32, and manually specify 5 element layers. Click Mesh Selected.

Swept Mesh Parameters	
Swept Mesh Parameters Predefined mesh sizes: Normal Subdomain selection Element Layers Sweep Direction Advanced 20 20 20 21 22 23 24 25 26 27 28 29 30 31 32 Select Remaining Function Support of the stribution selection Select Remaining	OK Cancel Apply Help
Reset to Defaults Remesh Mesh Selected	





VII. Computing the solution: Solver settings

Solver Parameters	
Analysis types	General Parametric Stationary Adaptive Optimization/Sensitivity Advanced Parameters Parameter Parameter Image(2.0e-7,1.0e-8,1.0e-6) Edit Parameter values: range(2.0e-7,1.0e-8,1.0e-6) Edit Linear system solver Linear system solver Linear system solver Image(2.0e-7,1.0e-8,1.0e-6) Preconditioner: Settings
Plot while solving	Adjust Solver Parameters as shown. Click OK and then click Solve (= button)

1

VIII. Postprocessing and visualization

• Modify the default Slice Plot to show three specific cross-sections on the simulation domain:

Plot Parameters	
Principal Streamlic General Slice	e Particle Tracing Max/Min Deform Animate osurface Subdomain Boundary Edge Arrow
Slice plot	
Slice data	
Predefined quantities:	Scattered electric field, x compon Range
Expression:	scEx Smooth
Unit:	V/m Recover
Slice positioning	
Number	of levels Vector with coordinates
x levels: 🔘 1	● 1e-9 Edit
y levels: 🔘 1	• 1e-9 Edit
z levels: 🔘 1	• -1e-9 Edit
Coloring and fill	
Coloring: Interp	olated 👻 Fill style: Filled 💌
Slice color	
⊙ Color table:	Rainbow 🔽 🗌 Reverse 🔽 Color legend
O Uniform color:	Color
	OK Cancel Apply Help



Evaluating and plotting cross-sections

Global Variables Plot					
Predefined quantities	Quantities to plot				
Sign factor for outward norm	sigma_abs sigma_abs_flux sigma_ext_near sigma_ext_OT sigma_near sigma_scat_OT				
Expression:					
sigma_scat_OT >					
Solutions to use	x-axis data				
Select via:	 Auto 				
2e-7	O Expression				
2.1e-7 💻					
2.2e-7	Line Settings				
2.3e-7	Title/Axis				
2.5e-7	Plot in: New figure V				
2.6e-7 🗸 🗸					
Timer					
Solution at angle (phase): 0 degrees					
ОК	Cancel Apply Help				

- Create a Global Variables Plot with the following expressions:
- sigma_abs
- sigma_abs_flux
- sigma_ext_near
- sigma_ext_OT
- sigma_near
- sigma_scat_OT



• This creates a plot of three distinct cross-sections calculated by two different methods each. Cross-sections are measured in m^2.





Radar Cross-Section

 Plot 4*pi*sigma_back in the Global Variables Plot to obtain the standard RCS (in m² units):



