# Mie scattering off plasmonic nanoparticle

Model documentation

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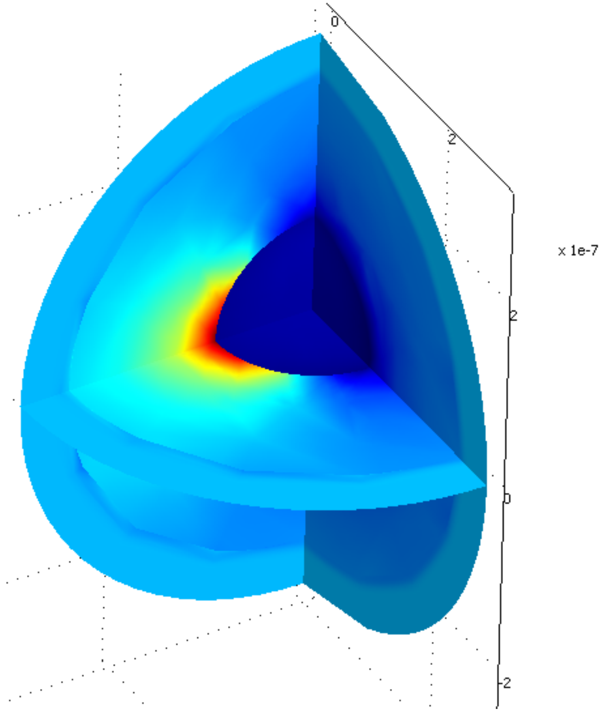
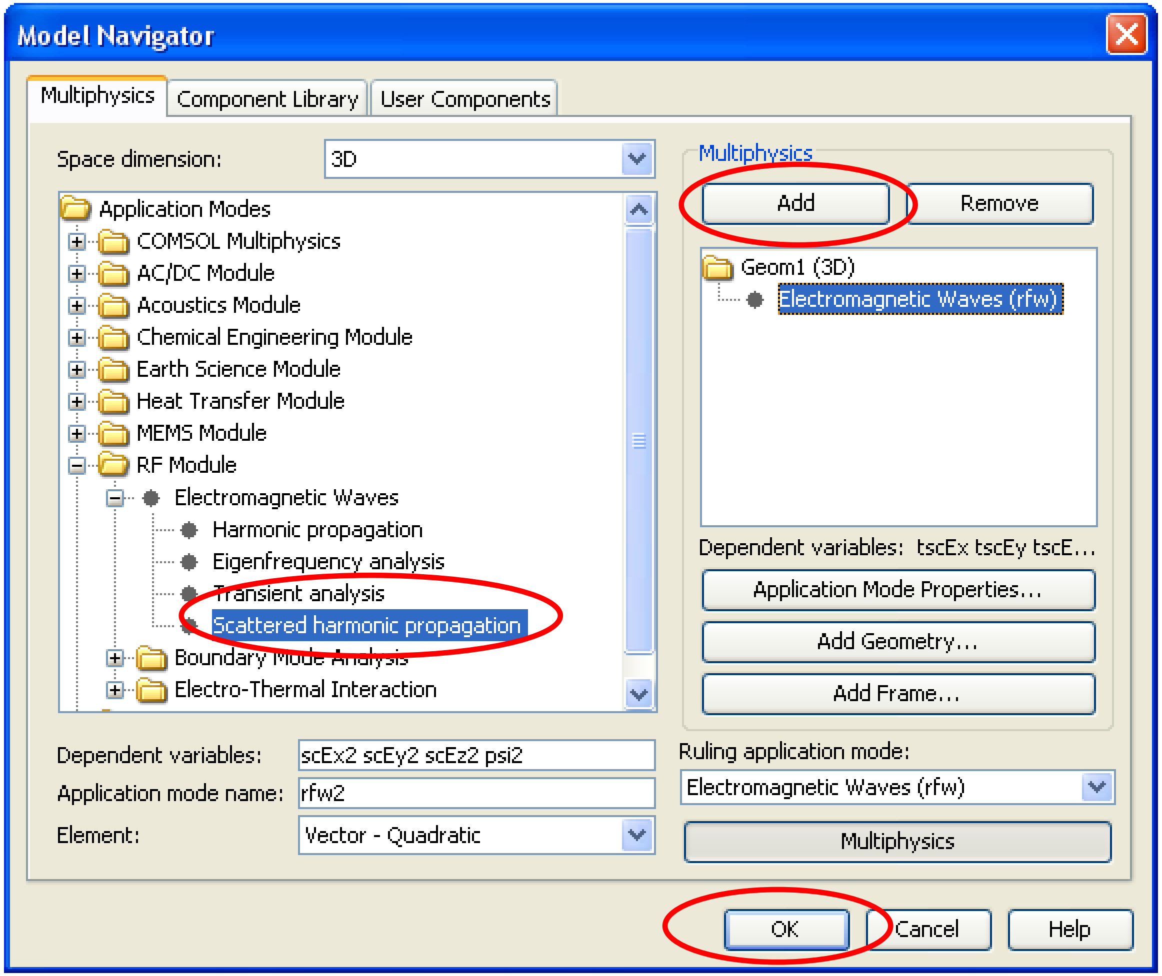
# Contents

# 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.

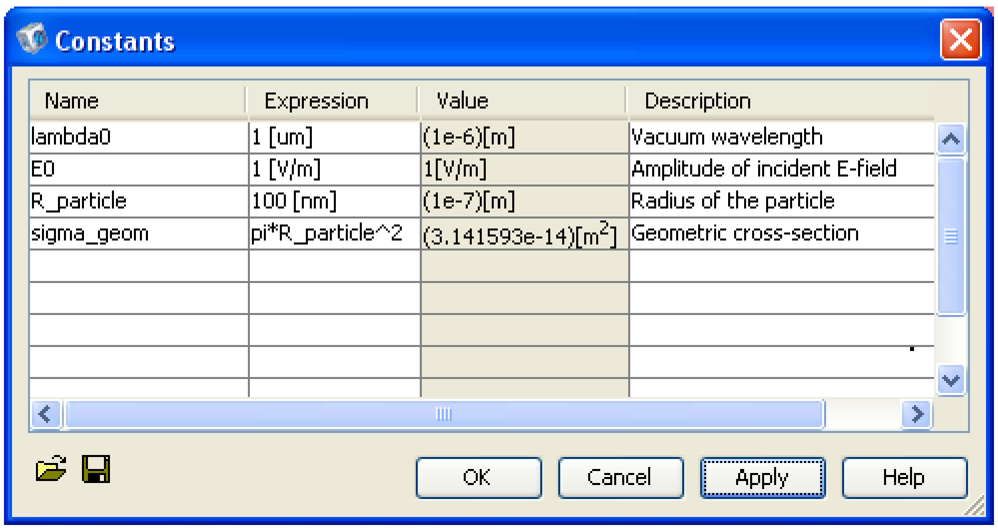


# II. Modeling in the Graphical User Interface: Model Navigator



# 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:




| Name | Expression | Value | Description |
|---|---|---|---|
| lambda0 | 1 [um] | (1e-6)[m] | Vacuum wavelength |
| E0 | 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 |

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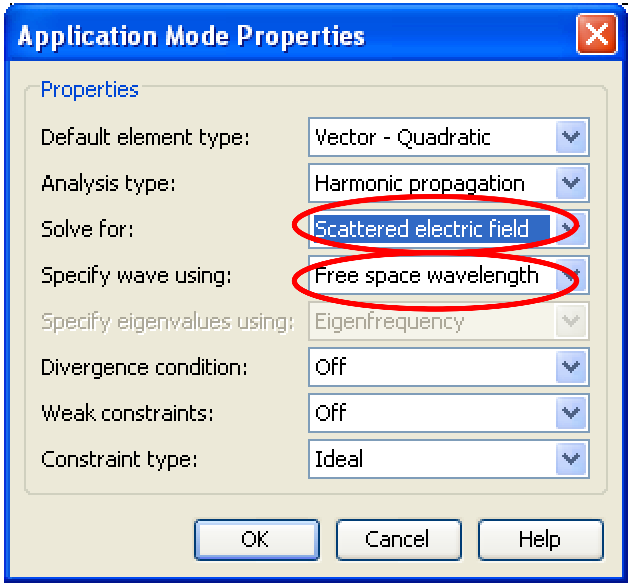
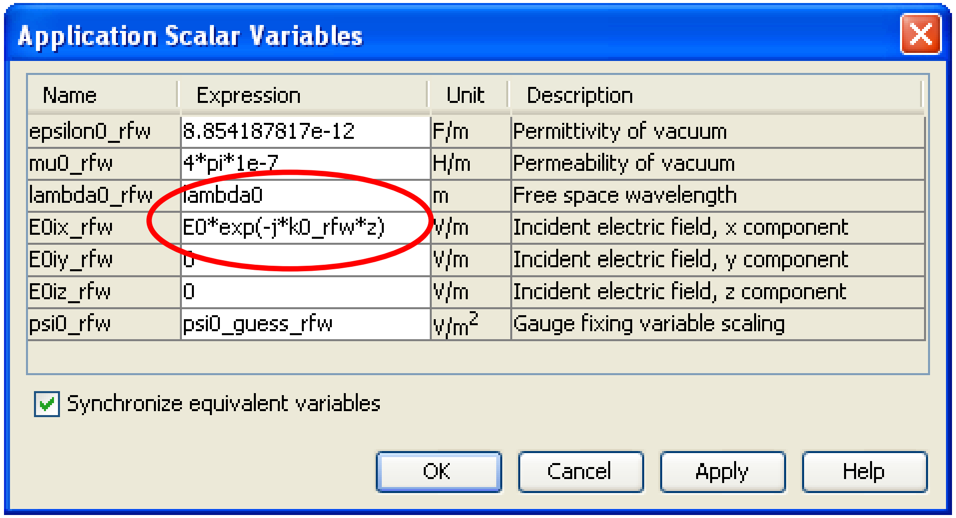
# Options and settings: Application Mode Properties

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



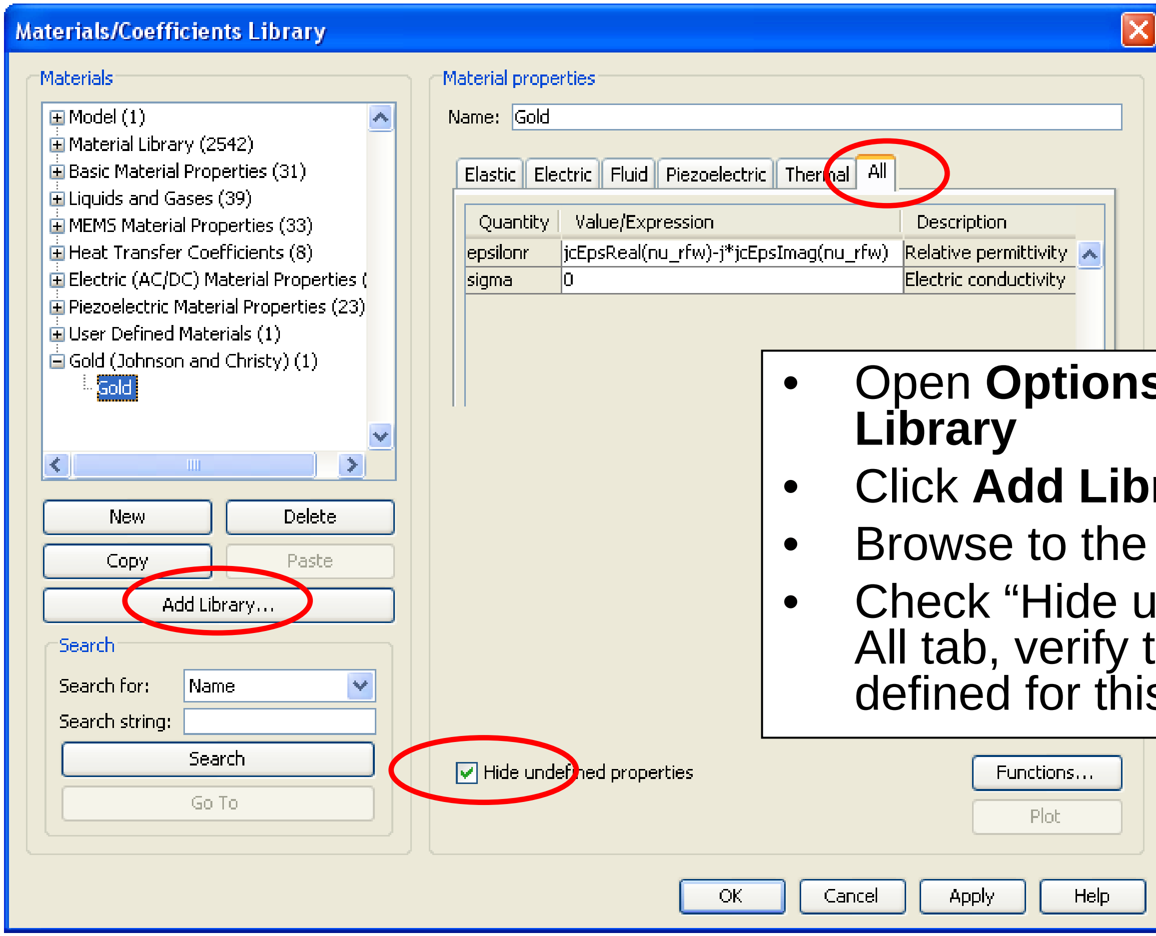
# Options and settings: Application Scalar Variables

- 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.




| 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 | E0*exp(-j*k0_rfw*z) | V/m | Incident electric field, x component |
| E0iy_rfw | 0 | 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 |

# Options and settings: Materials Library




- Open **Options>Materials/Coefficients Library**
- Click **Add Library…**
- Browse to the file gold_lib.xml, click OK
- Check “Hide undefined properties”, go to All tab, verify that Relative permittivity is defined for this material.

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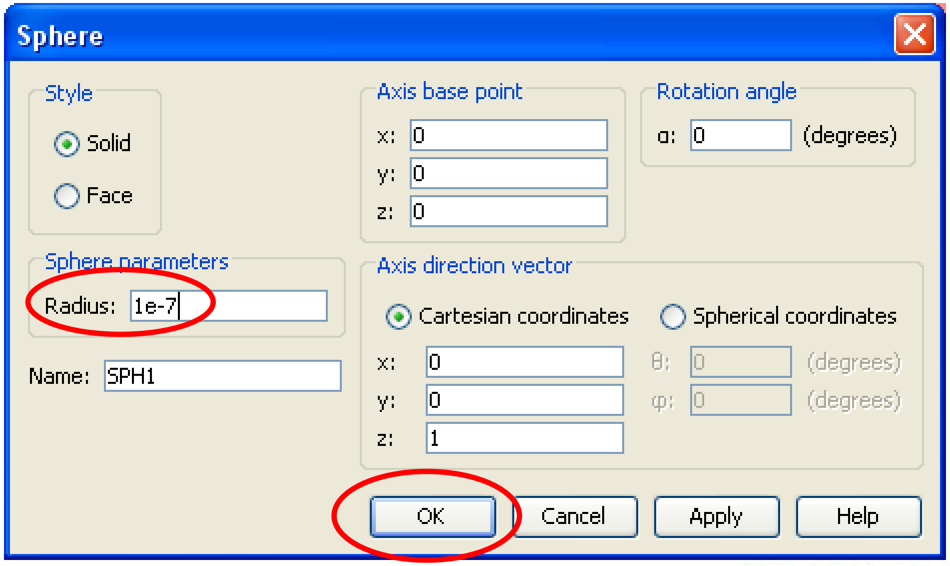
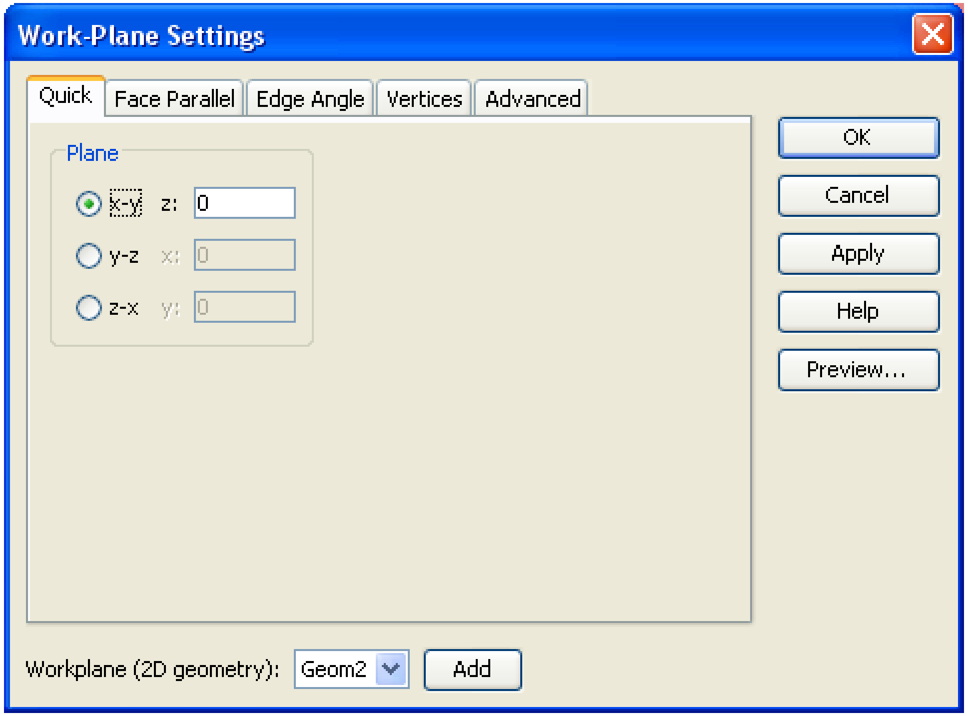
# IV. Geometry modeling

- 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.



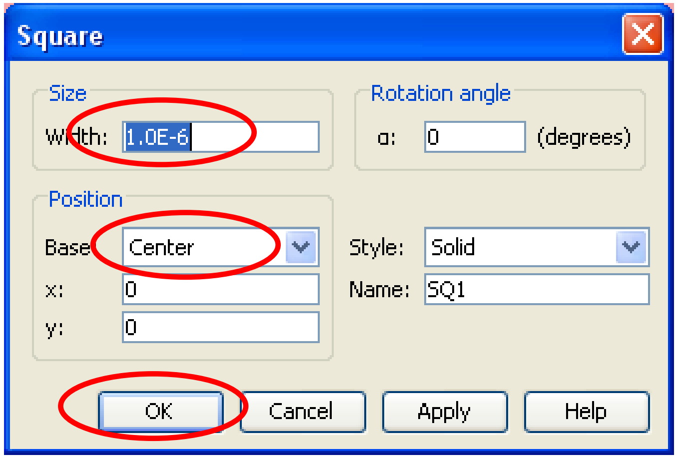
# Geometry modeling: create symmetry planes

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



# 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

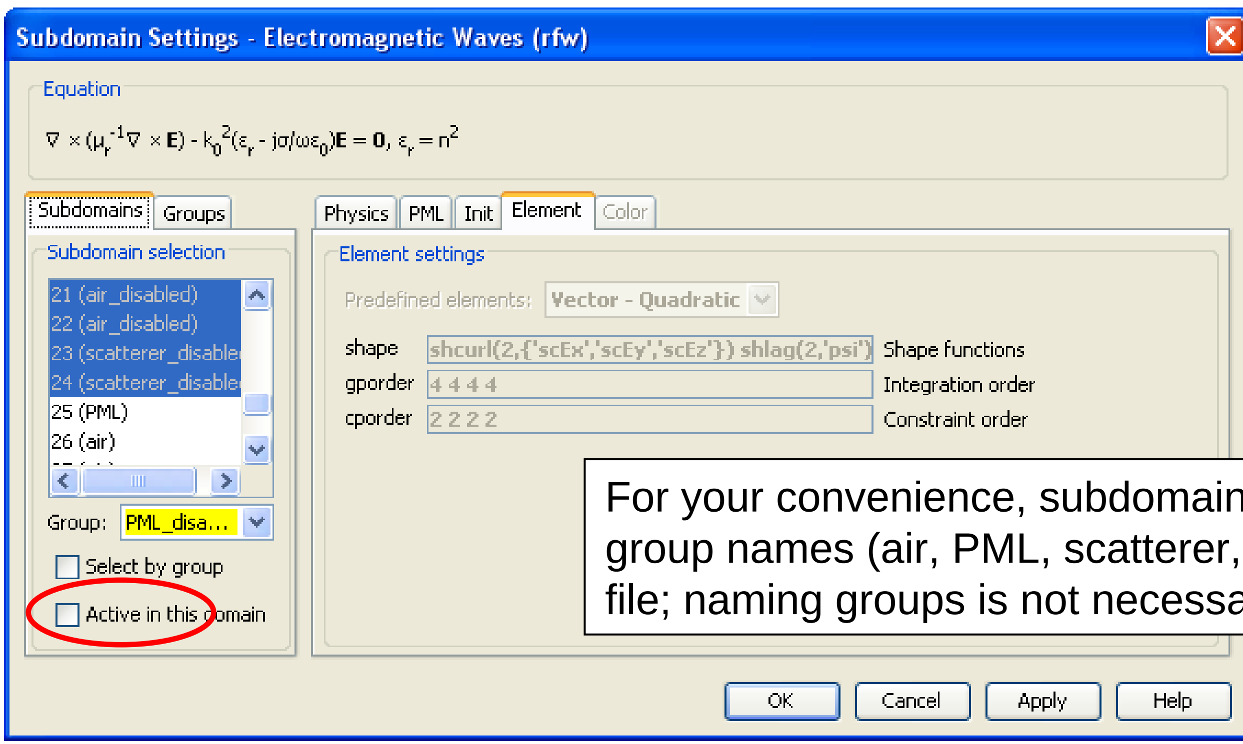
- Make sure the square object is selected. Click **Embed** from the **Draw** menu. This transfers the flat square object into the 3D geometry tab. This creates a symmetry plane at z=0.
- Open **Work-Plane Settings** again and create a y-z plane at x=0. This takes you to the 2D geometry tab. Embed the 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

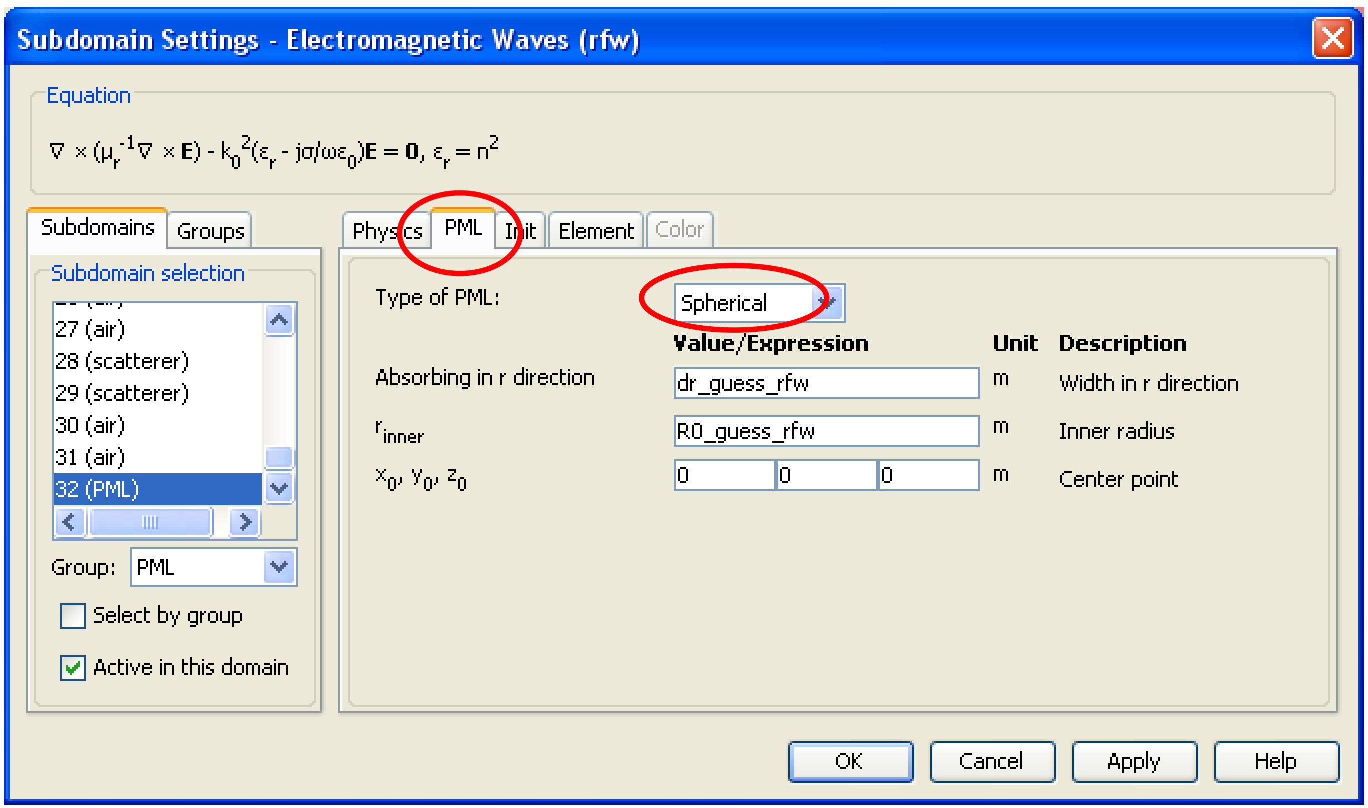
- Select subdomains 1-24, deselect the checkbox "**Active in this domain**".
- This disables equations on three quarters of the simulation domain, allowing you to use x=0 and y=0 symmetry planes later on.
- Note that z=0 is not a valid symmetry plane for Mie scattering: wave propagation direction (k=kz)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




For your convenience, subdomains are assigned group names (air, PML, scatterer, etc.) in this model file; naming groups is not necessary for calculations.

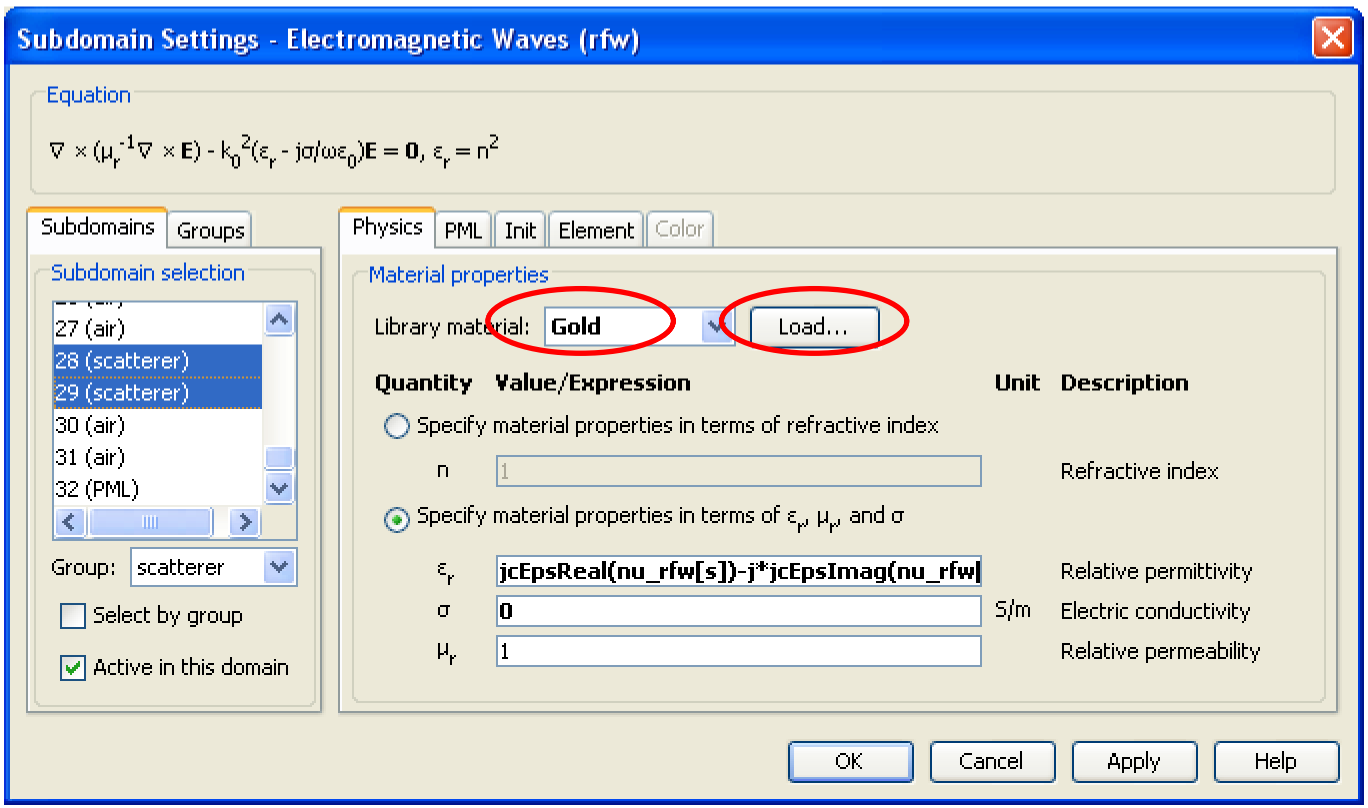
# Subdomain Settings: PMLs

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

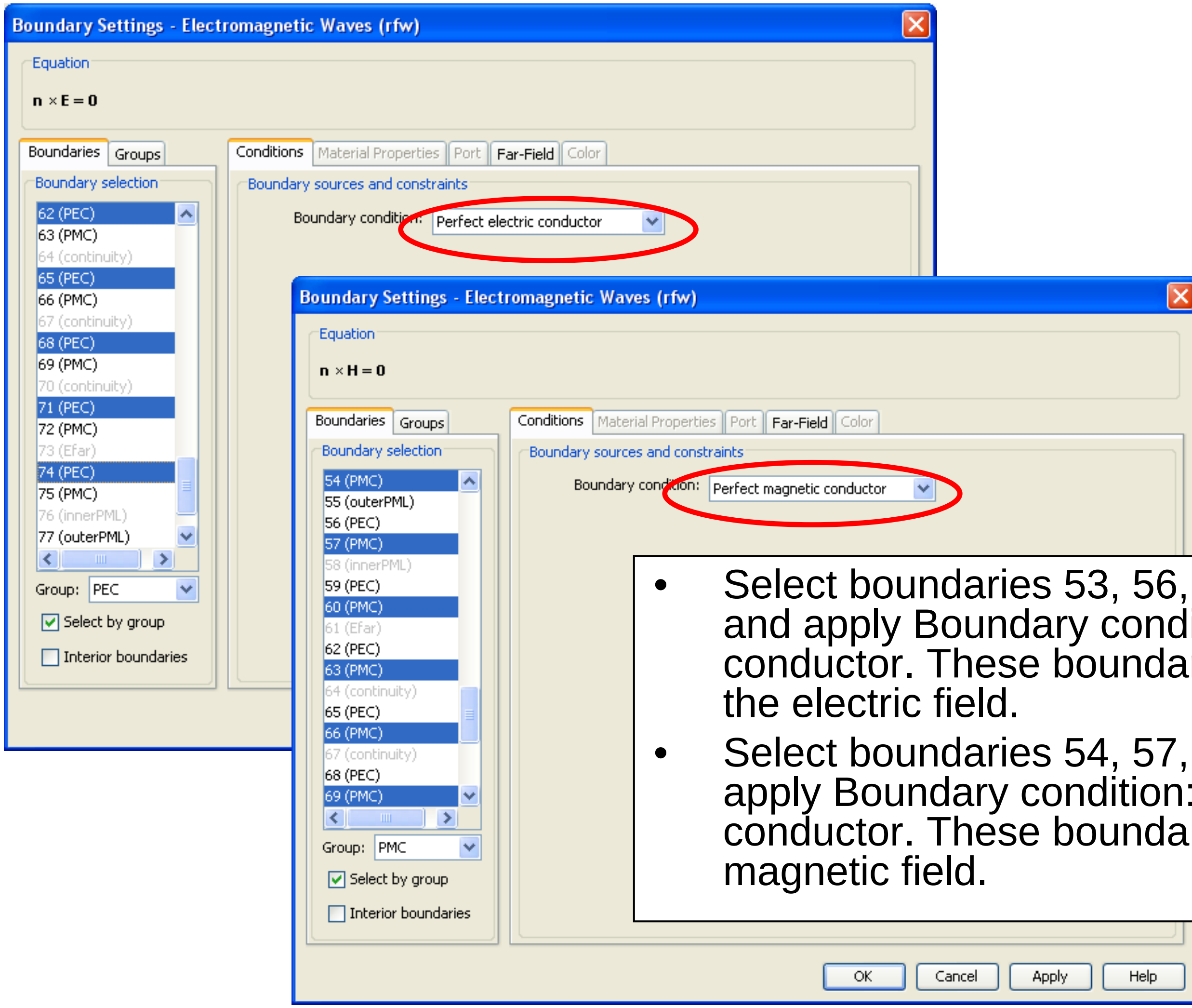


# Subdomain Settings: metal domains

- Select subdomains 28,29, click “**Load…**”, load Gold material and apply to these subdomains.



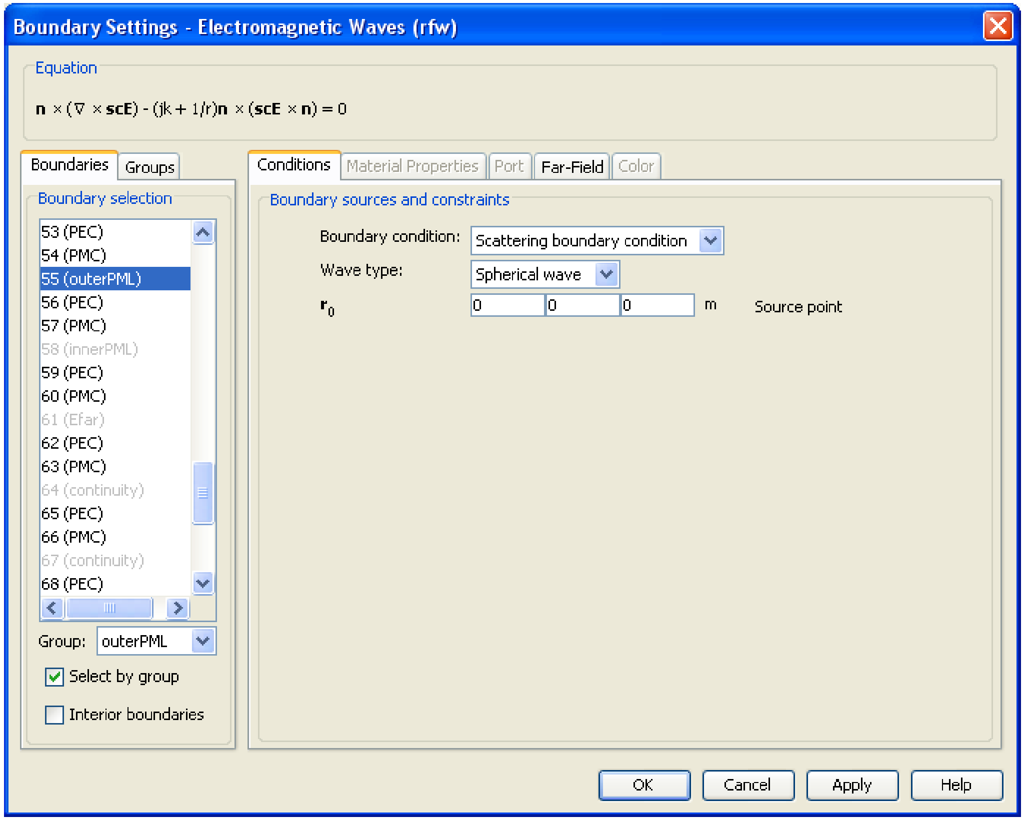
# Boundary Settings: symmetry planes




- Select boundaries 53, 56, 59, 62, 65, 68, 71, 74, and apply Boundary condition: Perfect electric conductor. These boundaries are perpendicular to the electric field.
- Select boundaries 54, 57, 60, 63, 66, 69, 72, 75, apply Boundary condition: Perfect magnetic conductor. These boundaries are orthogonal to the magnetic field.

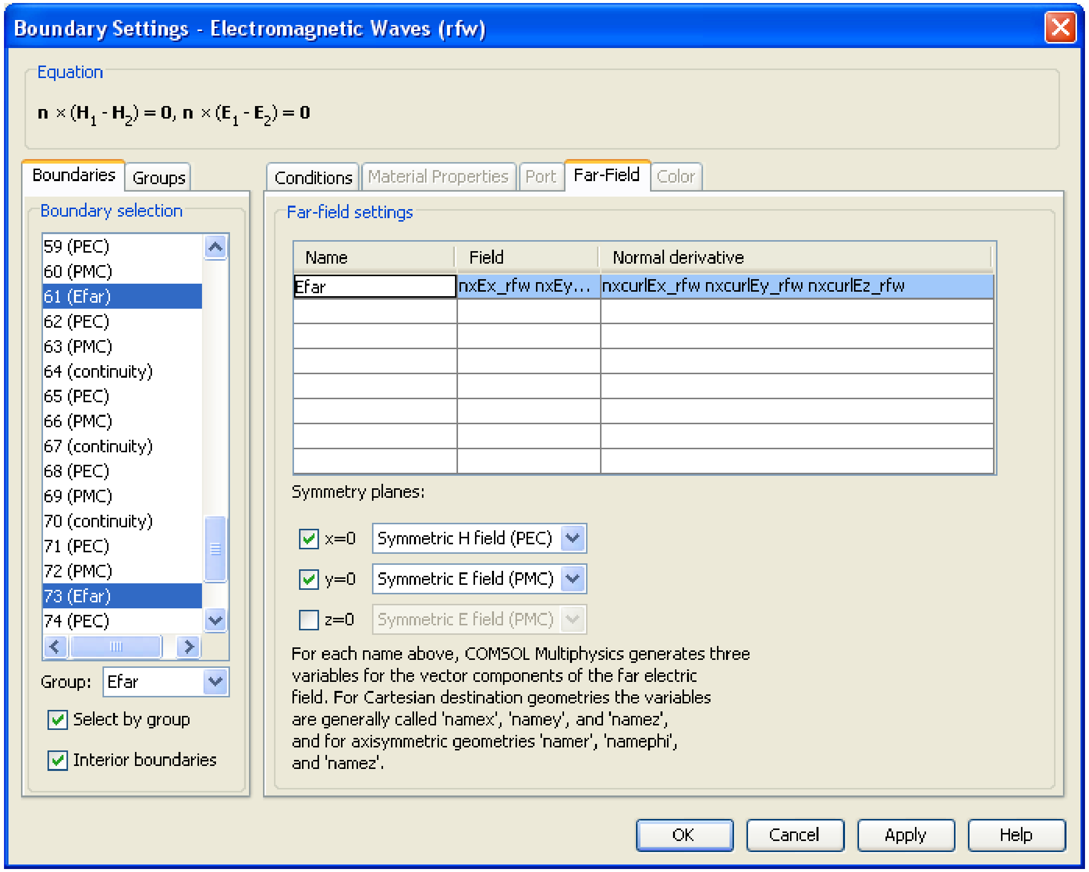
# Boundary Settings: exterior boundaries

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



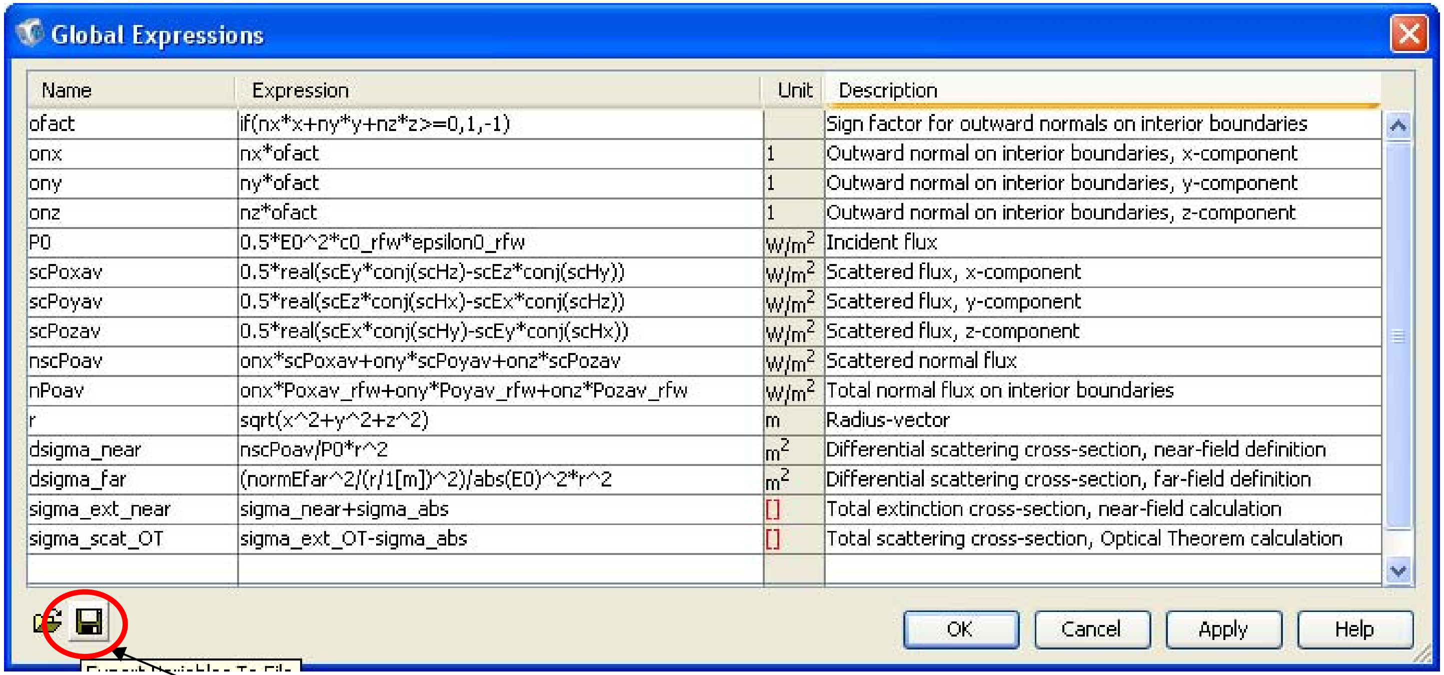
# Boundary Settings: Far-Field variables

- 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.



# Global Expressions

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



Global Expressions

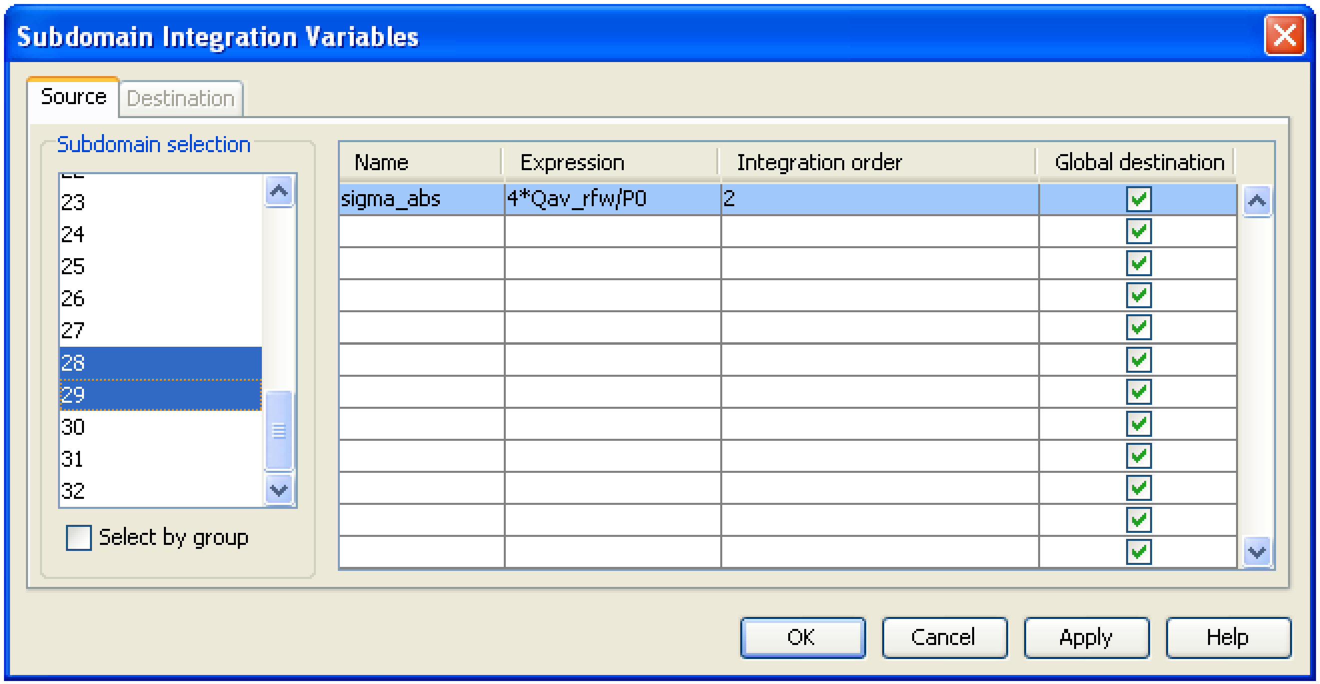
| Name | Expression | Unit | Description |
|---|---|---|---|
| ofact | if(nx*x+ny*y+nz*z>=0,1,-1) | | Sign factor for outward normals on interior boundaries |
| onx | nx*ofact | 1 | Outward normal on interior boundaries, x-component |
| ony | ny*ofact | 1 | Outward normal on interior boundaries, y-component |
| onz | nz*ofact | 1 | Outward normal on interior boundaries, z-component |
| P0 | 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 |
| r | 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 |



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

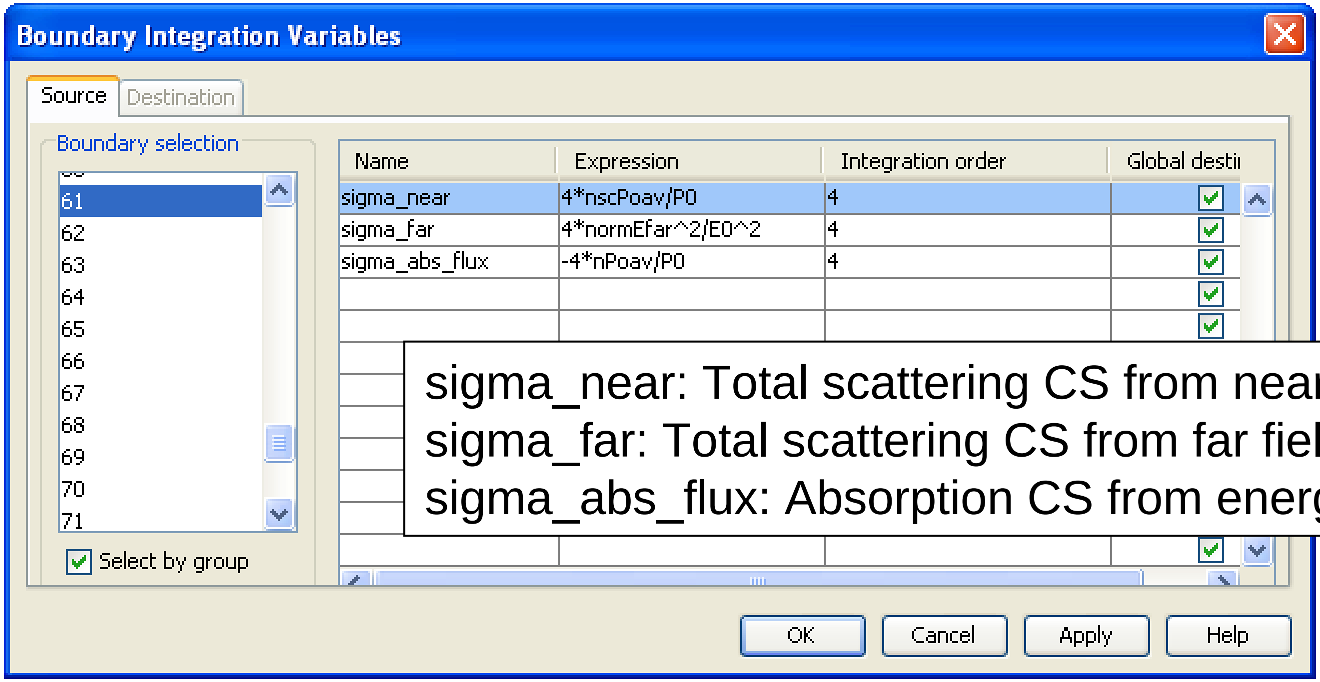
# Subdomain Integration Variables

On subdomains 28,29 define the following integration variable:



# Boundary Integration Variables

On boundaries 61,73 define the following integration variables:

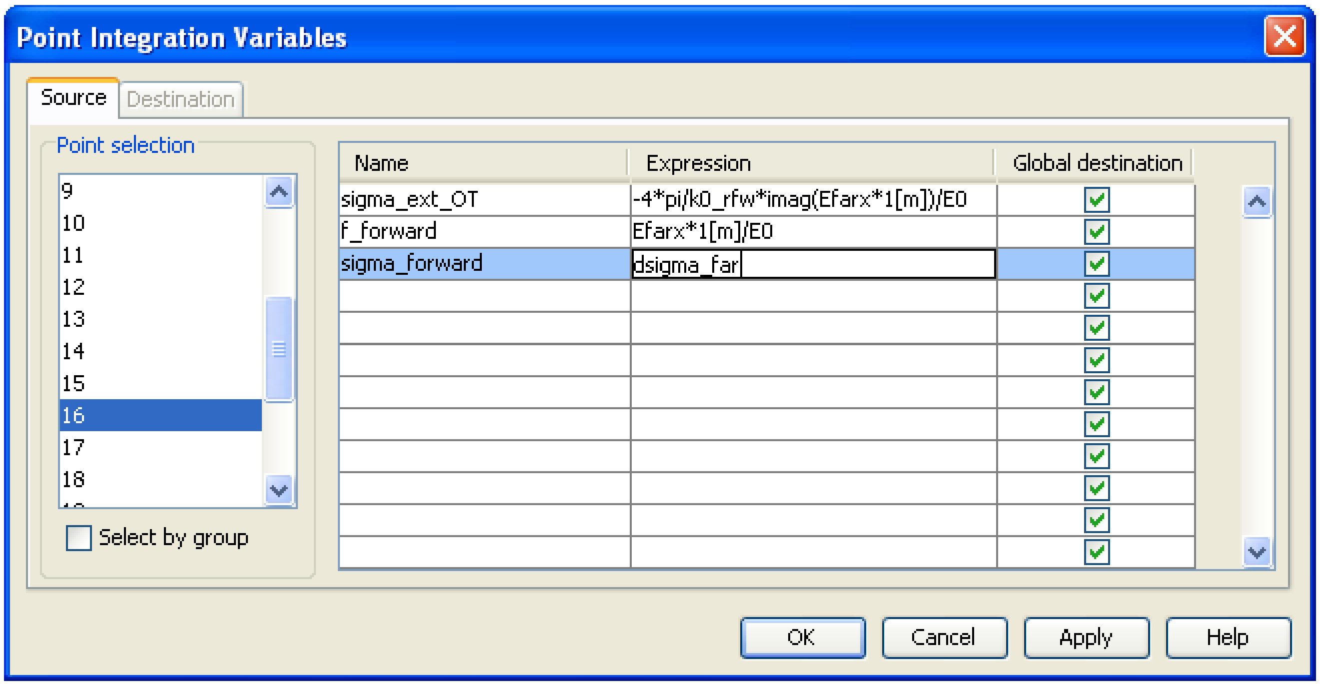



sigma_near: Total scattering CS from near fields
sigma_far: Total scattering CS from far fields
sigma_abs_flux: Absorption CS from energy conservation

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:

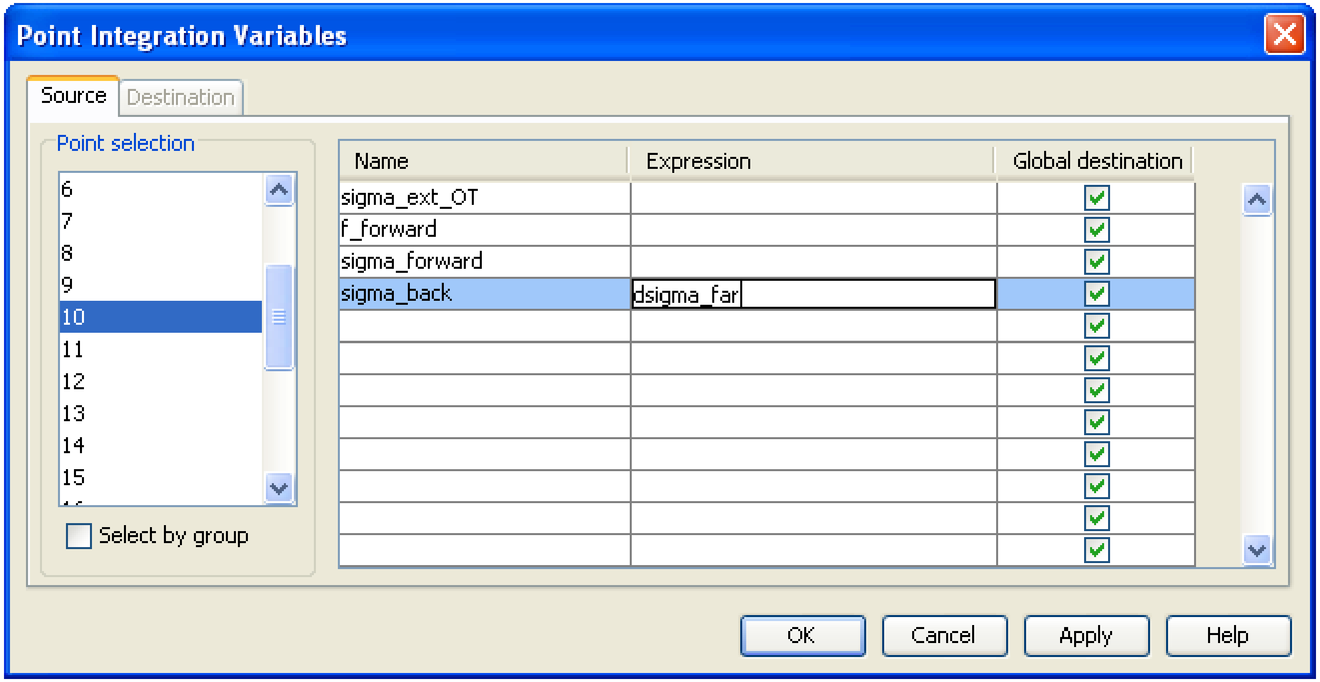



* The variable sigma_ext_OT represents the total extinction cross-section, calculated through the imaginary part of forward-scattering CS using the Optical Theorem (OT).
* Note: Far-Field variables such as Efarx are measured in units V/m*m=V and they actually represent the scattering amplitude rather than physical electric field.

# Point Integration Variables, cont'd

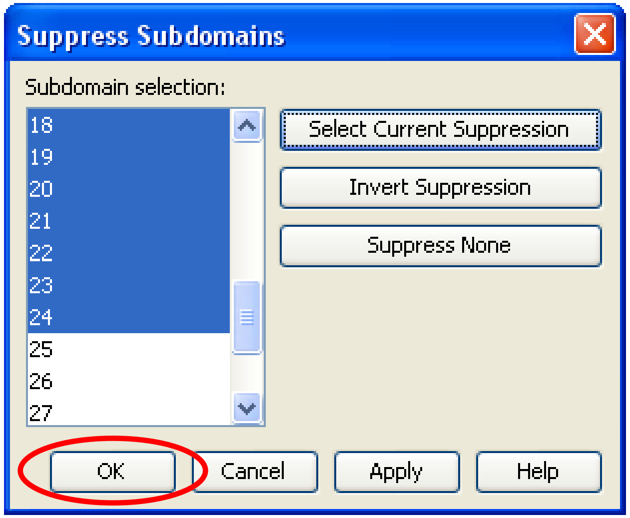
On point 10, define the variable sigma_back for back-scattering cross-section, i.e. differential scattering cross-section in the direction opposite to wave incidence.

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



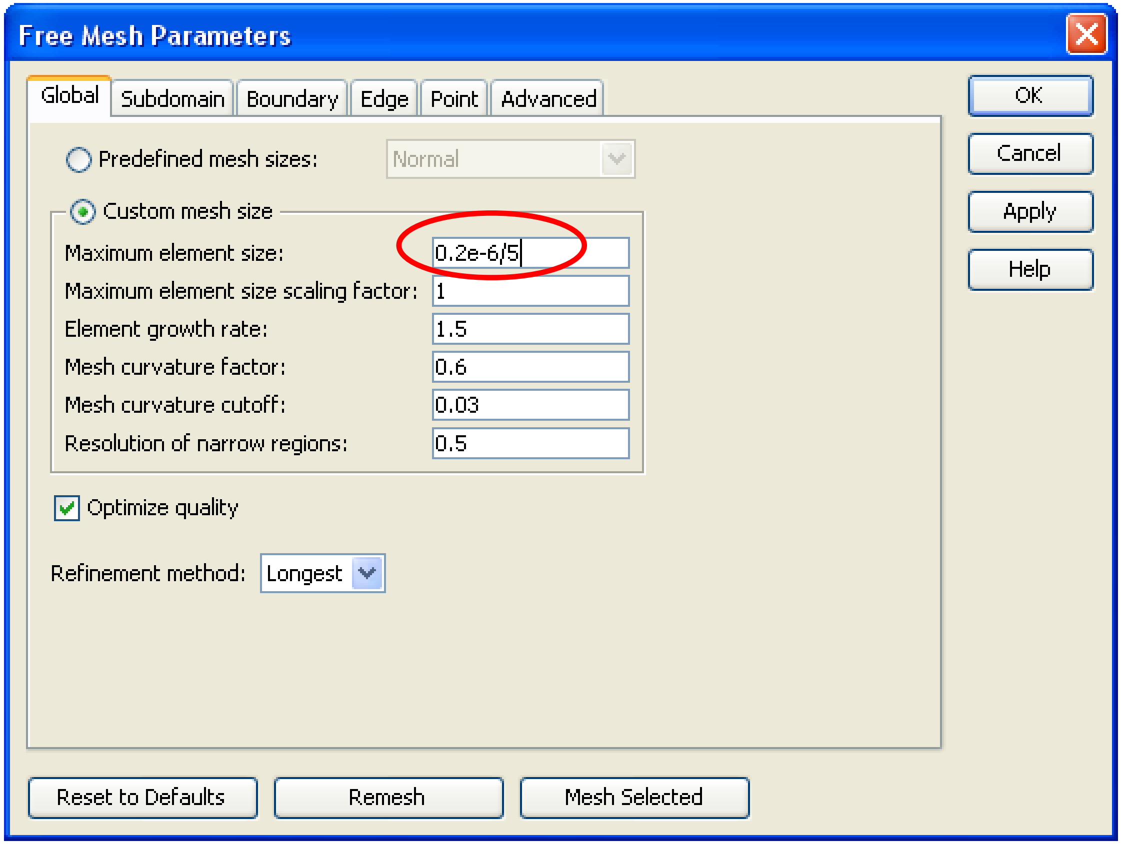
# VI. Mesh generation

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



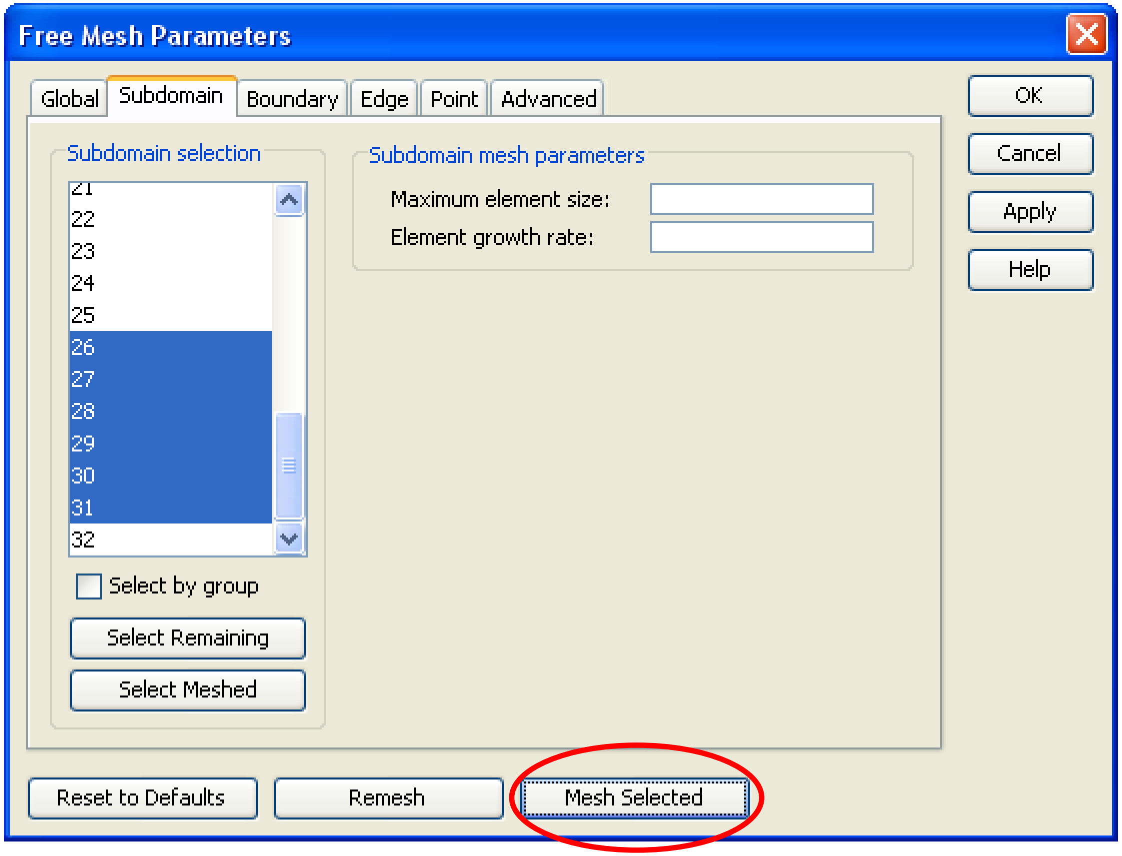
# Mesh generation, cont'd

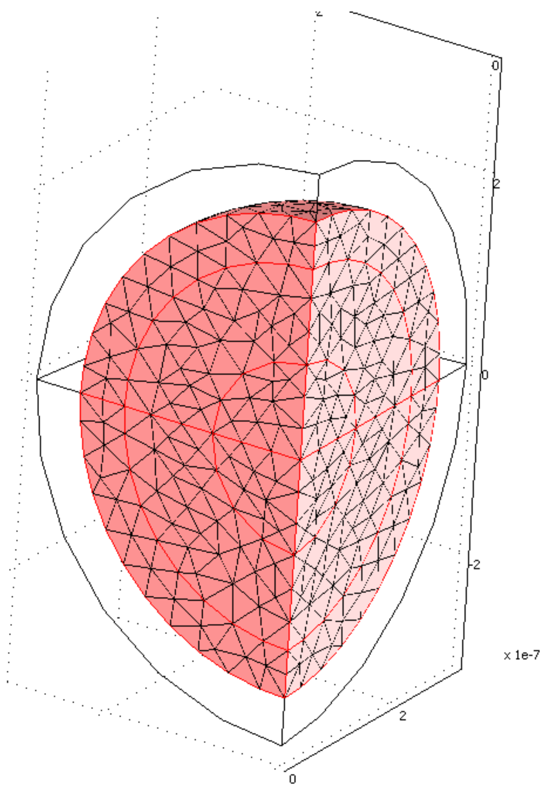
- In Free Mesh Parameters, constrain mesh element size to 0.2e-6/5.



# Mesh generation, cont'd

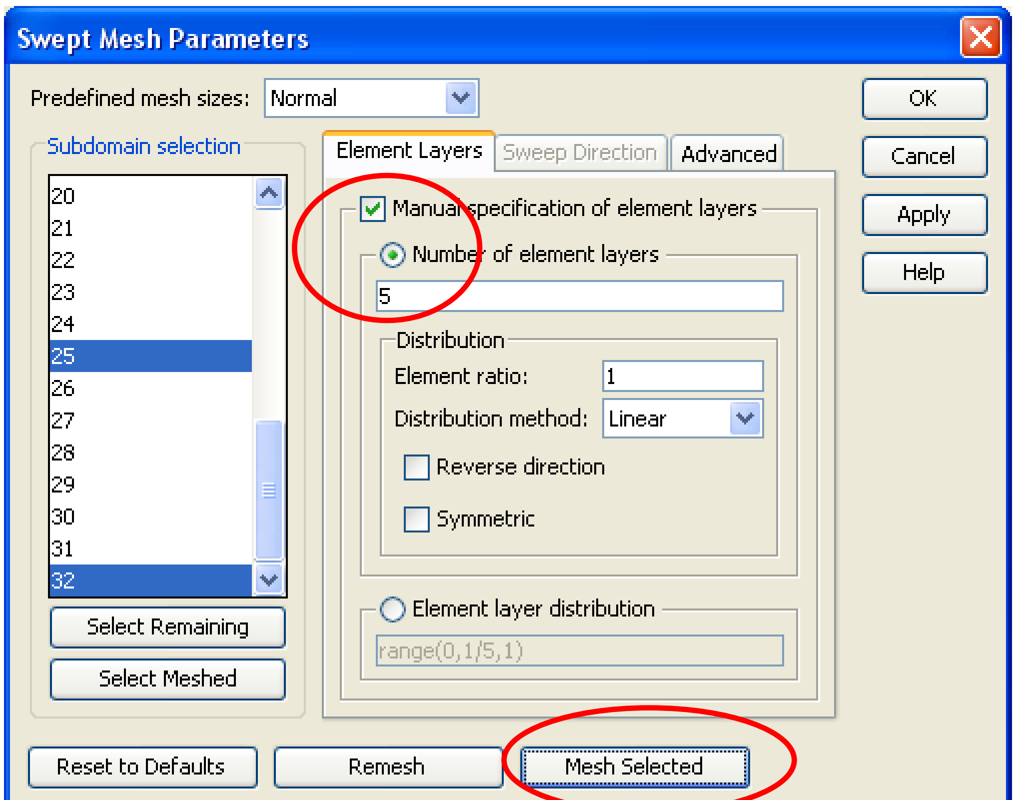
- On Subdomain tab, select subdomains 26-31. Click Mesh Selected.

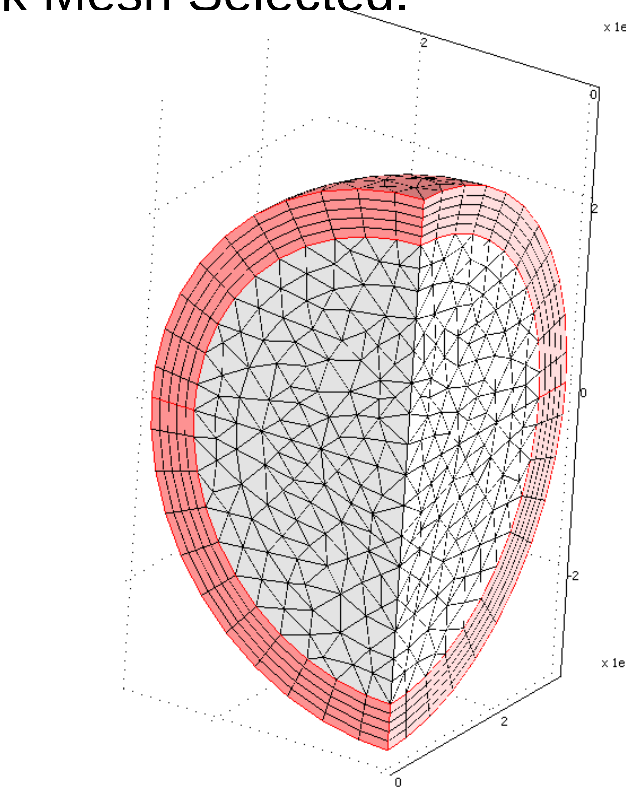


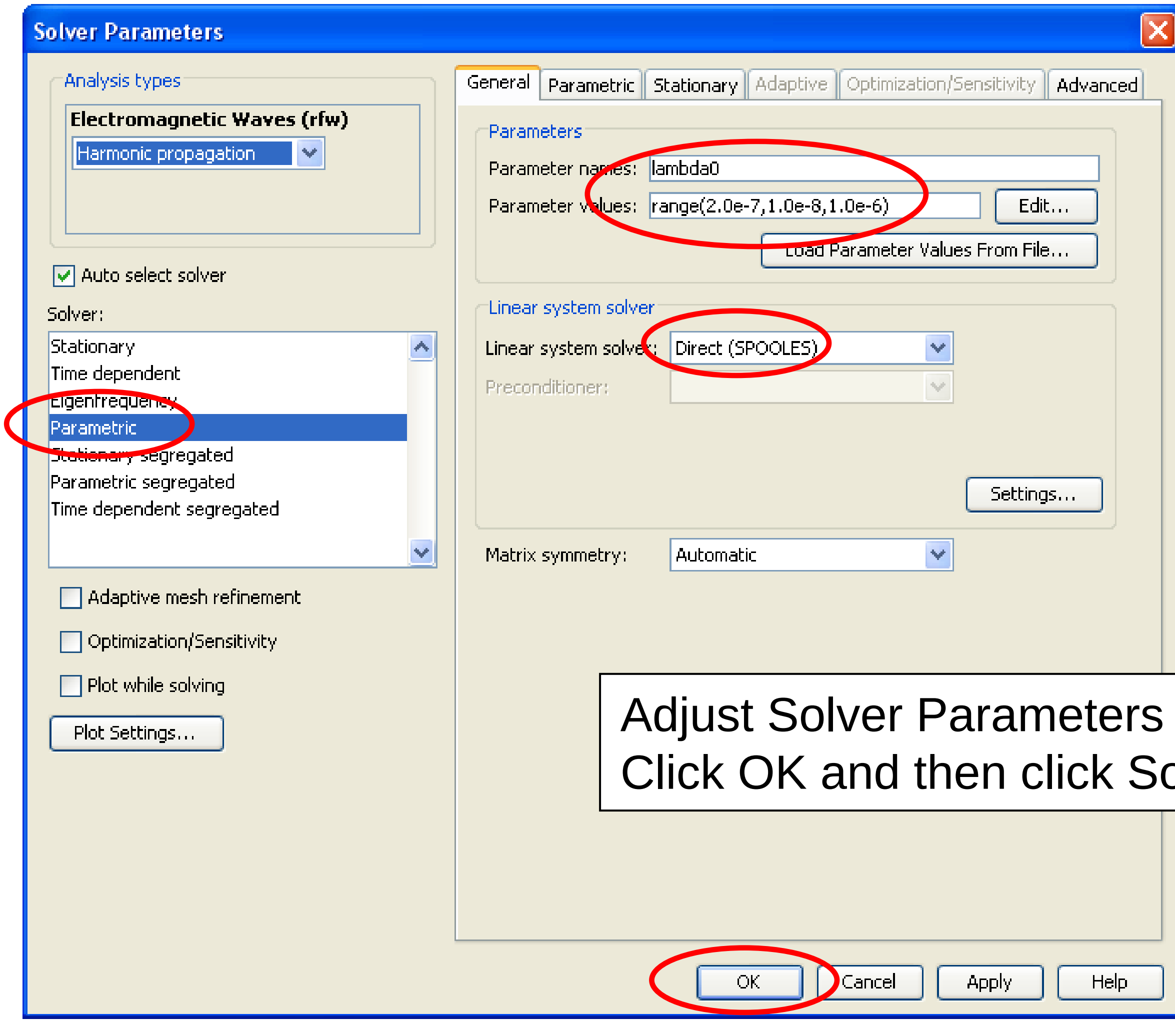
# Mesh generation, PMLs

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



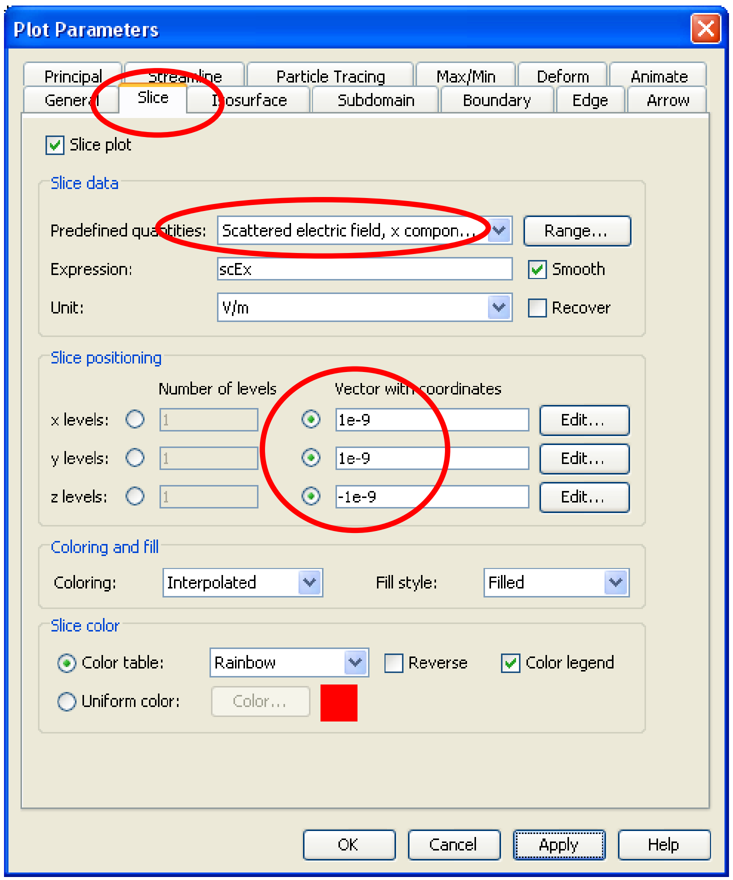
# VII. Computing the solution: Solver settings

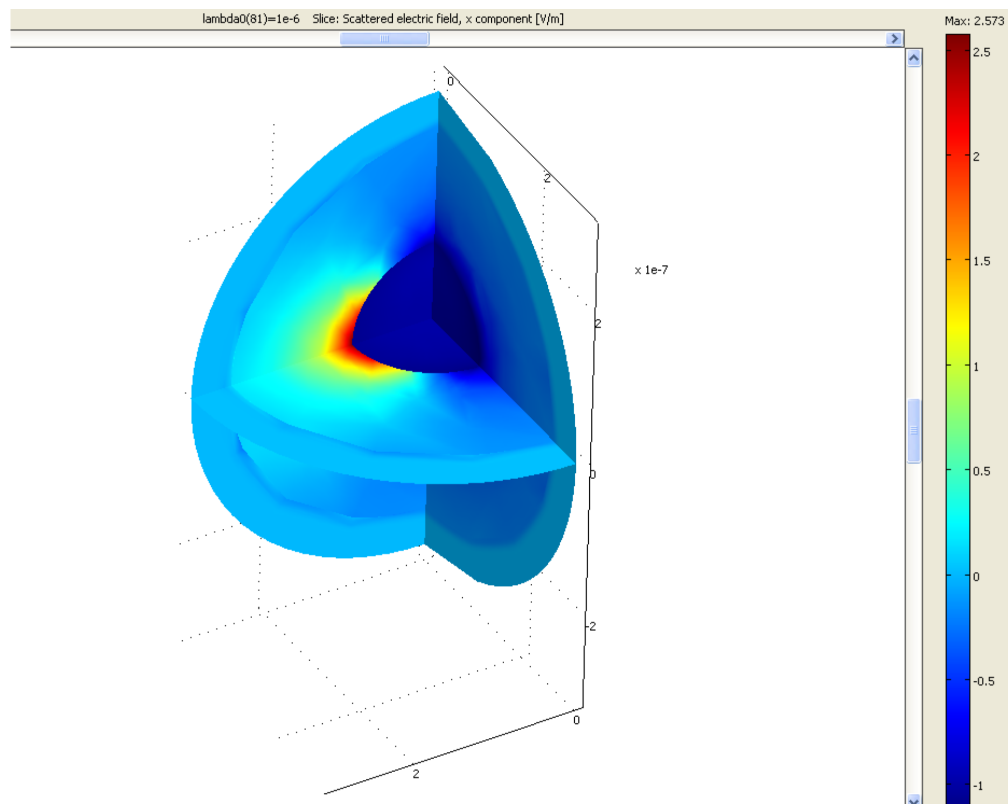



Adjust Solver Parameters as shown.
Click OK and then click Solve (= button)

# VIII. Postprocessing and visualization

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

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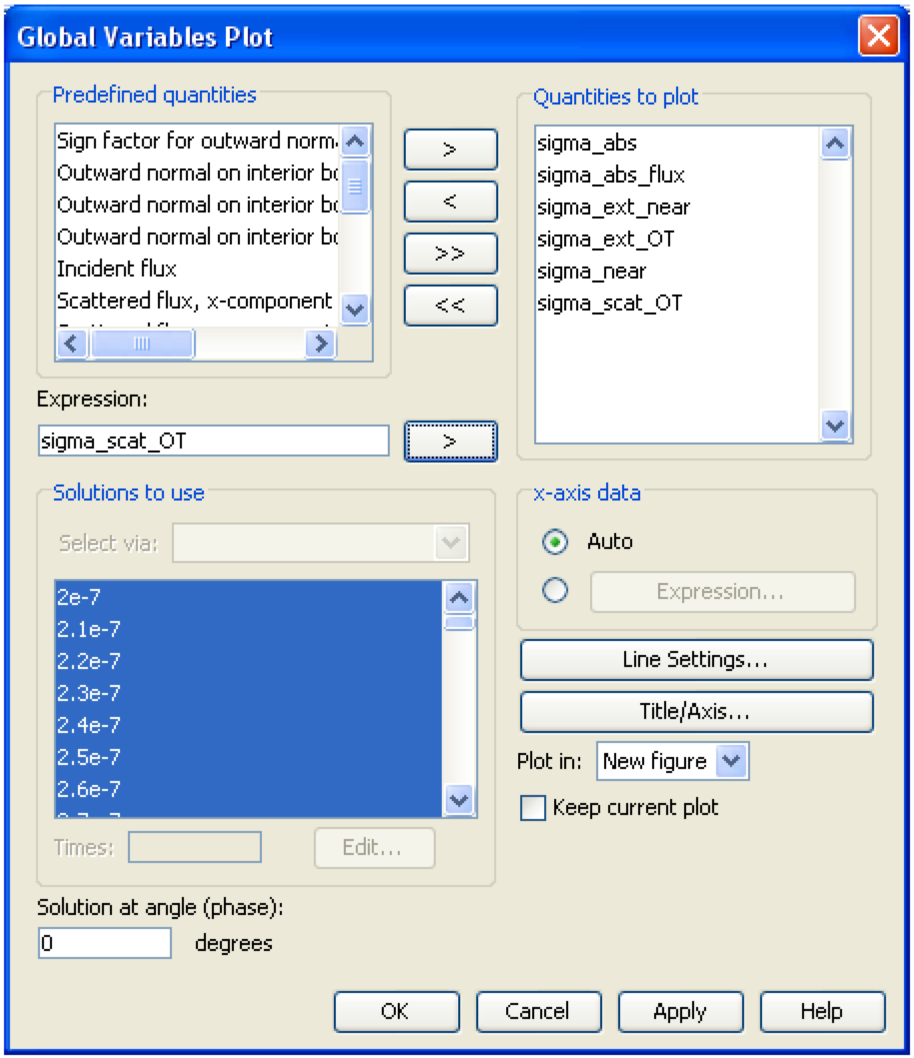
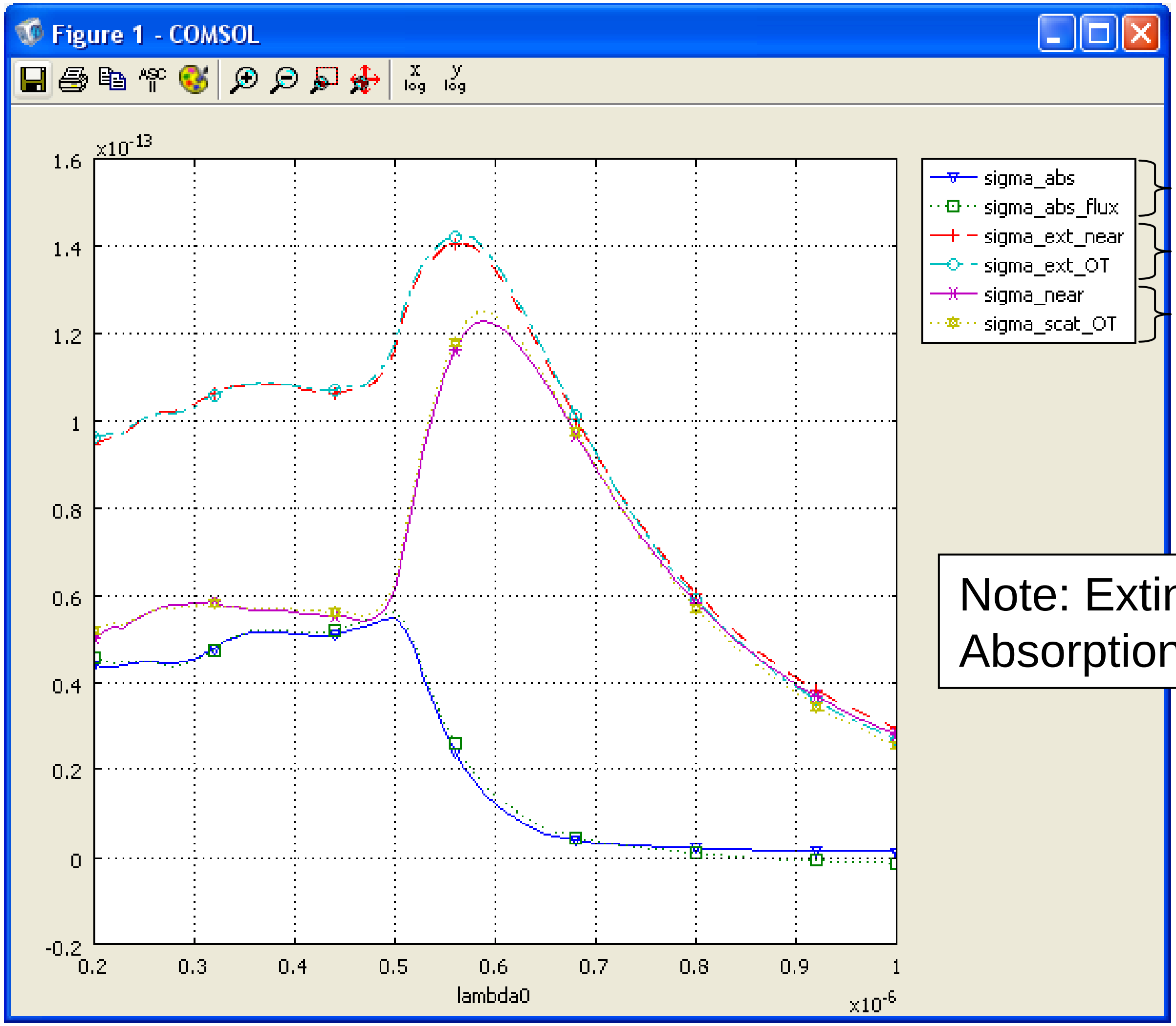
# Evaluating and plotting cross-sections




- 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.




Absorption CS
Extinction CS
Scattering CS

Note: Extinction CS= Absorption CS + Scattering CS

# Radar Cross-Section

- Plot 4*pi*sigma_back in the Global Variables Plot to obtain the standard RCS (in m^2 units):