Wavenology EM™

The SEM Solver for the Lithography and similar Applications

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June, 2020

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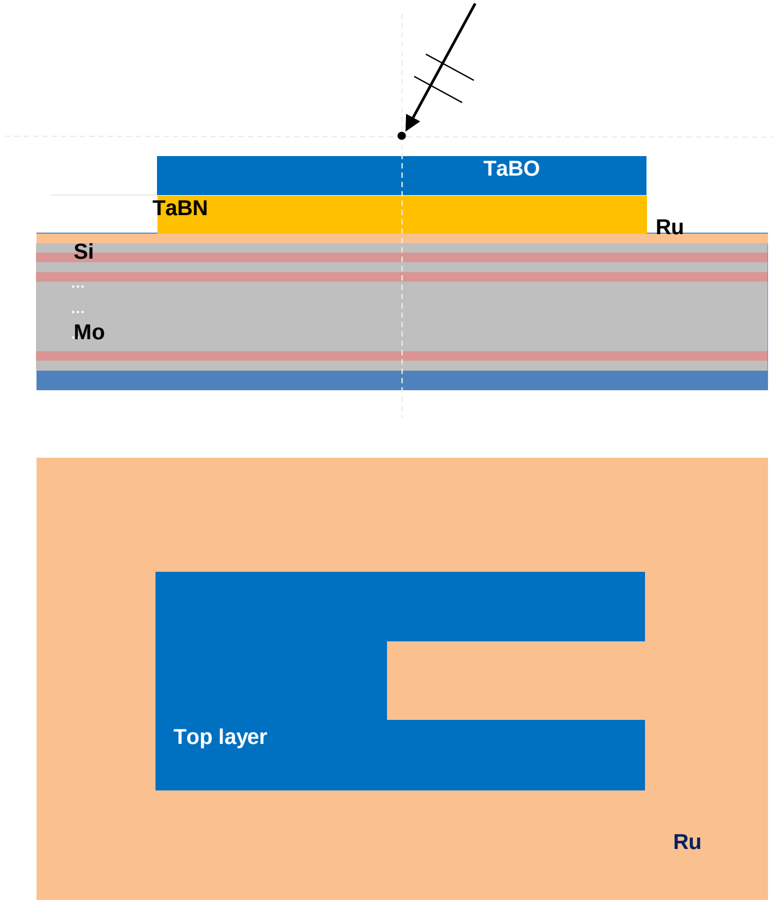
Introduction

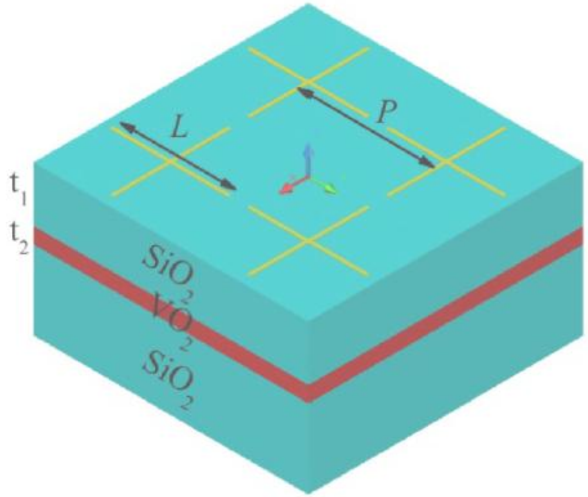
- Wavenology SEM solver is a spectrum EM solver, mainly focus on solving the near field distribution in lithography applications, or similar applications. These applications have following features
  - The incident wave is a plane wave propagating in Z, the plane wave can be tilted.
  - The boundary conditions in X & Y are bloch-periodic, in Z is open
  - The output field is E fields in user defined regions
  - Need to obtain the reflectance, transmittance and absorptance of the structures

Following is a typical structure for the EUV application simulated by the SEM solver

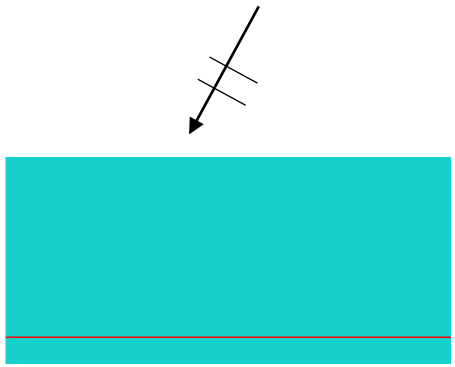


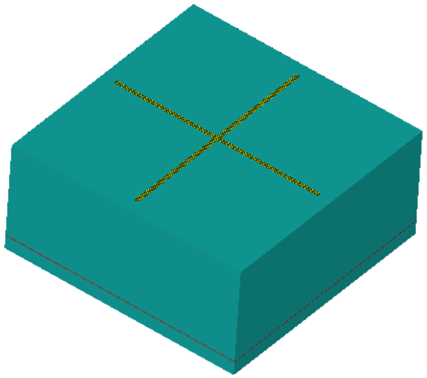
Following is a typical structure for other applications simulated by the SEM solver

Physical structure of Broadband Tunable Terahertz Absorber



Simulation model in the SEM solver





- From version 2.0.9 (Nov. 2019), there are two SEM solvers integrated in the Wavenology Litho Package

  - **Version 1 solver**[R1]: it solves the whole computational domain layer by layer. Due to the data for the whole domain need to be used, except small cases, it usually requires external data files to cache the temporary data. However, it is a direct solver, so it can solve all kinds of setting if the computer has enough resources: memory & storage.

  - **Version 2 solver**[R2]: it employs the Green's function for the layer media with Bloch periodic boundary to shrink the real computing region in the whole domain. By removing the calculation for the field in the layered background, this solver is **much faster** compared to the version 1 solver. Meanwhile, the memory requirement is **significantly reduced**. For a typical 10x10 wavelength EUV case, this solver is about **10 times faster** compared to the version 1 solver.

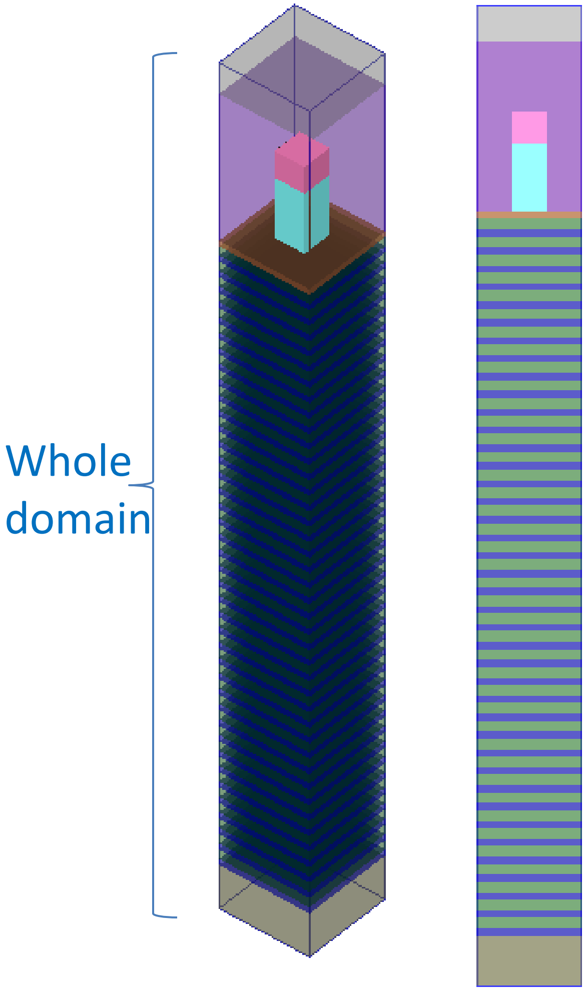
  With the same project setup, user can determine which solver will be used to simulate the project.

[R1] J. Niu, et al, "*Spectral element boundary integral method with periodic layered medium dyadic Green's function for multiscale nano-optical scattering analysis*", *Opt. Express*, 25(20), pp. 24199-24214, 2017.

[R2] Y. Mao, et al, "*Calderón preconditioned spectral-element spectral-integral method for doubly periodic structures in layered media*", *IEEE Trans. Antennas Propag.*, 68(7), pp. 5524-5533, 2020.

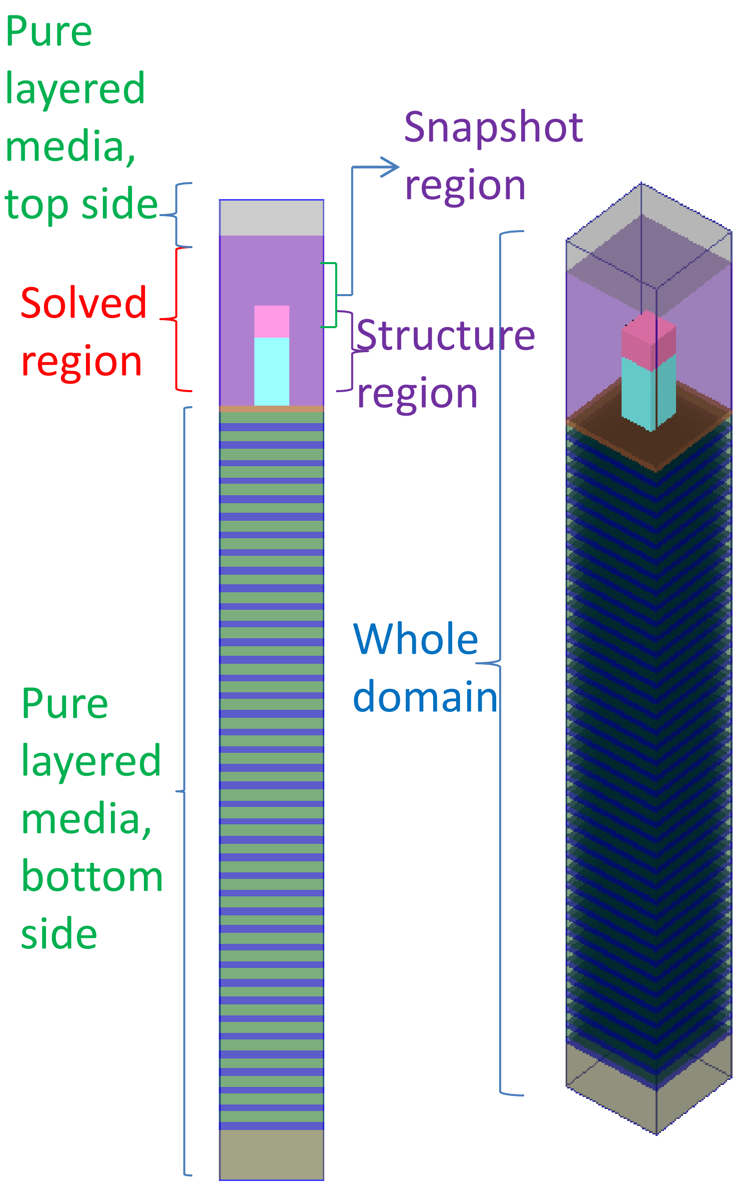
Comparison for 2 Solvers

- **version 1 solver**
  - For a case shown in the figure, the computational domain will include the whole region shown in the figure
  - All the fields in the computational domain will be solved. The solver is a direct solver.
  - The solver will detect the total memory requirement
  - If the required memory is very large, part of data will be swapped to data files in the hard drive
  - Due to the direct solver is used, this solver can obtain very **accurate results**. However, this solver is **not very fast** due to it need to solve all fields.



version 2 solver

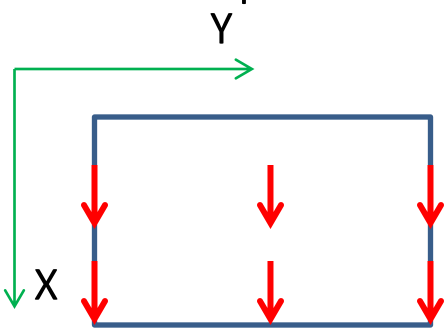
- For a case shown in the figure, the solved region will include the structure and receiver region only, as:
  - Zmin = min(Zmin of structure, Zmin of snapshot)
  - Zmax = max(Zmax of structure, Zmax of snapshot)
- Only the fields in **the solved region** will be solved
  - The number of unknown is determined by the size of solved region.
  - The size of solved region is related to the position of receiver also. Based on the feature of EUV applications, in order to reduce the number of unknowns, the receiver is better to be placed around the structure region
- The processing data all are in the memory
- This solver employs an iterative solver to solve the system. Therefore, the accuracy of the results is determined by the stop criteria.
- Compared to the version 1 solver, this solver requires **much less memory** and is **much faster**, but the result accuracy is not as good as that in the version 1 solver.
- In this solver, user can choose using double or single precision data to solve the system. For the single precision data, the memory requirement will be shrink to almost half. Even for the single precision data type, the pre-processing data is still in double precision. Therefore, the accuracy of result will be at a similar level for both two data types.

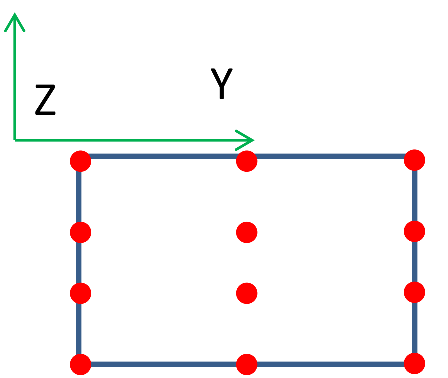


SEM Nodal Point

X, Y & Z components has it’s own nodal system
If we define the basis order as (nx=2, ny=2, nz=3)

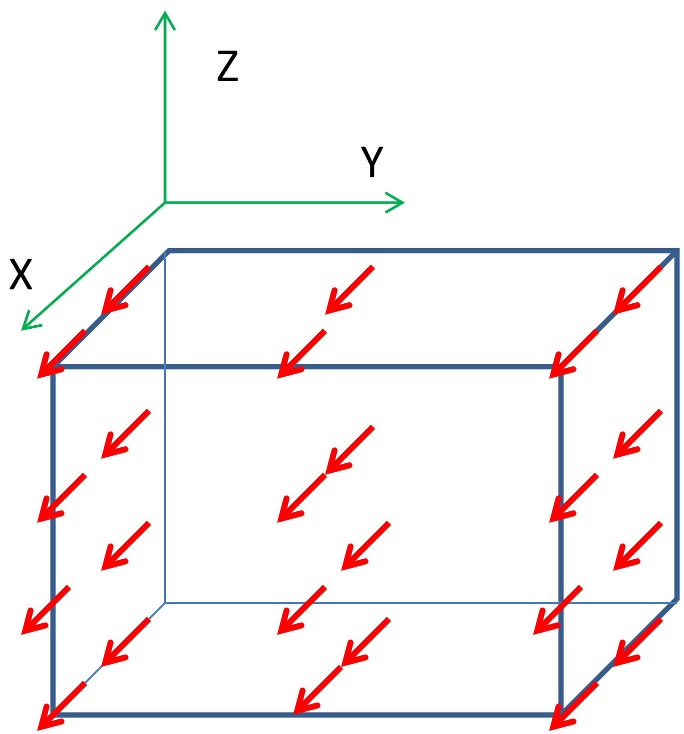
X Component





The tangent components can touch the cell boundary. The normal components can’t touch the cell boundary.

As shown in left top figure, X component can touch the XZ face of a cell, but will not touch the XY face.



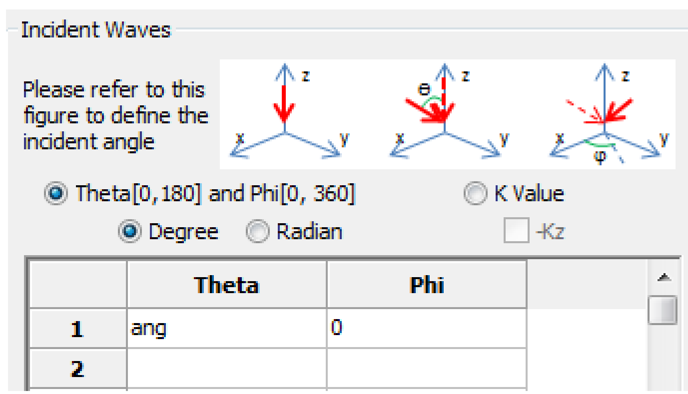
- note:
  - We suggest to use an order >= 3 in the main propagation direction, not matter the size of cell in the main propagation direction. For an order = 4, in general, it will provide a better solution compared to order = 3.
  - For solver 2, if the cell size in Z is about 1 wavelength, we suggest that the order in Z should be at least 5.

Incident Plane Wave

To define the incident direction of the plane wave, user can input

1) The incident angle directly, or
2) The propagation constant K of the plane wave

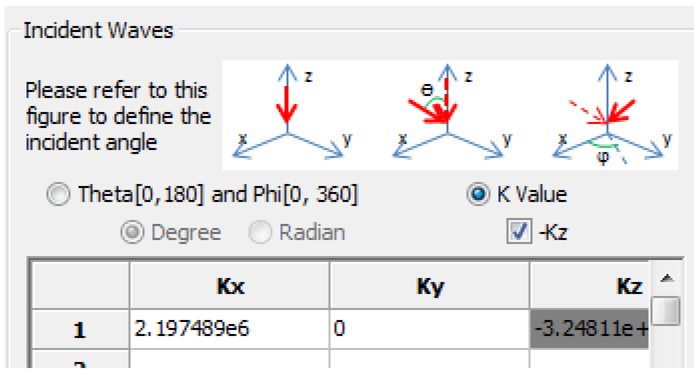
The incident angle (ϴ, φ) definition



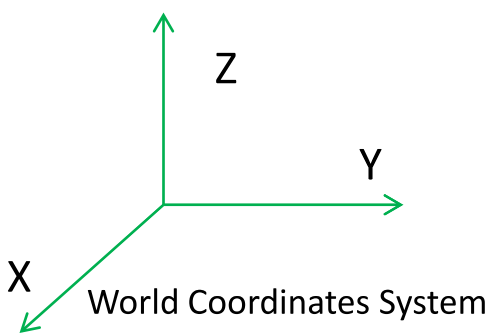
The propagation constant K

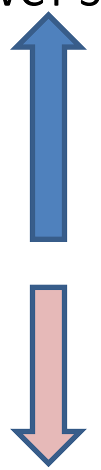
User need to input the (K_x, K_y) for the 1st layer the incident wave hit the space, and the sign of K_z (the value of K_z will be calculated by GUI) .

- For the wave propagates from –Z to +Z, the 1st layer is the bottom layer
- For the wave propagates from +Z to -Z, the 1st layer is the top layer



Sign of Kz in WCT SEM solver





propagation -Z -> +Z
Kz: +|Kz| (Positive sign)

propagation +Z -> -Z
Kz: -|Kz| (Negative sign)

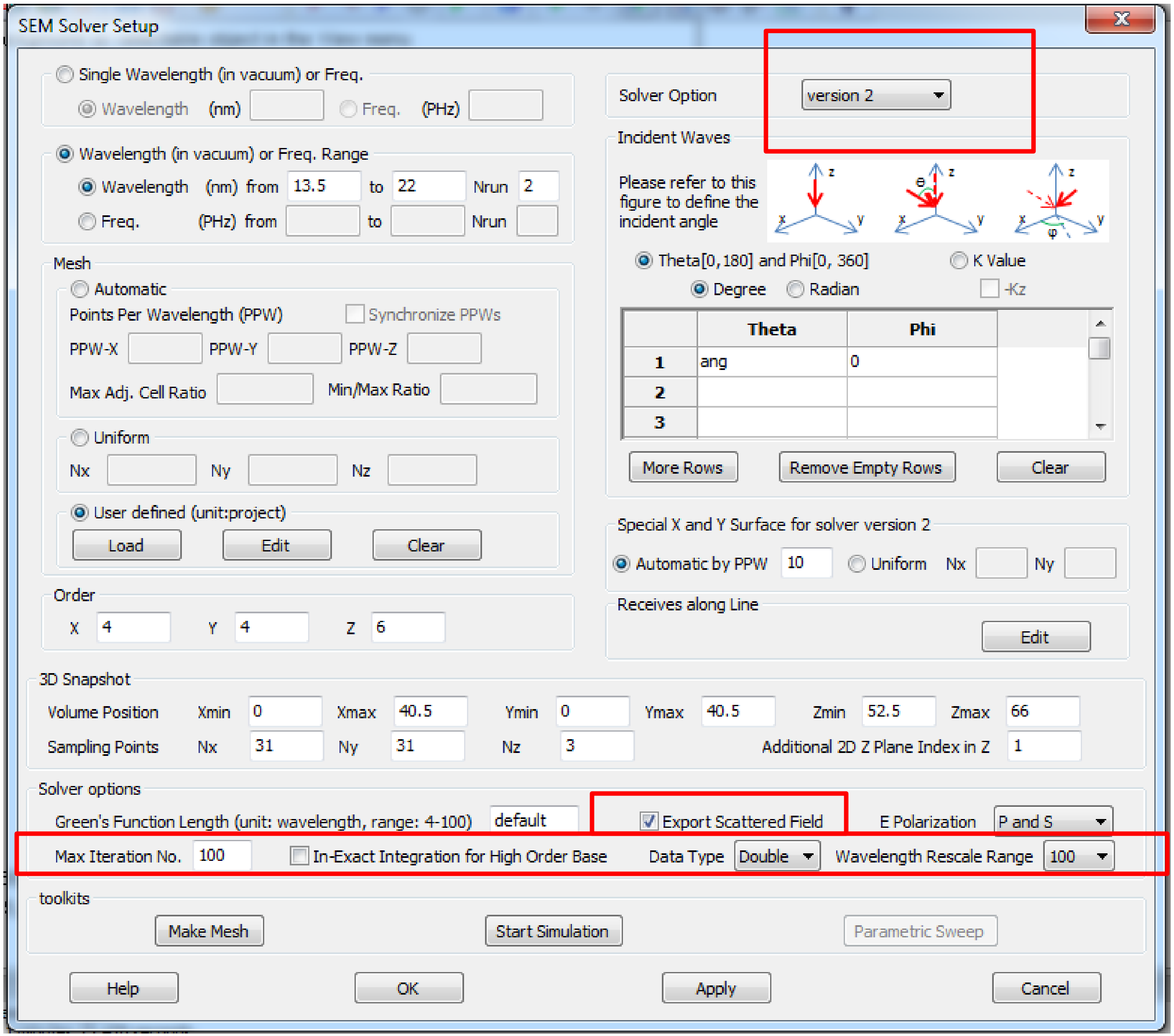
Project Setting

In order to start a WCT SEM simulation, user need to define following general settings.
Here, we assume user already know how to use WCT GUI to create a WCT EM project. If user doesn't familiar with it, please refer to the WCT EM manual or the embedded manual in the WCT GUI.

1. The domain size, boundary conditions, and 3D geometries for a regular EM simulation
2. Working wavelength (or frequency). The wavelength is that in the vacuum.
3. Meshing setting for the SEM solver (not the mesh setting for the FDTD solver)
4. The order in the SEM solver
5. Incident plane wave. The input can be incident angle (θ,Φ), or propagation constant
6. Snapshot definition to export the E field
7. Solver type: version 1 or version 2

8. For the version 2 solver, there are more options
   1) The max iteration number
   2) E field polarization: P & S polarization together, P polarization only, S polarization only
   3) Data type in solving: double precision, or single precision

The SEM solver setup dialog



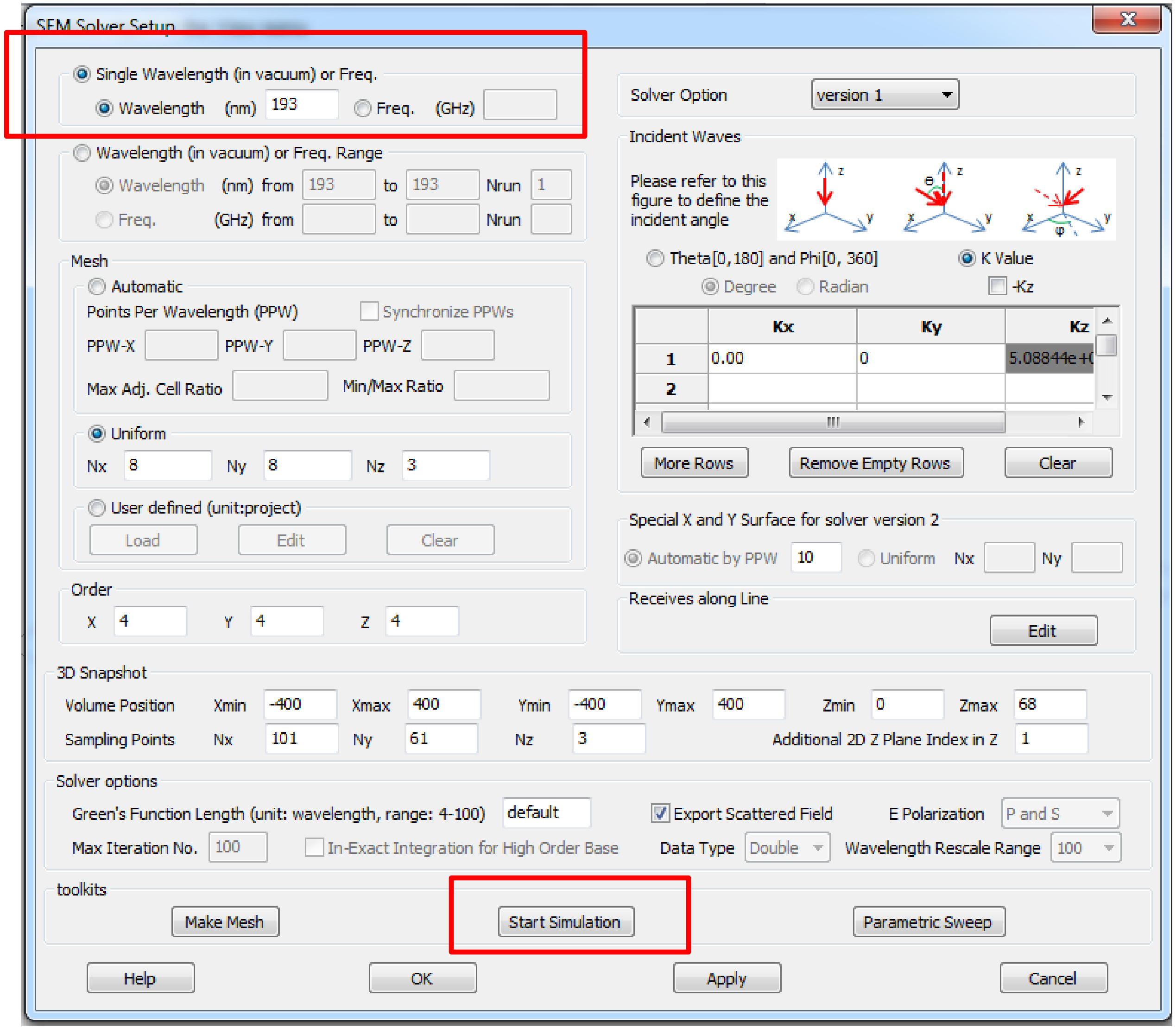
Switch solver

Options for solver version 2 only

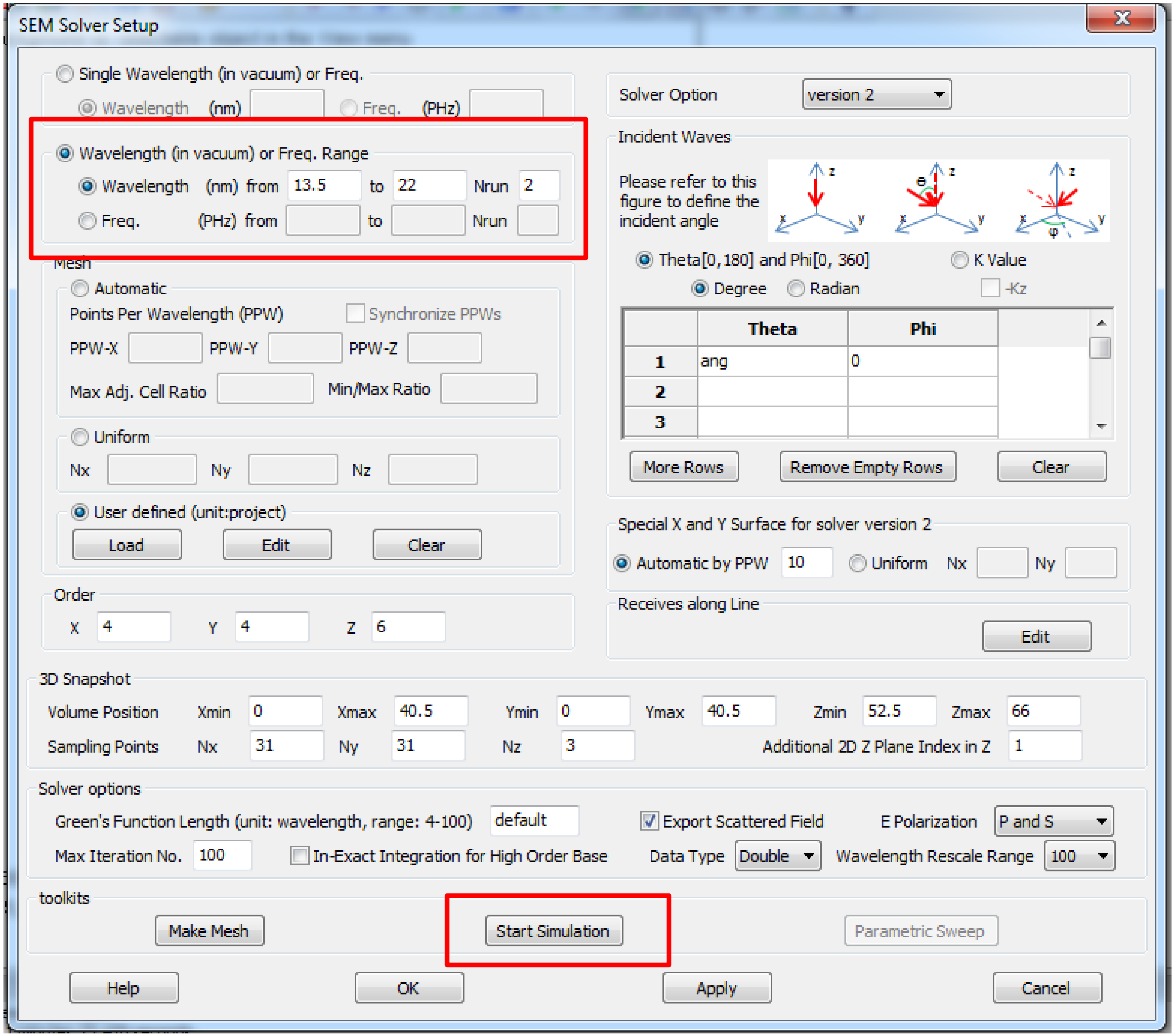
Simulation Types

- Single Simulation
  - Simulate the project with a fixed setup
- Sweeping Frequency/Wavelength
  - Simulate the project by a range of freq./wavelength, and export the simulation results for each freq./wavelength
- Parametric Sweeping
  - Design the project with variables, simulate the project by a range of variables, export the simulation results for each value of the variables
- Sweep the mask pattern
  - Define the mesh in X & Y as fixed arrays, align/shift the geometries to match the mesh grid by the mask pattern editor, batch simulate the pattern. More details can be referred to Appendix I: the mask editor

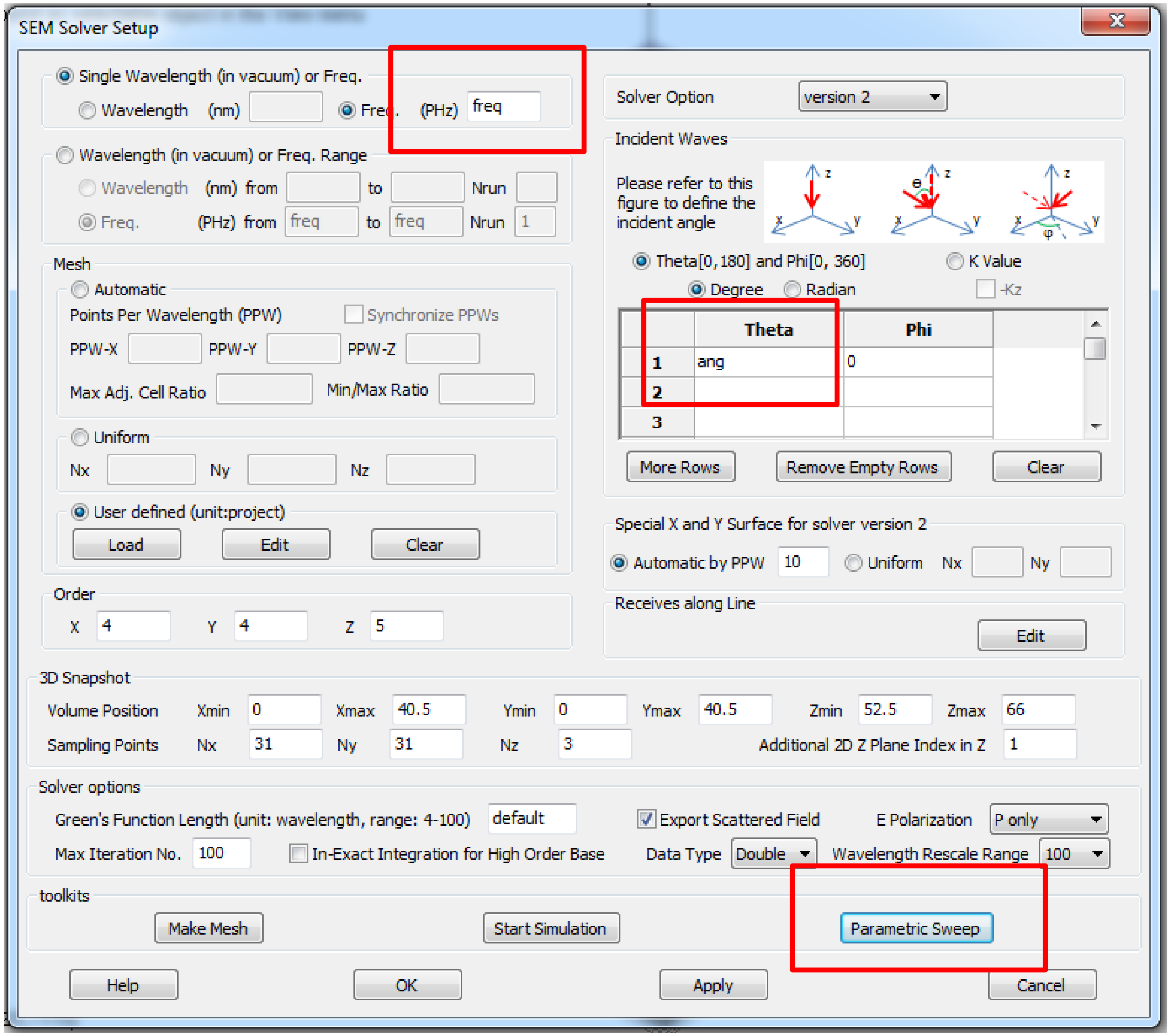
Set up & Start a Single simulation



Sweeping Frequency/Wavelength



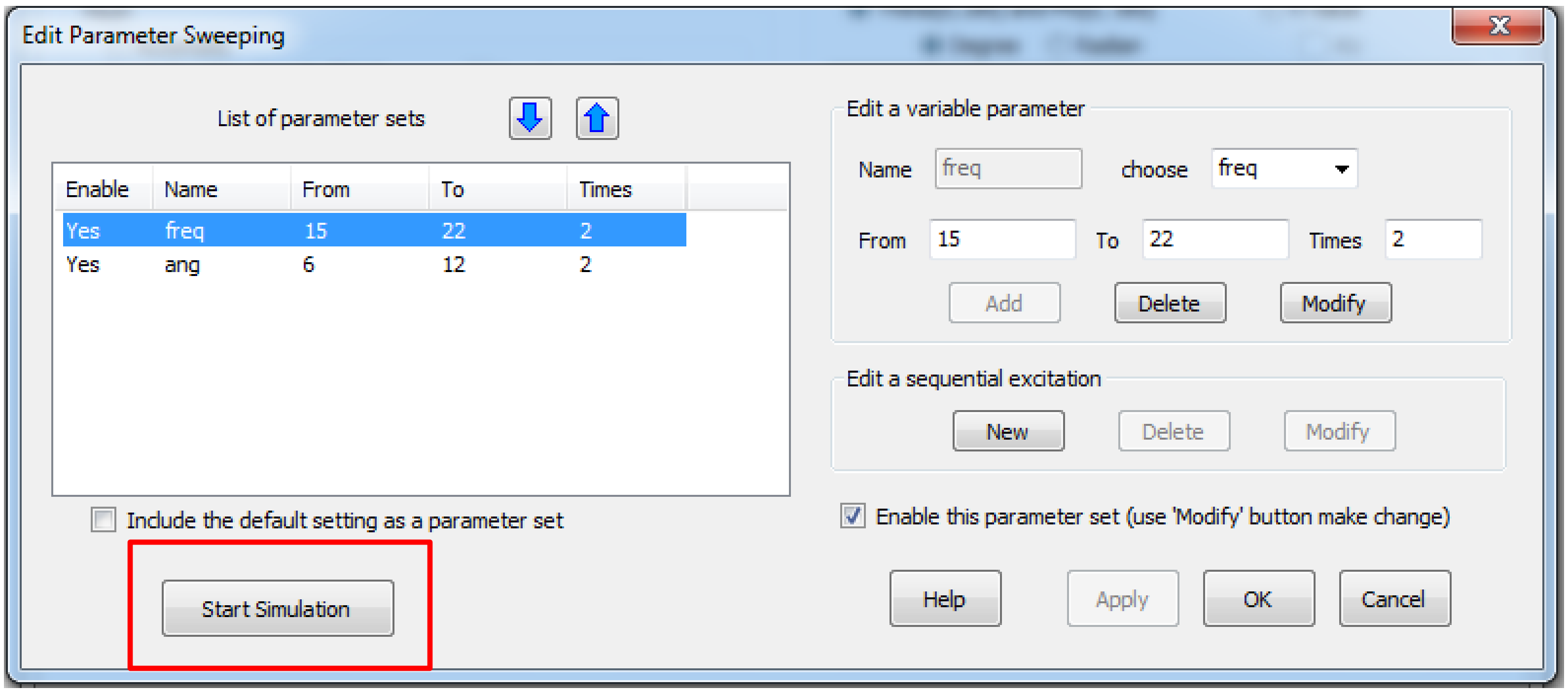
Parametric Sweeping



In the GUI, almost all inputs can be defined by variables, including the geometry parameters, source definition, working frequency, etc.

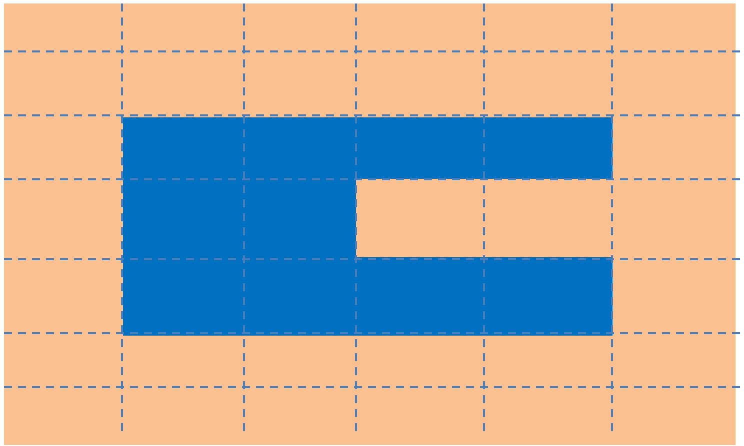
Here, the project working frequency and the source incident angle are defined by variables, we are sweeping these 2 variables

Define the sweeping variables and the sweeping range



Sweep Mask Pattern

- For typical Lithographic applications, the base layers, including the Si/Mo bilayers and the Si substrate, are fixed. Only the absorber layer and the capping layer (mask layers) will be variant in different applications. Meanwhile, the structures in mask layers can be decomposed by fixed size boxes due to the fundamental element shape in the lithographic application is fixed. Based on these features, WCT GUI provides an editor to generate the mask pattern in a simple way for Lithographic applications and similar applications .
- The usage of the mask pattern editor and sweeping on the mask pattern can be referred to here



Simulation Results

1. General simulation result for a single simulation
   - P polarized plane wave source and S polarized plane wave source
   - Total fields
   - Scattered fields
   - Snapshot for cubic volume
   - Snapshot in rectangular 2D plane (one Z cross-section in the volume snapshot)
   - Receiver array along lines
   - Reflectance, transmittance, absorptance
2. Sweeping Frequency/Wavelength
   - Data file names for each simulation in the sweep
   - The single data file for all reflectance, transmittance, absorptance
3. Parametric sweeping
   - Data file names for each simulation in the sweep
   - The single data file for all reflectance, transmittance, absorptance
   - The variables' value table for each simulation in the sweep
4. Sweep mask pattern
   - Please refer to the Appendix I

General Simulation Result for a Single Simulation

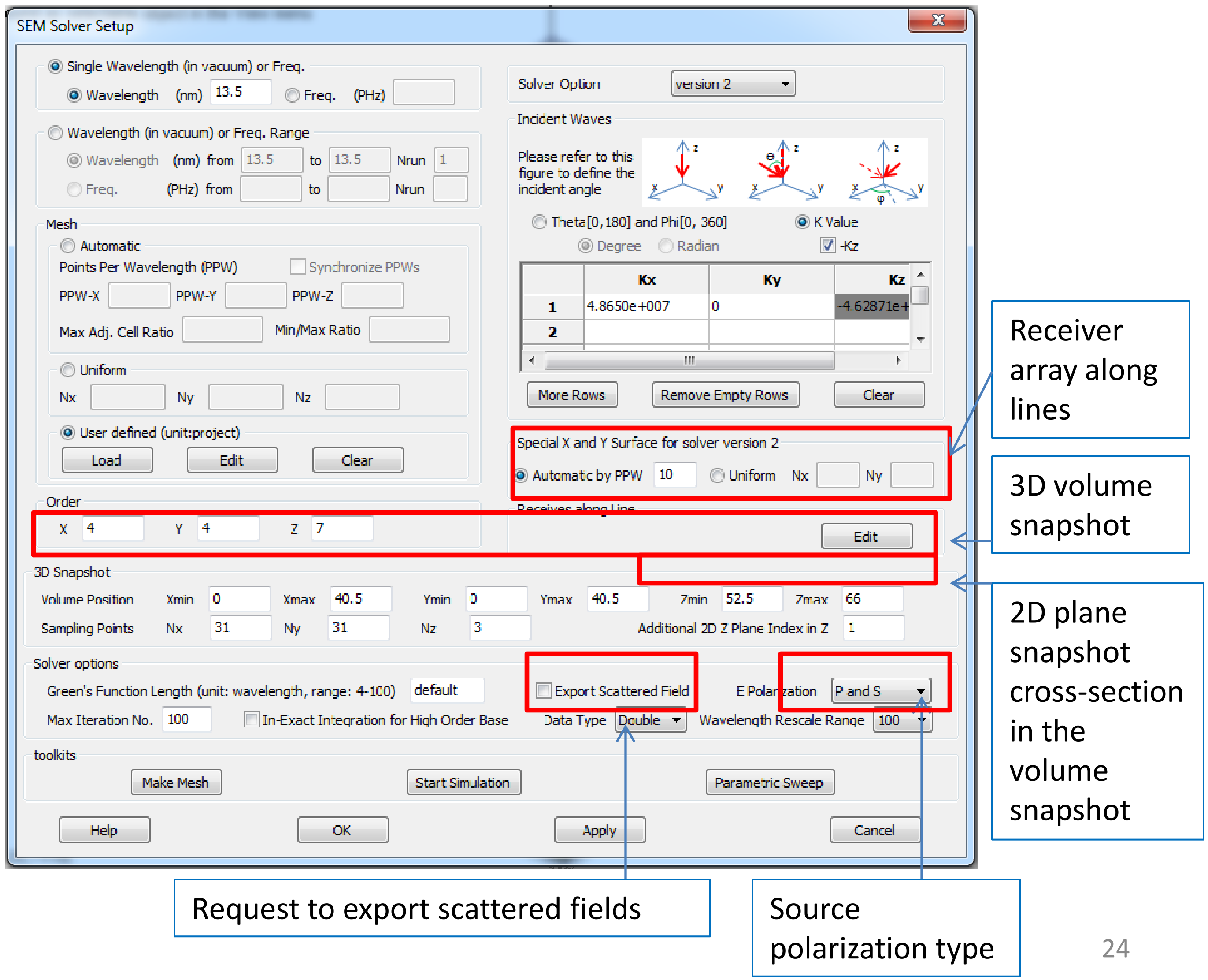
For a incident plane wave, there are 2 possible polarization: P & S, user can determine which polarization will be used in the simulation, or use both 2 polarizations.

The total fields for

- ➢ 3D volume snapshot
- ➢ 2D planar snapshot
- ➢ Receiver array

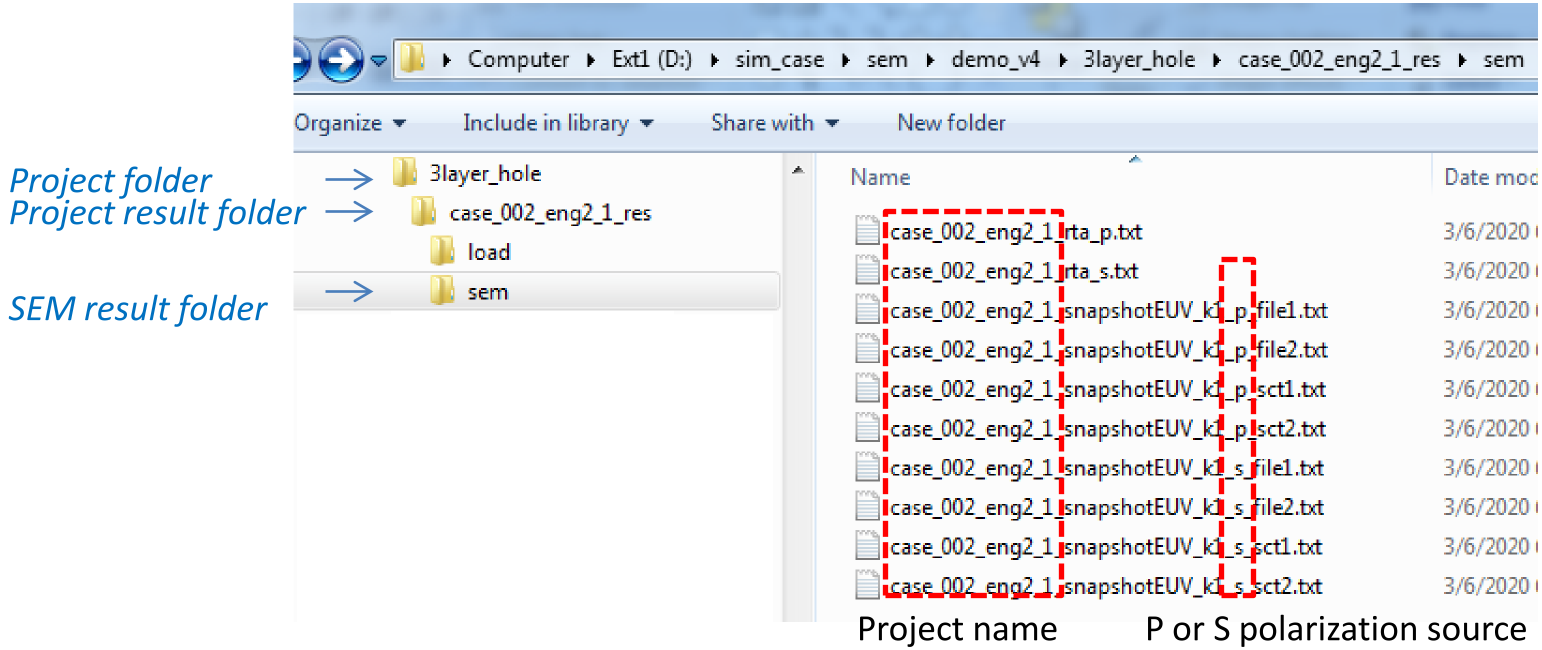
will be always exported.

The scattered fields on above position will be exported by request.



Data file name & format for exported data

The data files will be stored in the sub-folder:
Project_folder\Project_name_res\sem



xxx_file1.txt: 2D planar snapshot **E** total field
xxx_file2.txt: 3D volume snapshot **E** total field
xxx_sct1.txt: 2D planar snapshot **E** scattered field
xxx_sct2.txt: 3D volume snapshot **E** scattered field
xxx_rta...txt: Reflectance, transmittance, absorptance
xxx_RecvArray_p_tot.txt: **E** total field at receiver array for P polarization source
xxx_RecvArray_s_sct.txt: **E** scattered field at receiver array for S polarization source

Here, "xxx" is the project name

Data file format

Basically, all SEM data files are ASCII text files.

1) 2D/3D Snapshot data file format is 9 column array as following

X	Y	Z	Ex real	Ex imag	Ey real	Ey imag	Ezreal	Ez imag

here, the coordinates (x,y,z) of the sampling point use the project unit. For example, if the project unit is nm, the (x,y,z)=(1,2,3) is (x,y,z)=(1nm, 2nm, 3nm)

The sampling positions in the snapshot is generated by following for-loop

```
for x
    for y
        for z
```

Appendix II has an example of using Matlab code to load and show the snapshot data.

2) For the receiver array along lines, data file format is 9 column array as following

X	Y	Z	Ex real	Ex imag	Ey real	Ey imag	Ezreal	Ez imag

Receiver array along line 1 (rows 1–3)

Receiver array along line 2 (rows 4–6)

here, the coordinates (x,y,z) of the sampling point use the project unit. For example, if the project unit is nm, the (x,y,z)=(1,2,3) is (x,y,z)=(1nm, 2nm, 3nm)

3) For the data file for reflectance, transmittance, absorptance, there are 2 rows. 1st row is the comment, 2nd row is data. Following is an example

```
%Reflectance, transmittance, absorptance
0.187338    0.553233    0.259429
```

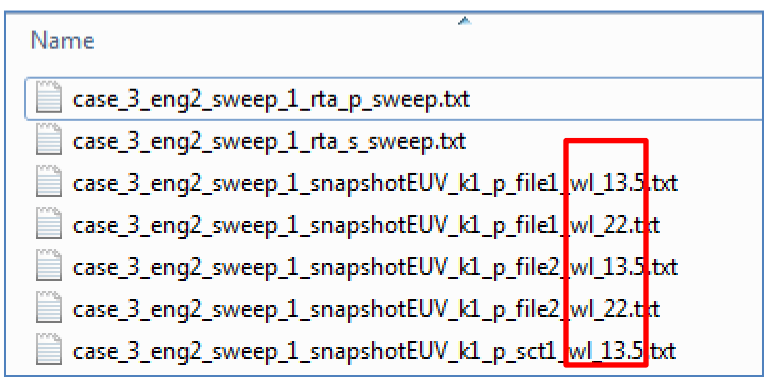
Simulation Result for Sweeping Freq/Wavelength

Basically, each freq/wavelength in the sweep will generate following independent data files

- ➢ Snapshot for cubic volume
- ➢ Snapshot in rectangular 2D plane (one Z cross-section in the volume snapshot)
- ➢ Receiver array along lines

Only all reflectance, transmittance, absorptance will be stored in the same data file

Following is part of data files for freq sweeping case



As can be seen, there is string as “**wl_xxx**” in the file name, which means: **wavelength=xxx**
This string is used to distinguish the case setup for this sweep.

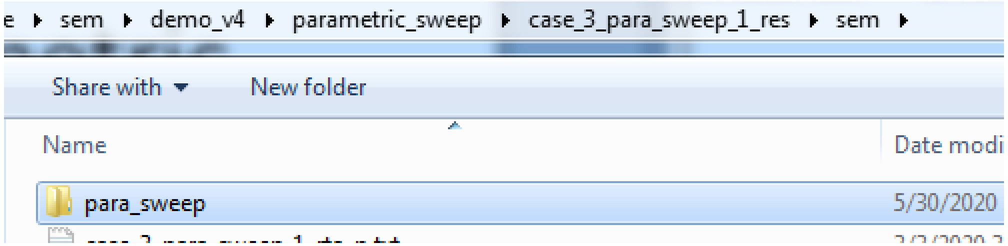
Cont.

For the data file for reflectance, transmittance, absorptance, there is clear comment in the file. Following is an example

```
% Wave Computation Technology SEM solver freq. sweep result for reflectance, transmittance and absorptance.  Version 1.0
% Reflectance     transmittance     absorptance
% wl=13.5
0.605693      0.285223      0.109084
% wl=22
0.00176385      0.912923      0.0853132
```

Simulation Result for Parametric Sweeping

The sweeping result will be stored to the sub-folder “para_sweep” under the SEM result folder “sem”.

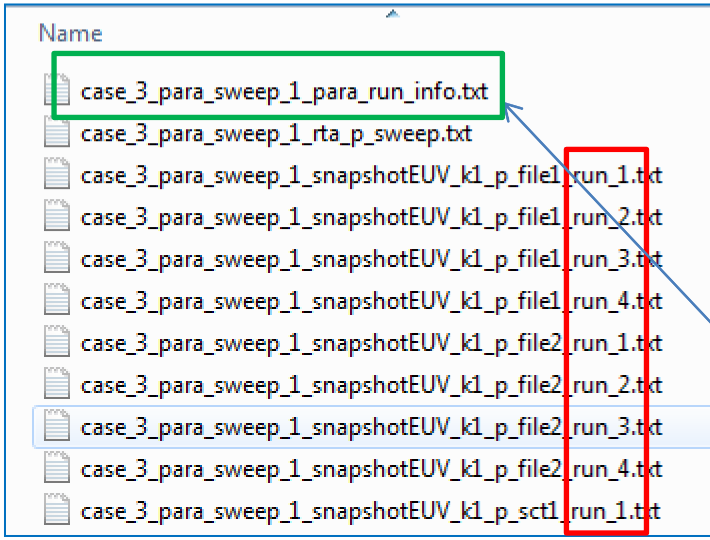


Each case in the sweeping will generate following independent data files

- Snapshot for cubic volume
- Snapshot in rectangular 2D plane (one Z cross-section in the volume snapshot)
- Receiver array along lines

Only all reflectance, transmittance, absorptance will be stored in the same data file

Following is part of data files for parametric sweeping case



As can be seen, there is string as "**run_x**" in the file name, which means it is xth case in the sweep, the corresponding values for all paramters can be refer to the file "xxx_para_run_info.txt"

Here is an example of the "xxx_para_run_info.txt"

Run=1, Paramaters: freq = 15; ang = 6
Run=2, Paramaters: freq = 15; ang = 12
Run=3, Paramaters: freq = 22; ang = 6
Run=4, Paramaters: freq = 22; ang = 12

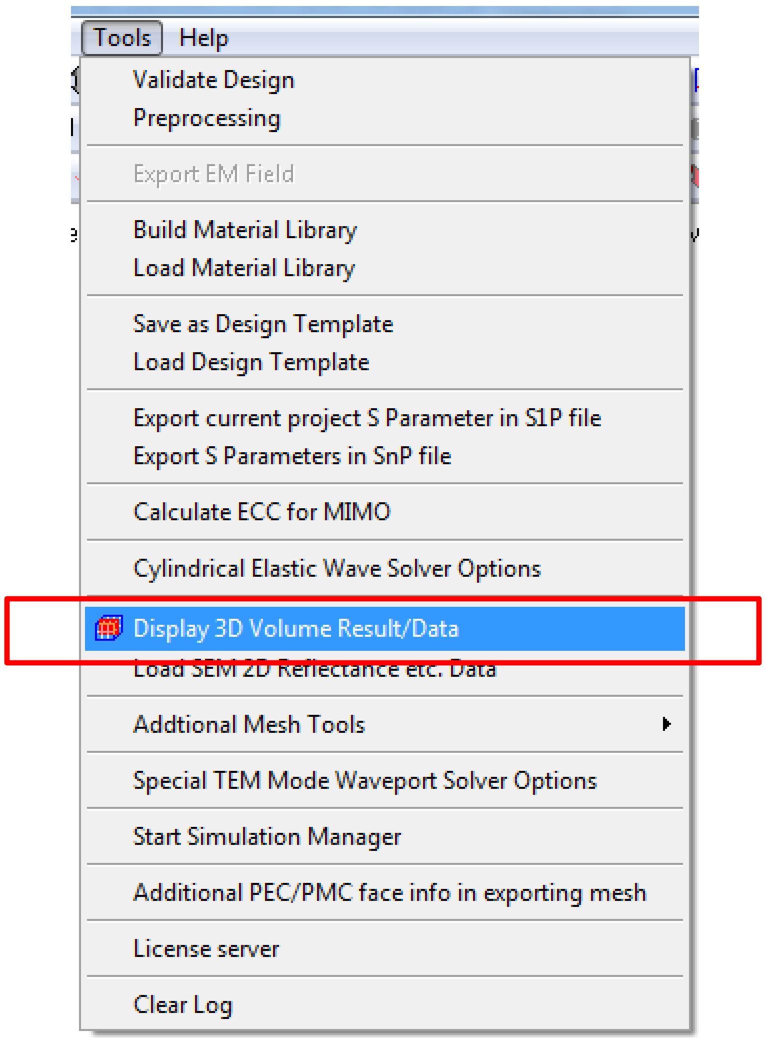
For the data file for reflectance, transmittance, absorptance, there is clear comment in the file. Following is an example

```
% run = 1, paramter: freq = 15; ang = 6
0.0351881      0.886933      0.0778788
% run = 2, paramter: freq = 15; ang = 12
0.030703      0.886425      0.0828717
% run = 3, paramter: freq = 22; ang = 6
0.594399      0.298691      0.10691
% run = 4, paramter: freq = 22; ang = 12
0.136531      0.793829      0.0696406
```

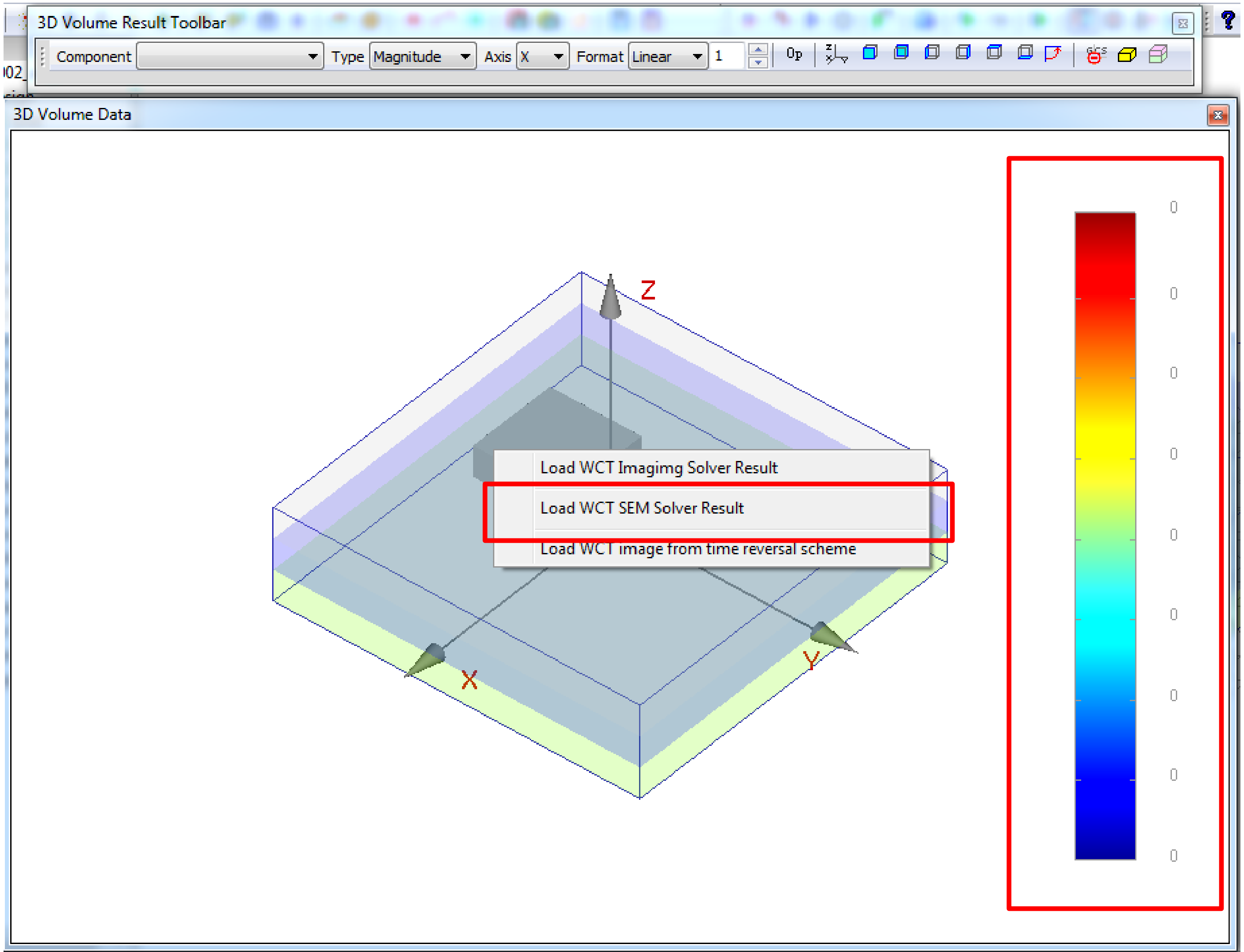
Display Simulation Results

3D & 2D snapshot

After the SEM simulation, use this menu item to load the 2D or 3D snapshot data



In the new canvas, right click mouse to popup a menu to load SEM simulation result

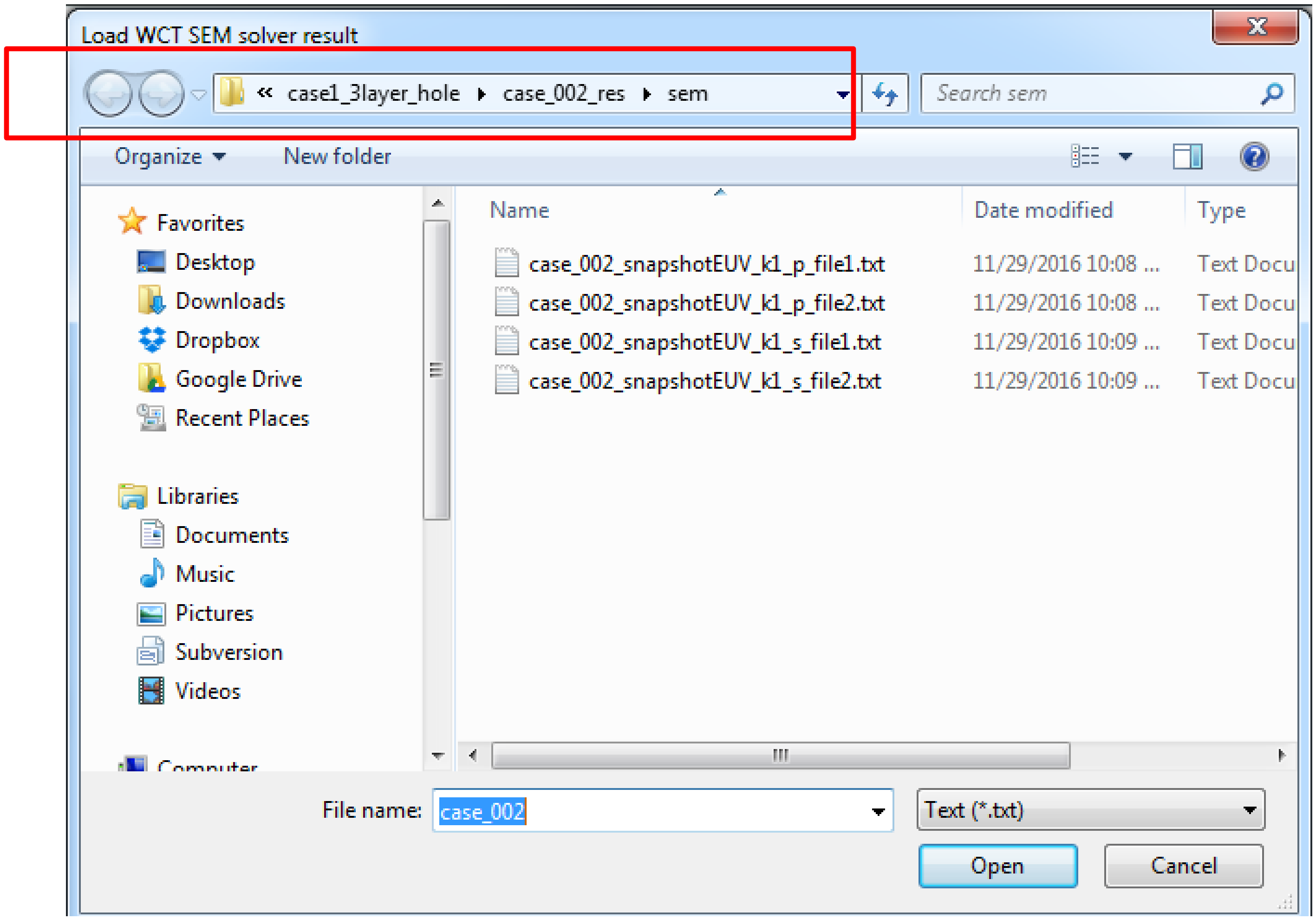


Note: in displaying the SEM snapshot data. The data range for the colorbar include all data in the data file.

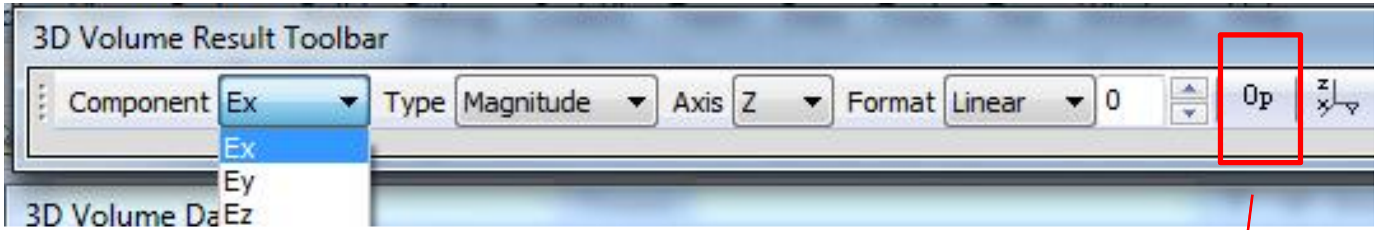
For the "xxxx_x_file2.txt", it is the volume snapshot data. Therefore, the shown single frame may not cover the full range the data range shown by the colorbar.

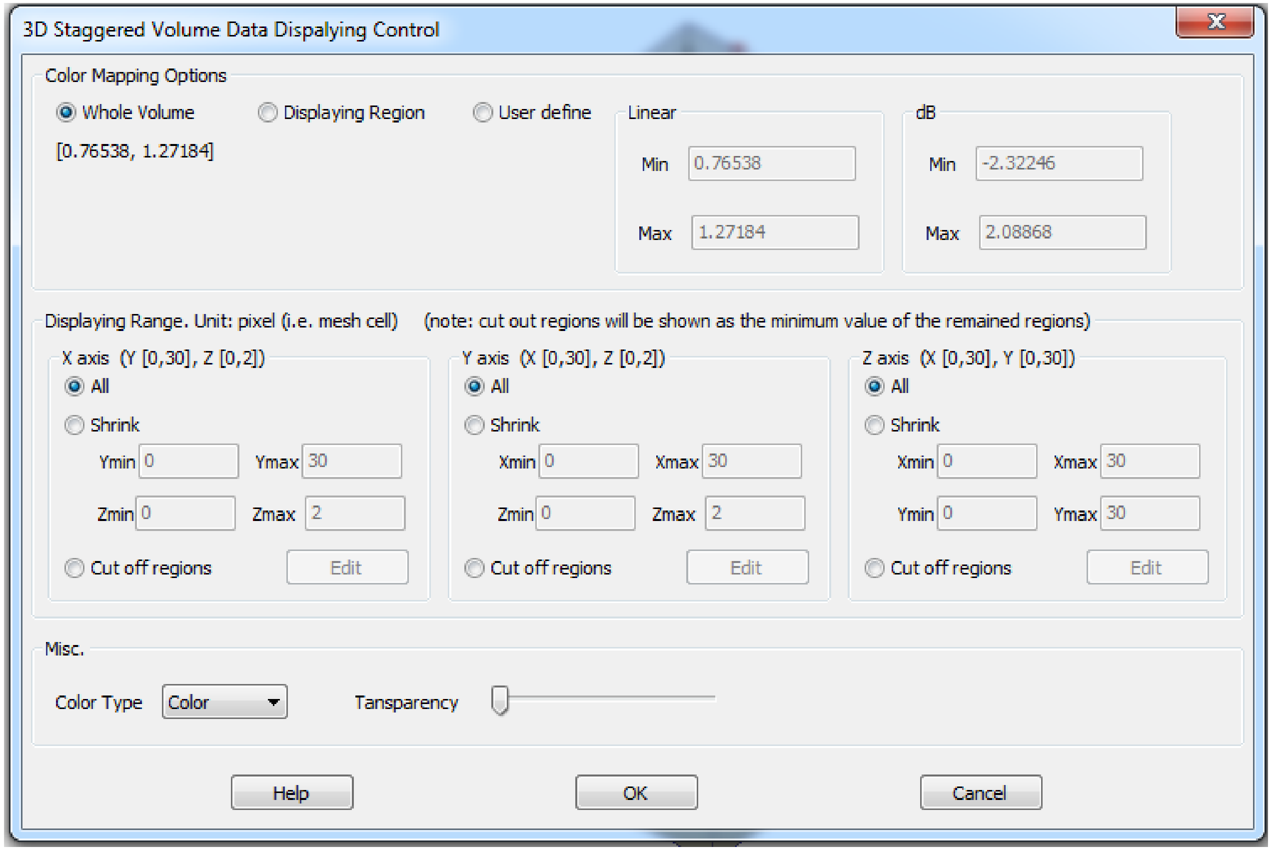
For the "xxxx_x_file1.txt", it is a single frame in the volume snapshot. Therefore, the shown single frame will cover the full range shown by the colorbar.

If the project has the SEM simulation result, the data folder is automatically set to this simulation's result folder

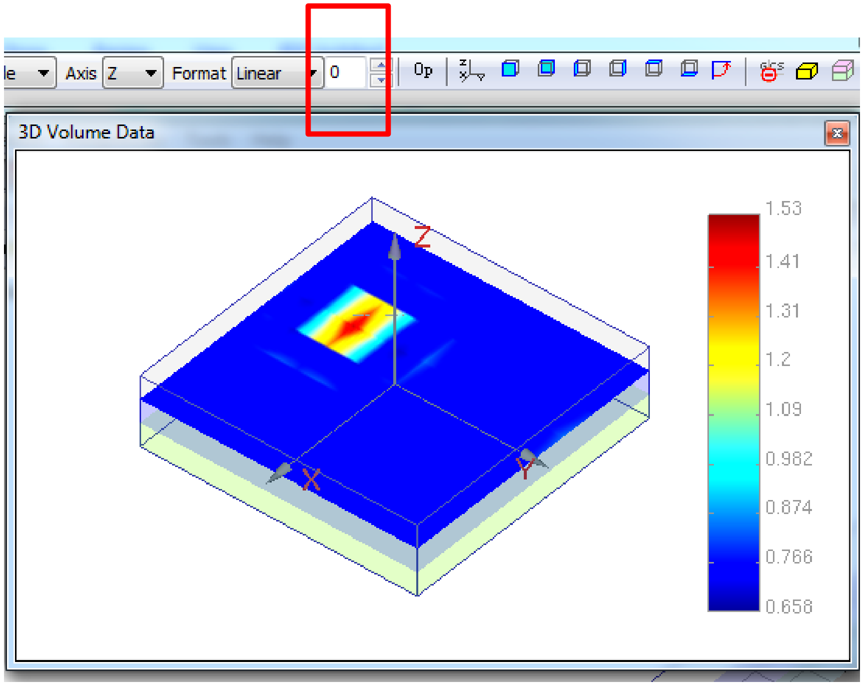


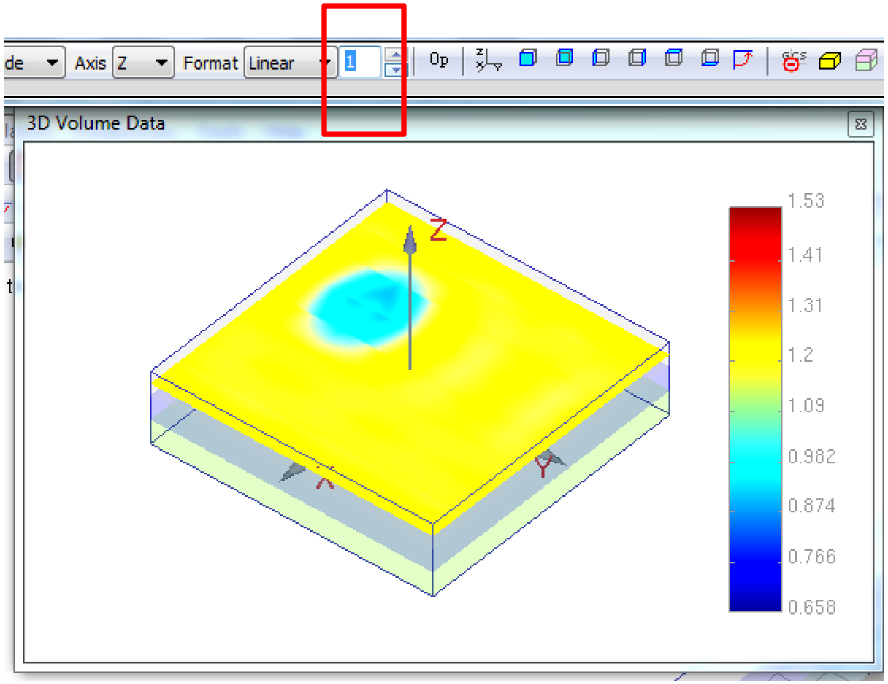
The toolbar has many options to control different components, displaying type, etc.





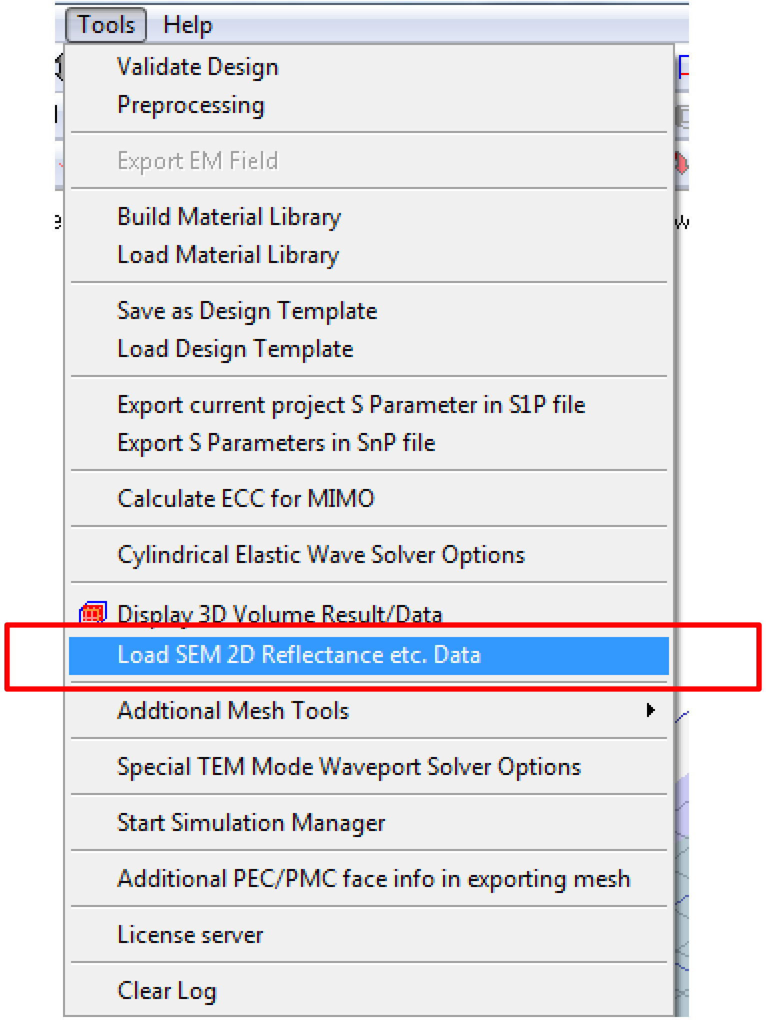
Use the frame index to show different cross-sections



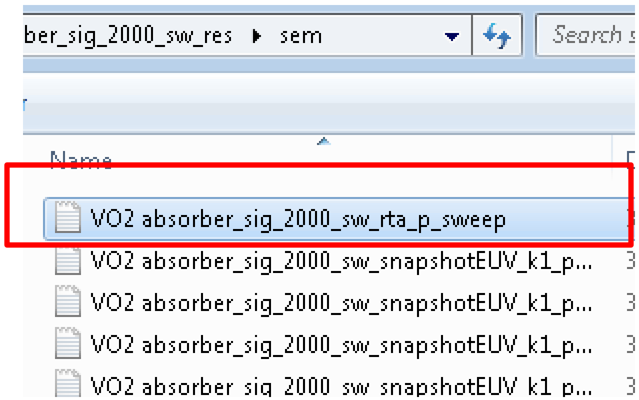


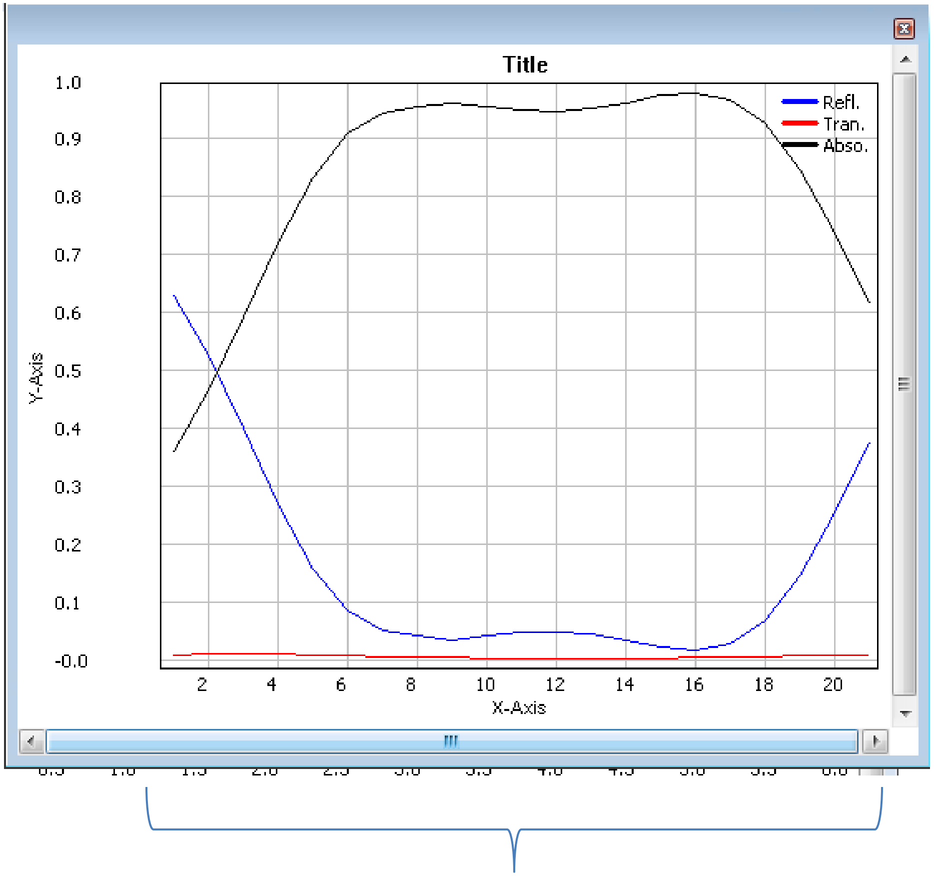
1D reflectance, transmittance, absorptance curve in freq/wavelength sweeping

In the sweeping, all reflectance, transmittance and absorptance are stored in the same file, it can be loaded in GUI and displayed as 1D curves



If the project has the SEM simulation result, the data folder will be automatically set to the simulation's result folder: "xxxx_res/sem".
Load the file "xxx_rta_..._sweep.txt", the curves will be shown as following



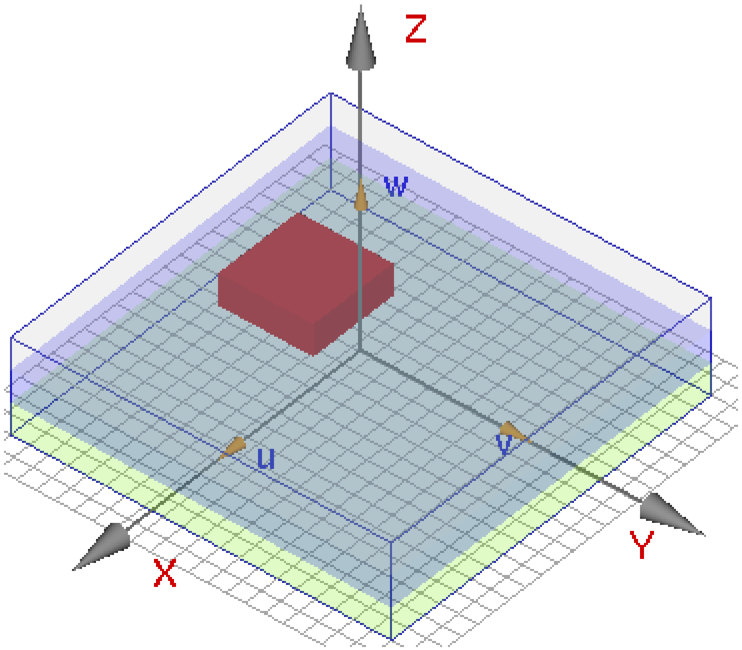


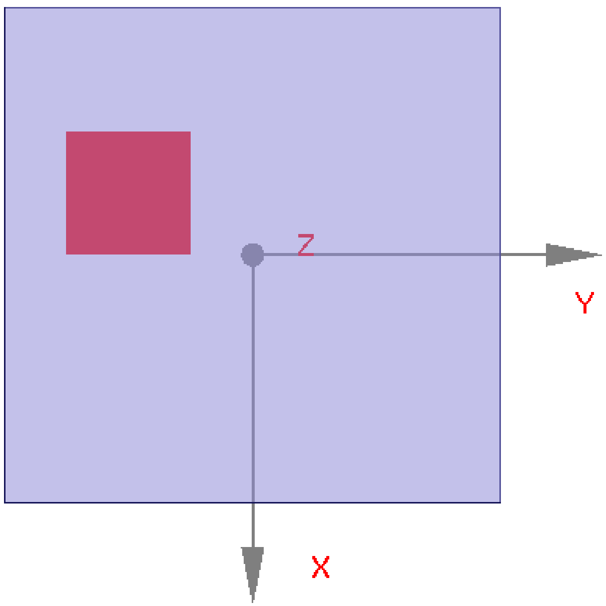
X axis is the case index in the sweeping

Demo

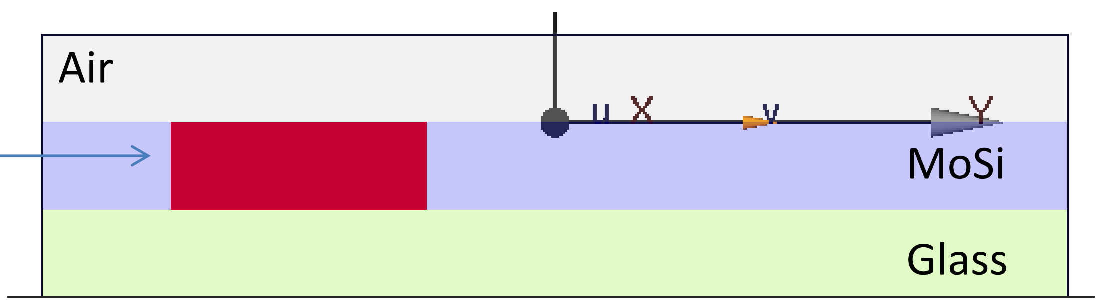
Here, we will show how to build the project for SEM simulation purpose, including the cases for the single simulation and the sweeping simulation.

Demo (1): Simulate a 3 layers structure with a hole



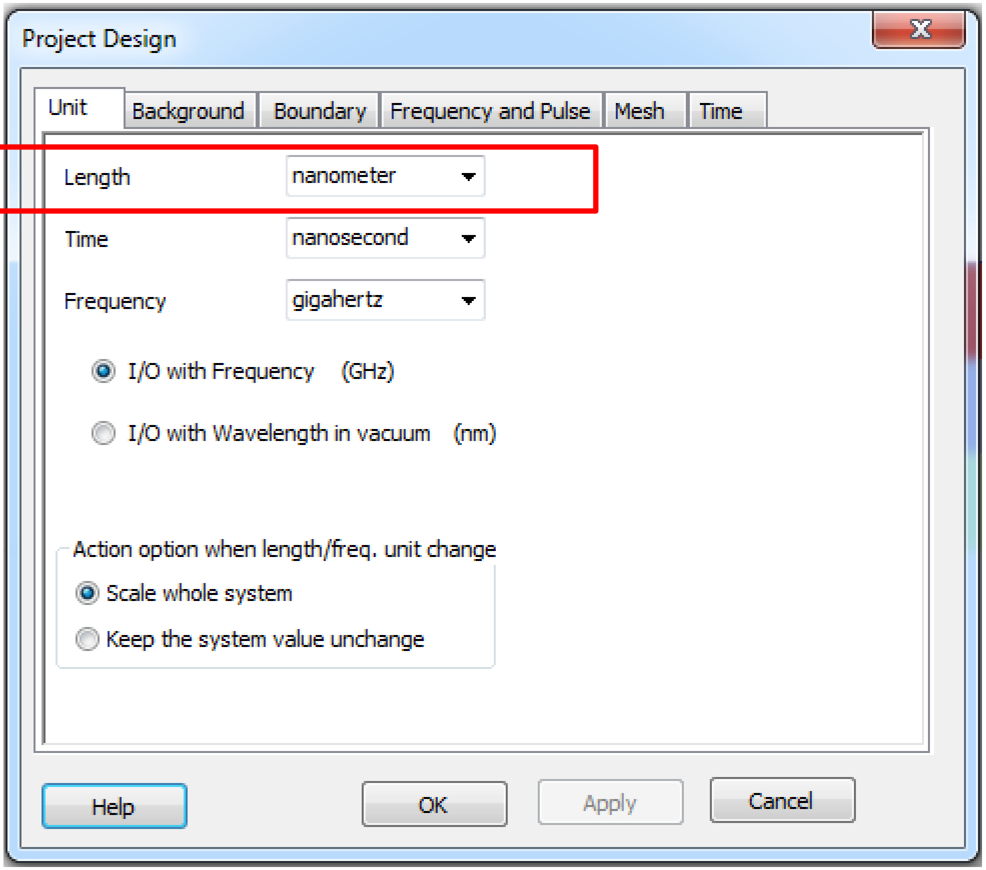


This red box is an air box in MoSi layer

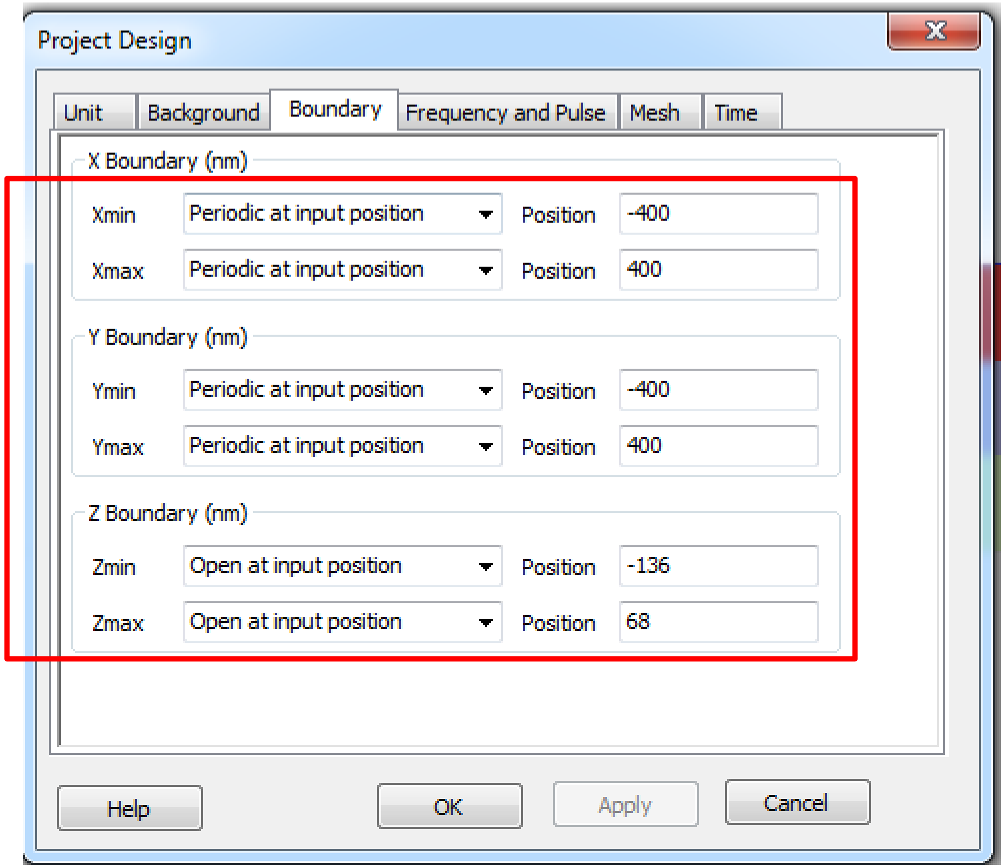


1. Define project unit as

Use nanometer as length unit

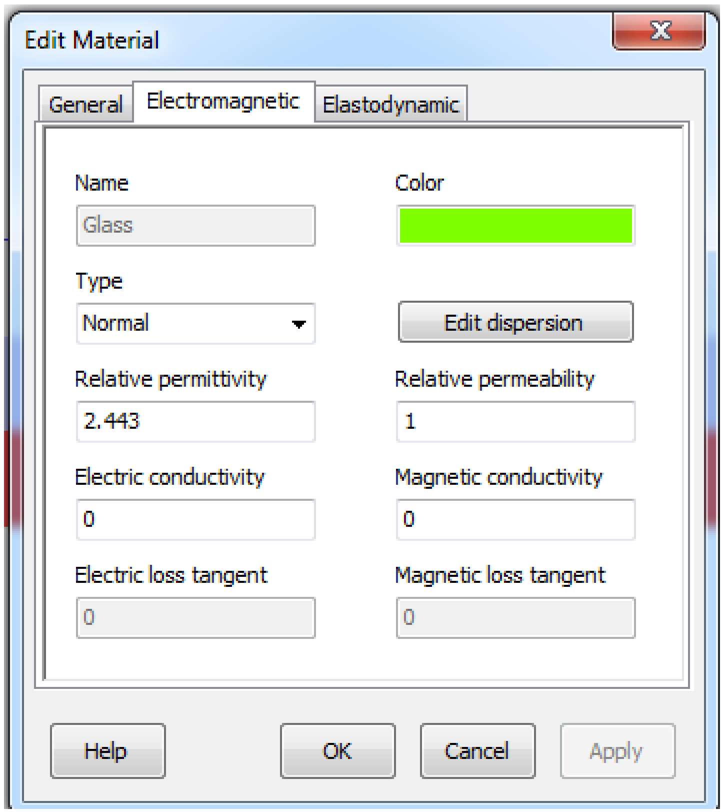


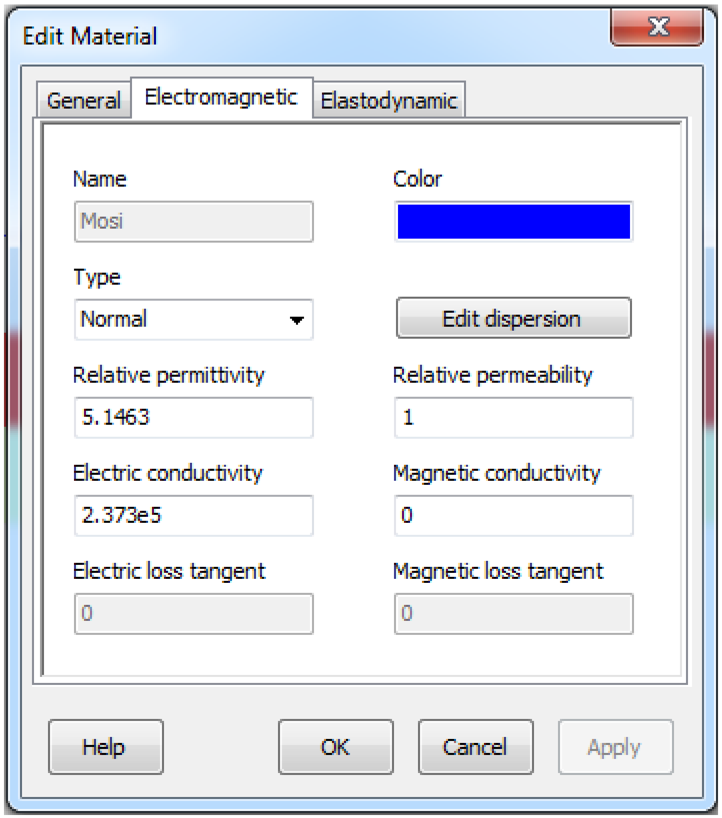
2. Boundary conditions as



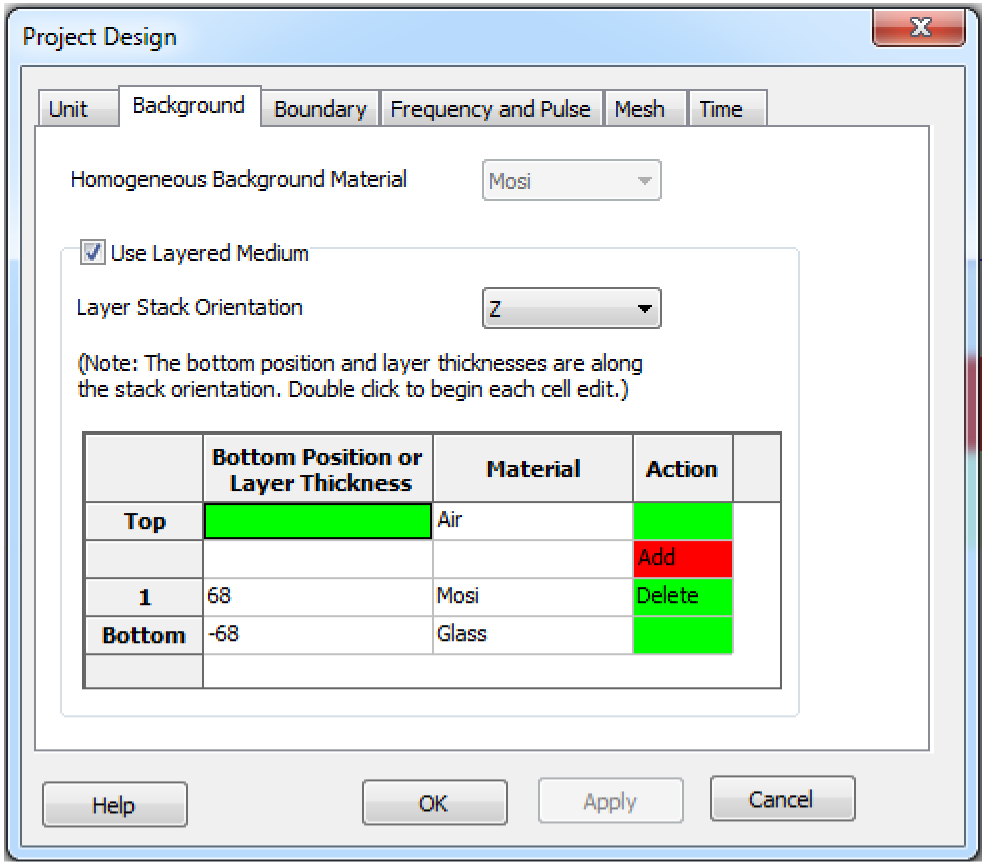
X & Y are periodic, Z is open

3. Define new material Glass & Mosi as

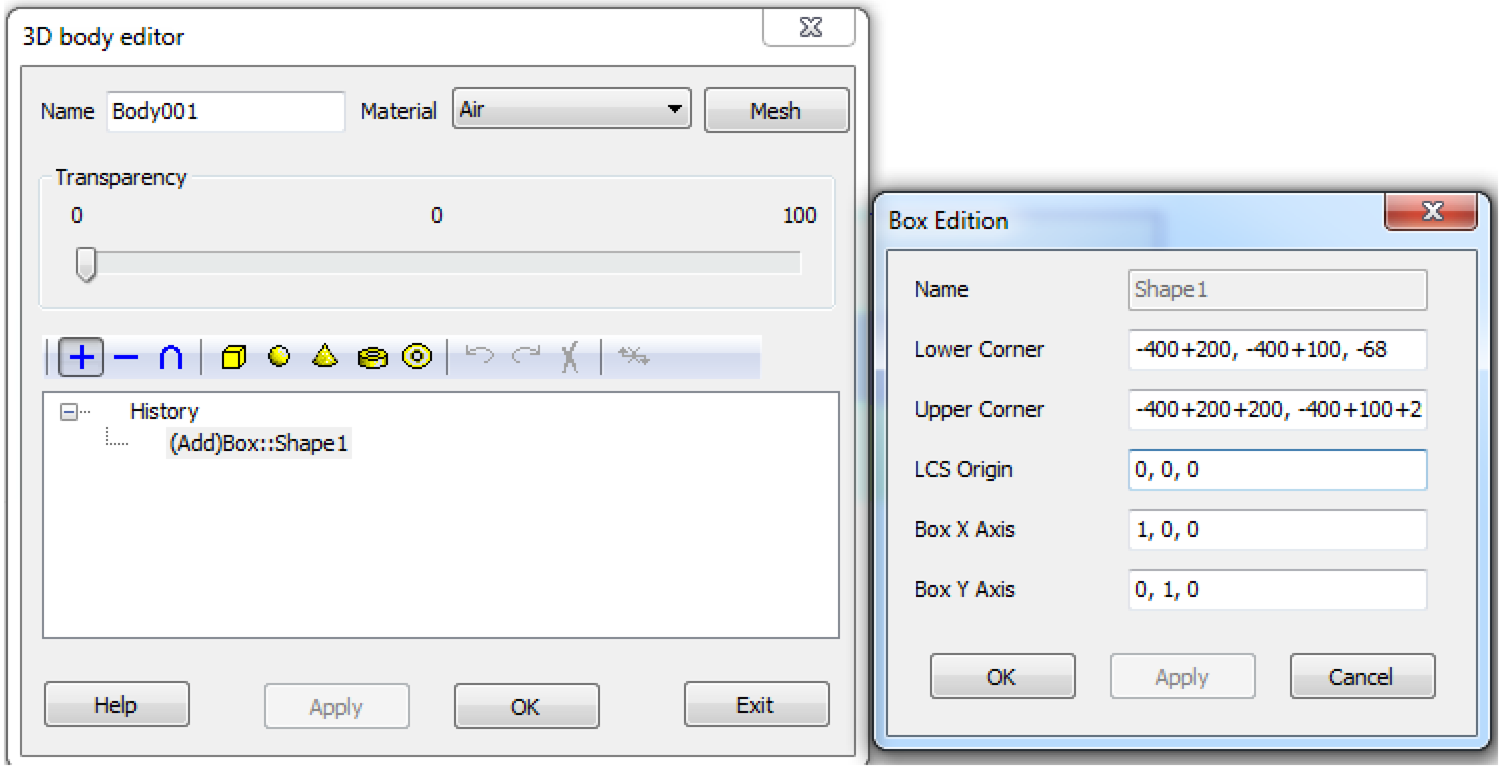




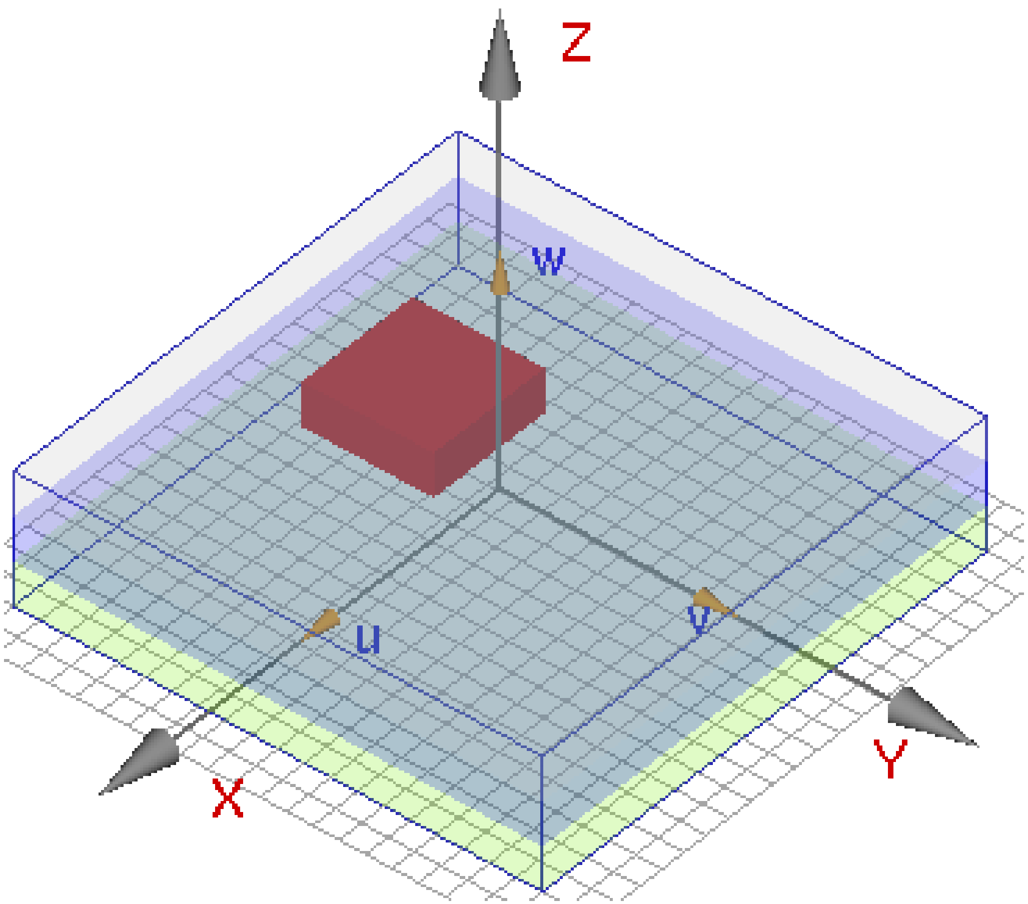
4. Define layered background



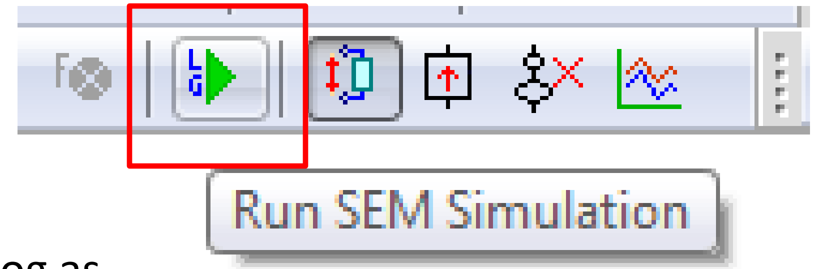
5. Place an air box in the correct position



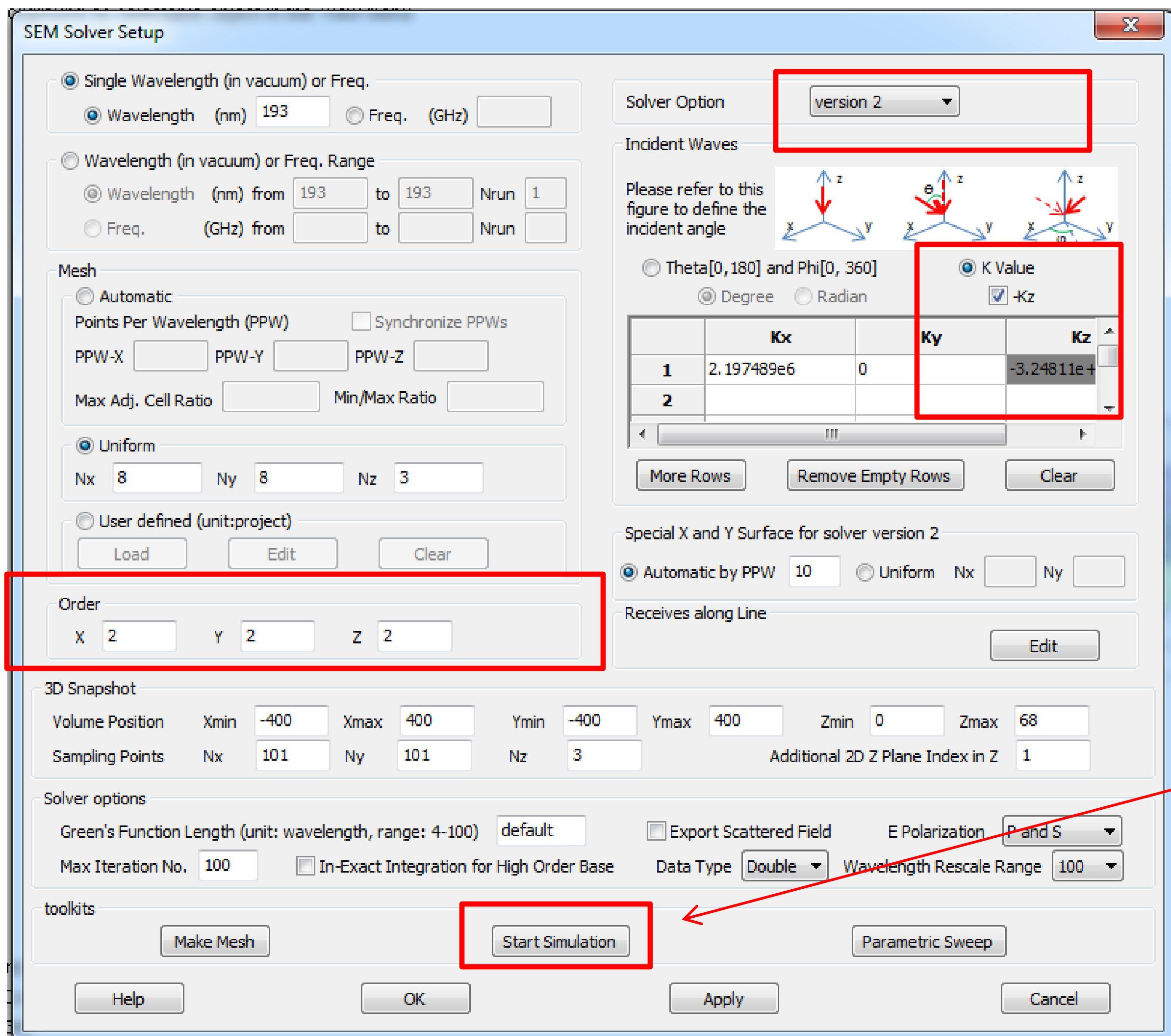
After these steps, a physical environment is build as following. Then, we will setup the SEM solver to get the near field distribution



In WCT GUI, click this button



Popup the SEM solver setting dialog as

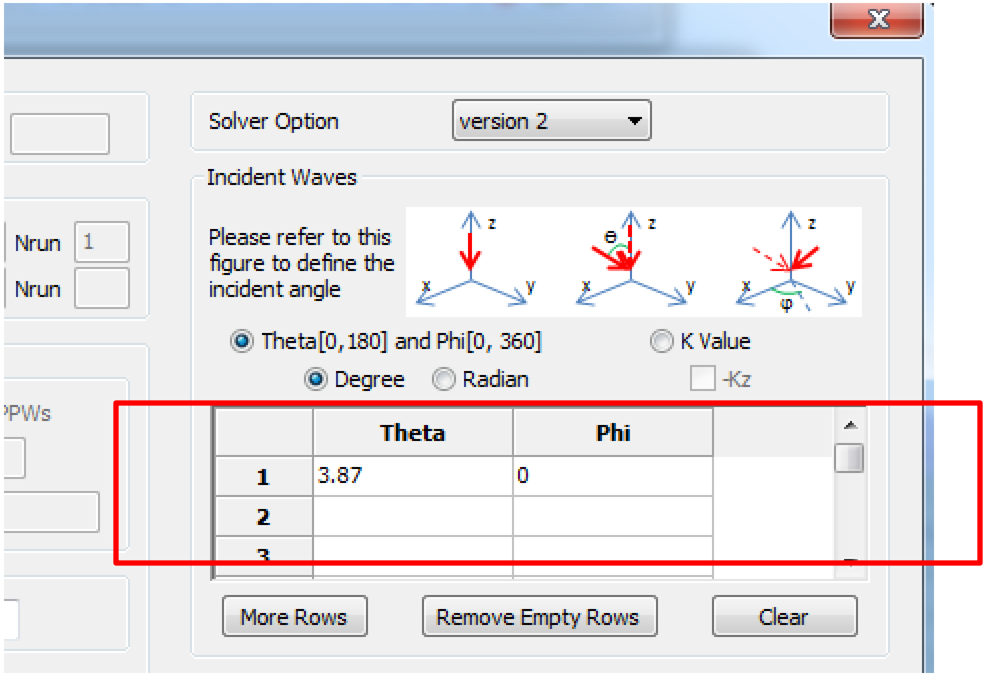


The sign of K is explained in this page

For the meaning of order, please read the next page

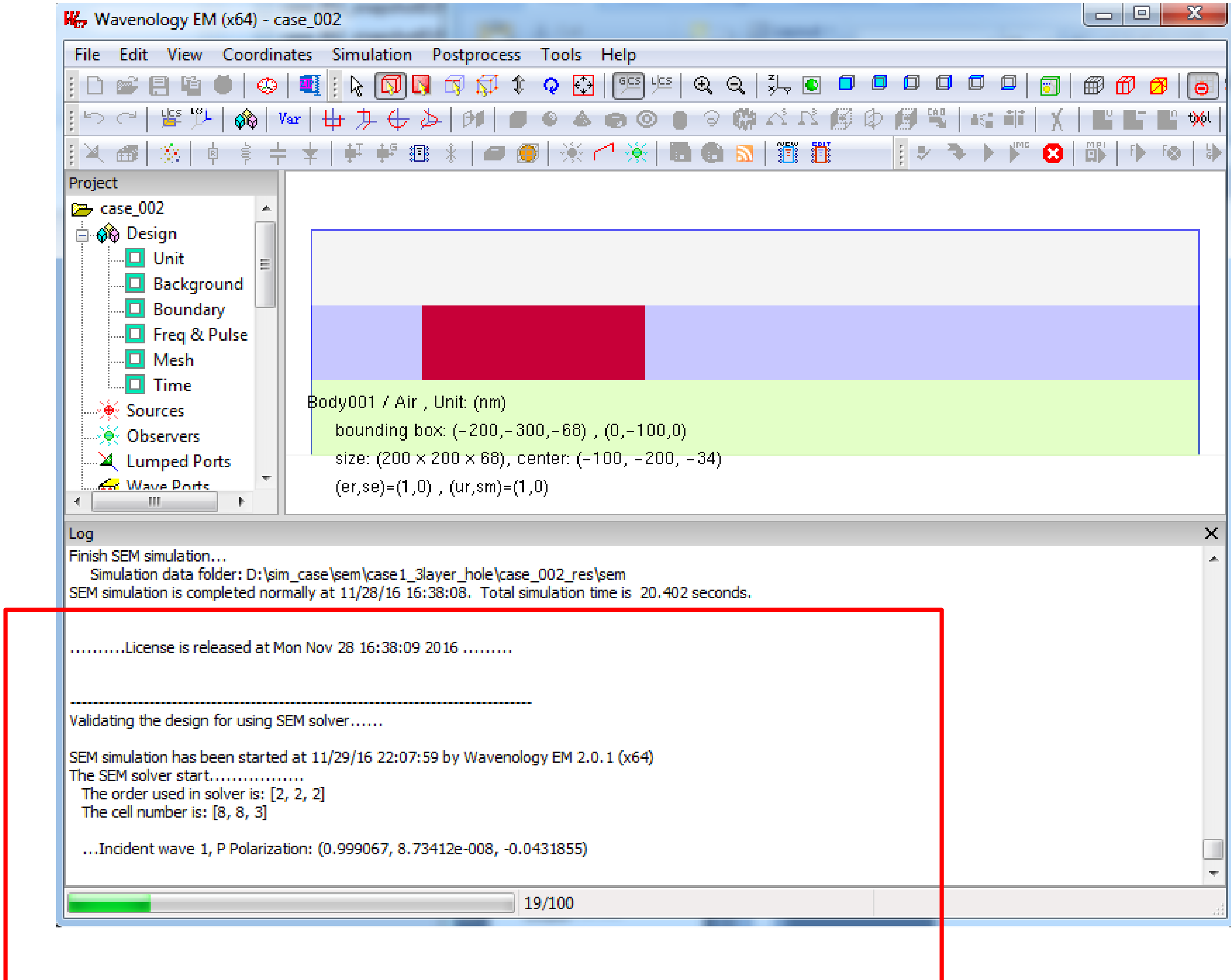
Click this button to start the SEM simulation

The incident wave can also be set up by the incident angle directly, as following



Both 2 setup for the incident wave will obtain the same simulation results.

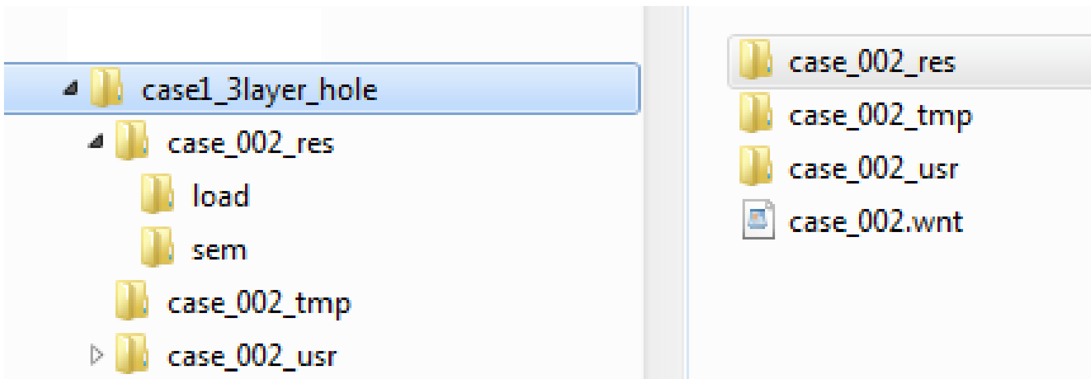
After the SEM simulation start, the simulation progress and status will be shown in WCT GUI



Simulation Results

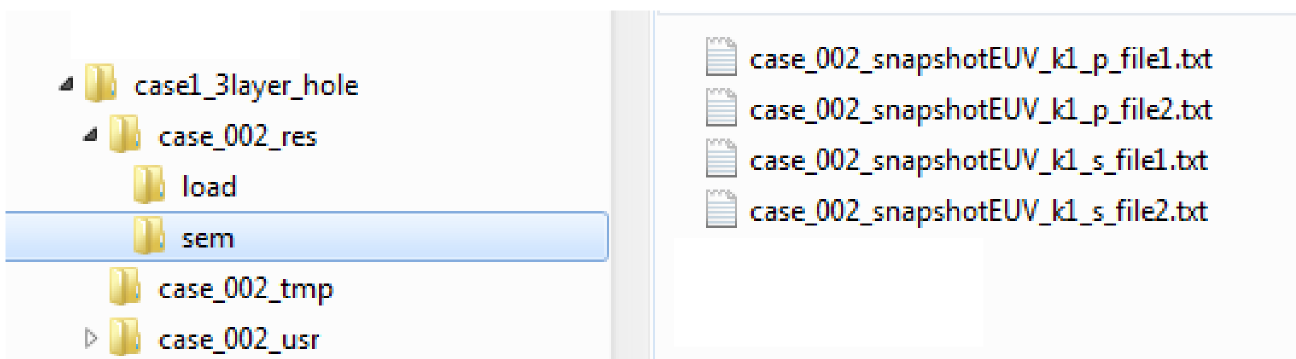
The simulation result is stored in the sub-folder: xxxx/xxxx_res/sem.
Here, xxxx is the project name.

(1) Total field only (don't set the "export scattered field" flag)



Each plane wave will create 4 files

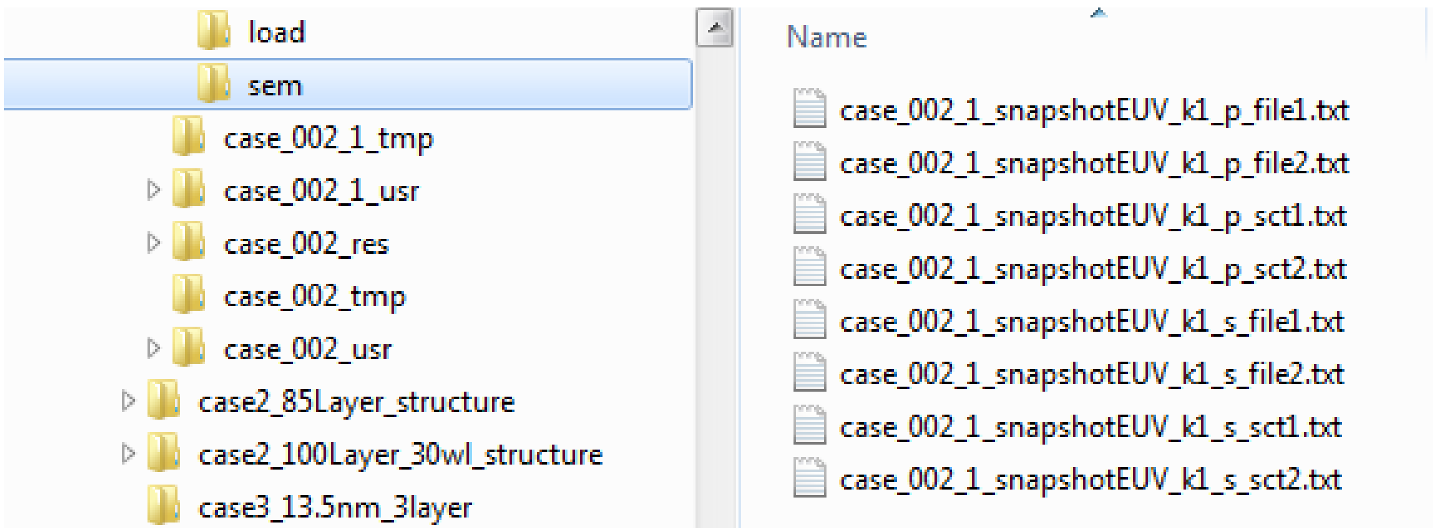
- xxxx_p_file2.txt: p polarization, the volume snapshot data
- xxxx_p_file1.txt: p polarization, additional 2D snapshot data
- xxxx_s_file2.txt: s polarization, the volume snapshot data
- xxxx_s_file1.txt: s polarization, additional 2D snapshot data



(2) Total field with scattered (set the "export scattered field" flag)

Each plane wave input will create additional 4 files for scattered field for corresponding total field

- xxx_p_sct2.txt: p polarization, the volume snapshot data
- xxx_p_sct1.txt: p polarization, additional 2D snapshot data
- xxx_s_sct2.txt: s polarization, the volume snapshot data
- xxx_s_sct1.txt: s polarization, additional 2D snapshot data



➢ SEM simulation data file format: TEXT

Each row has the E field at one sampling point.

The number of data is defined in the solver’s snapshot definition part. The output file includes the E field data only, there is not nX, nY, nZ and range information

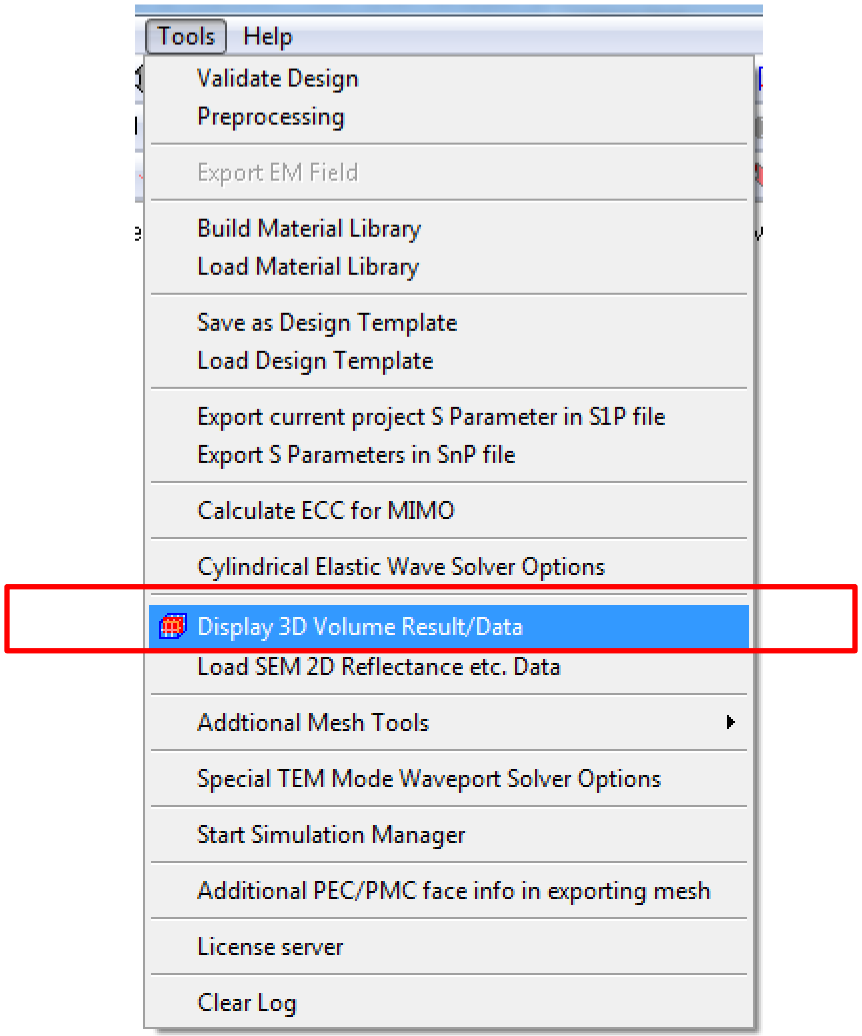
row

Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9
Pos. x	Pos. y	Pos. z	Real(ex)	Imag(ex)	Real(ey)	Imag(ey)	Real(ez)	Imag(ez)

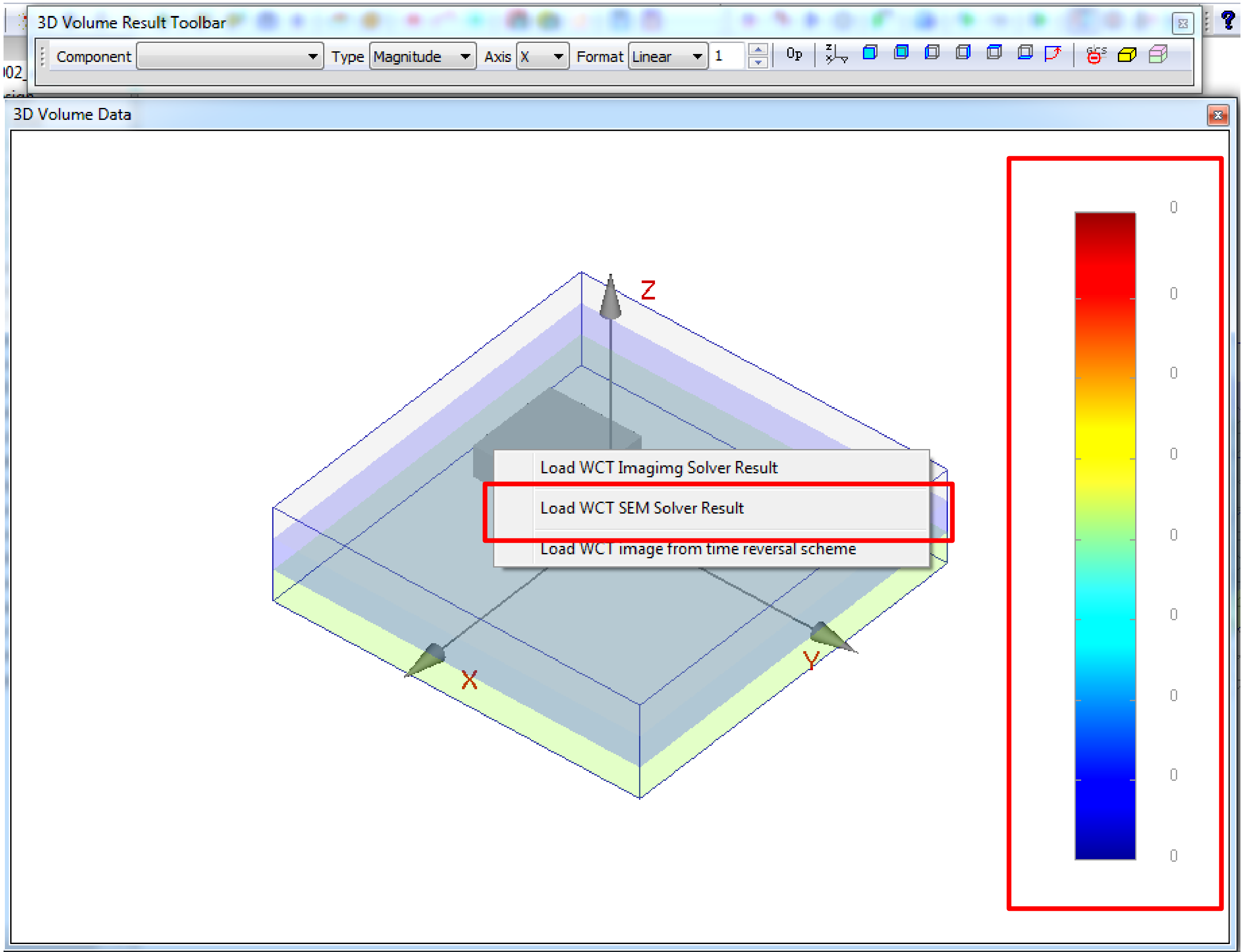
The for loop to generate the data is:

```
for x
    for y
        for z
```

Displaying 3D/2D SEM Snapshot in the GUI



In the new canvas, right click mouse to popup a menu to load SEM simulation result



Note: in displaying the SEM snapshot data. The data range for the colorbar include all data in the data file.

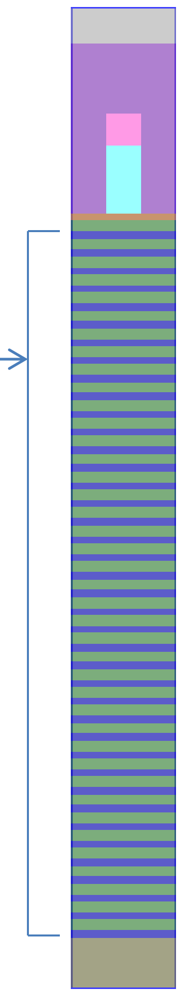
For the "xxxx_x_file2.txt", it is the volume snapshot data. Therefore, the shown single frame may not cover the full range the data range shown by the colorbar.

For the "xxxx_x_file1.txt", it is a single frame in the volume snapshot. Therefore, the shown single frame will cover the full range shown by the colorbar.

Demo (2): Building a EUV case with 85 layered structures

Because the demo case 1 is already go through the whole procedure of simulating a WCT SEM project. Here, we will demonstrate how to build the layered background in a EUV simulation.

For a typical EUV case, there are 40 bi-layers at the domain bottom, there are 2 ways to build these layers,



- use array of boxes: these boxes touches the XY boundary
  - advantage: in general, 3 actions are required to build this 80 layers
  - disadvantage: when this case need to modify the size in X or Y, user need to modify the boundary position and boxes size also, each direction need 1-2 actions

- build 80 layers one by one manually in the layered background setting
  - advantage: when this case need to modify the size in X or Y, user only need to modify the boundary position, 1 action
  - disadvantage: user need to build 80 layers one by one, 80 actions for the 1st case.

Following is the steps to build these 80 layers

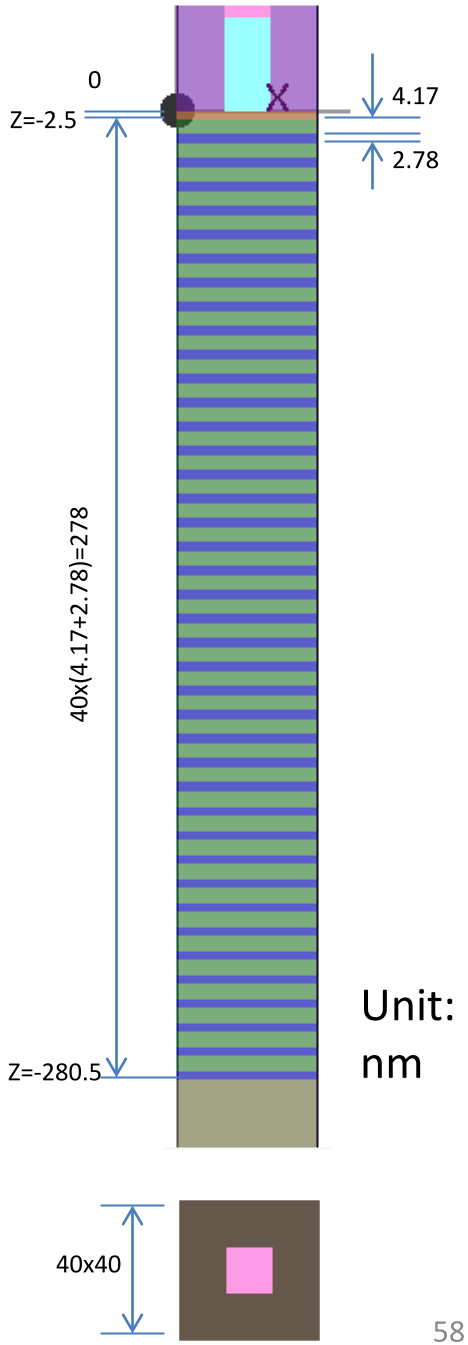
We assume the materials used in this project has been created, the materials for this bi-layers is **layer1** and **layer2**, respectively. The project's unit in length is ***nm***.

The Z position of bottom layers is shown as the figure,

The layer with the material layer1 has a thickness as 2.78 nm; the layer with the material layer2 has a thickness as 4.17 nm.

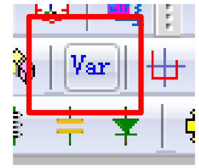
The Z position of the lowest interface for these bi-layers is -280.5 nm, as shown in the figure.

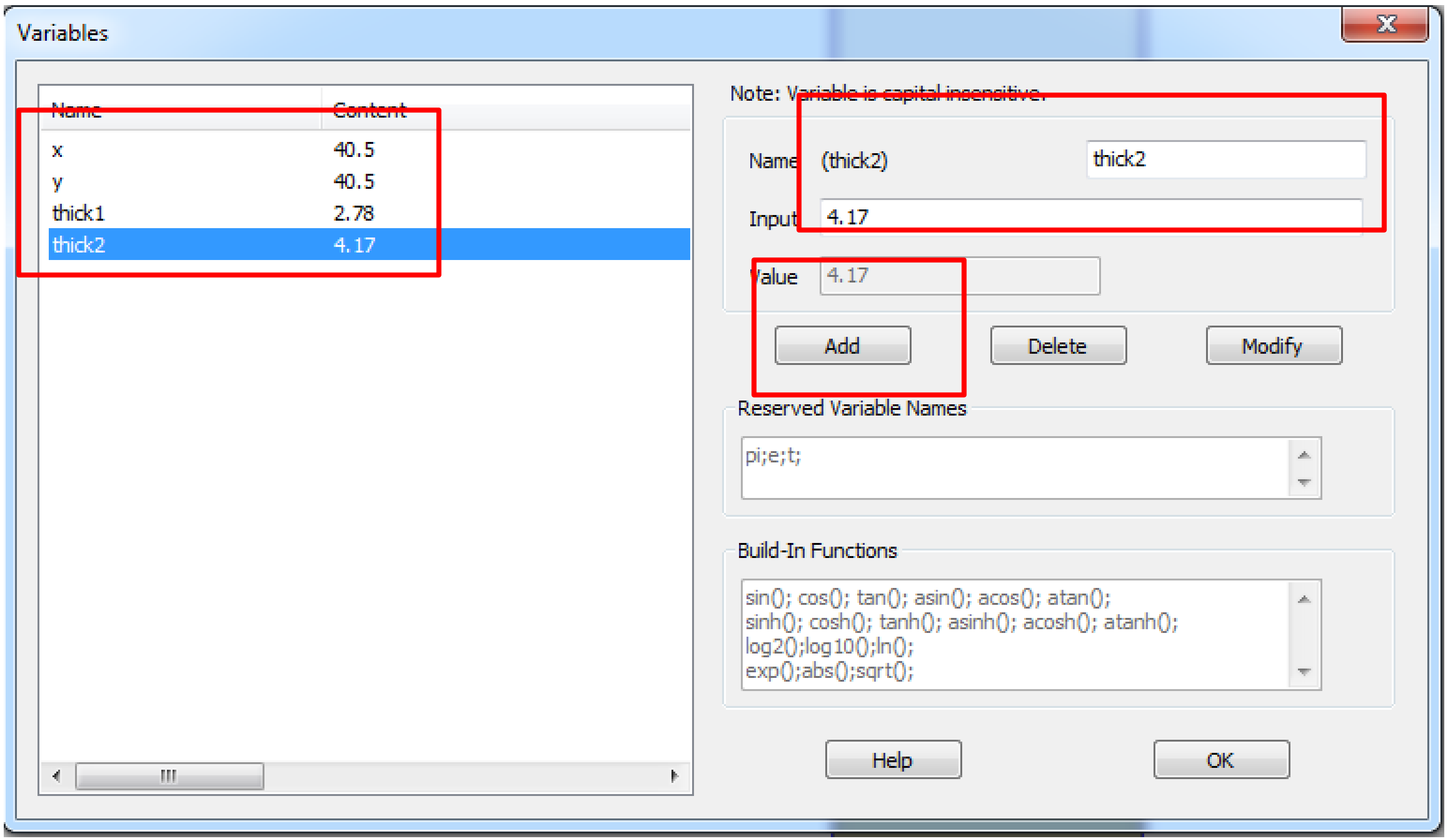
The domain size in X and Y both are 40 nm.



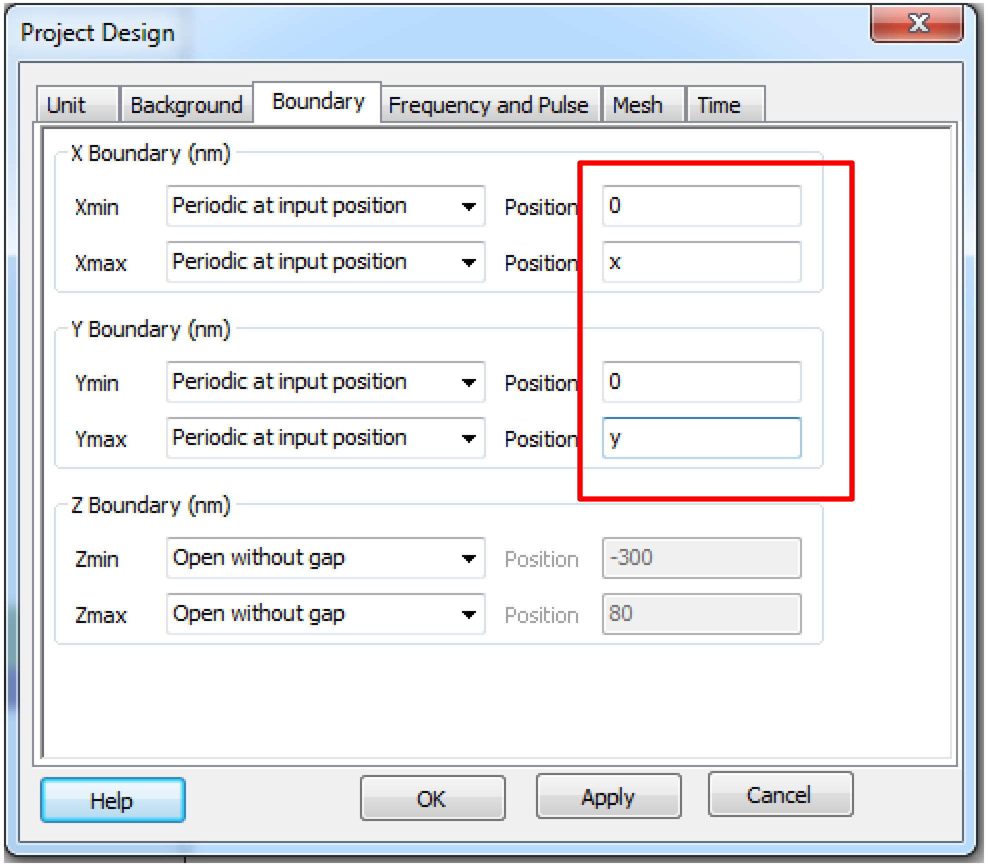
Method (1): Using “Array Copy” on 2 boxes to generate 40 bi-layers

1. We define variables: x=40.5, y= 40.5, thick1=2.78, thick2=4.17

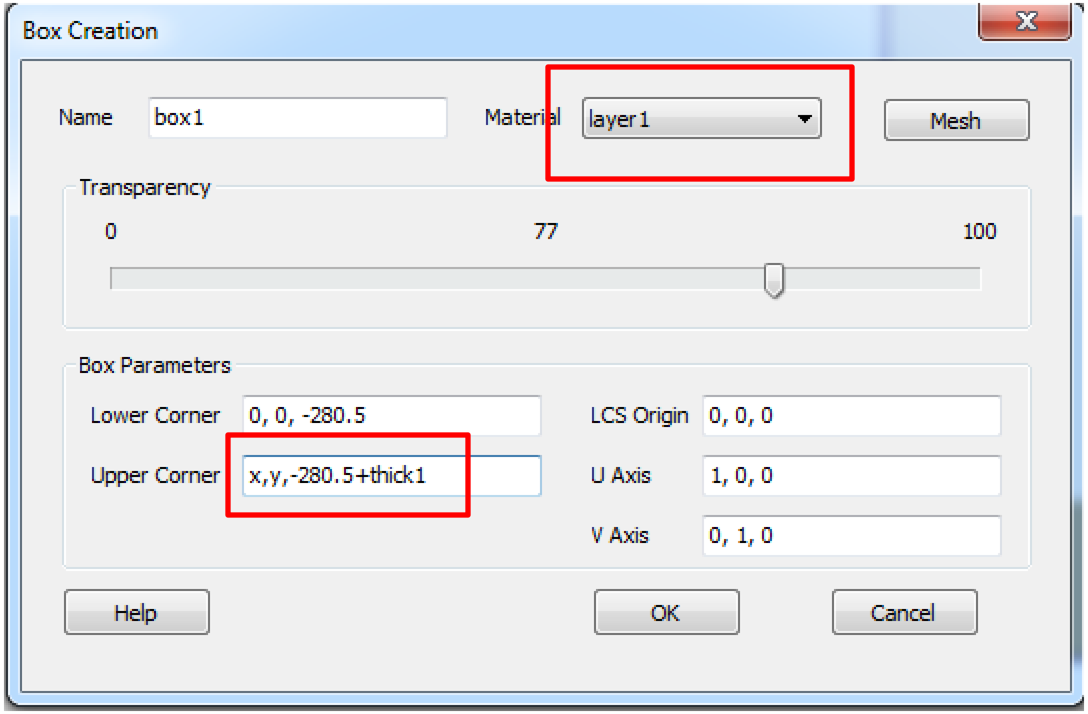




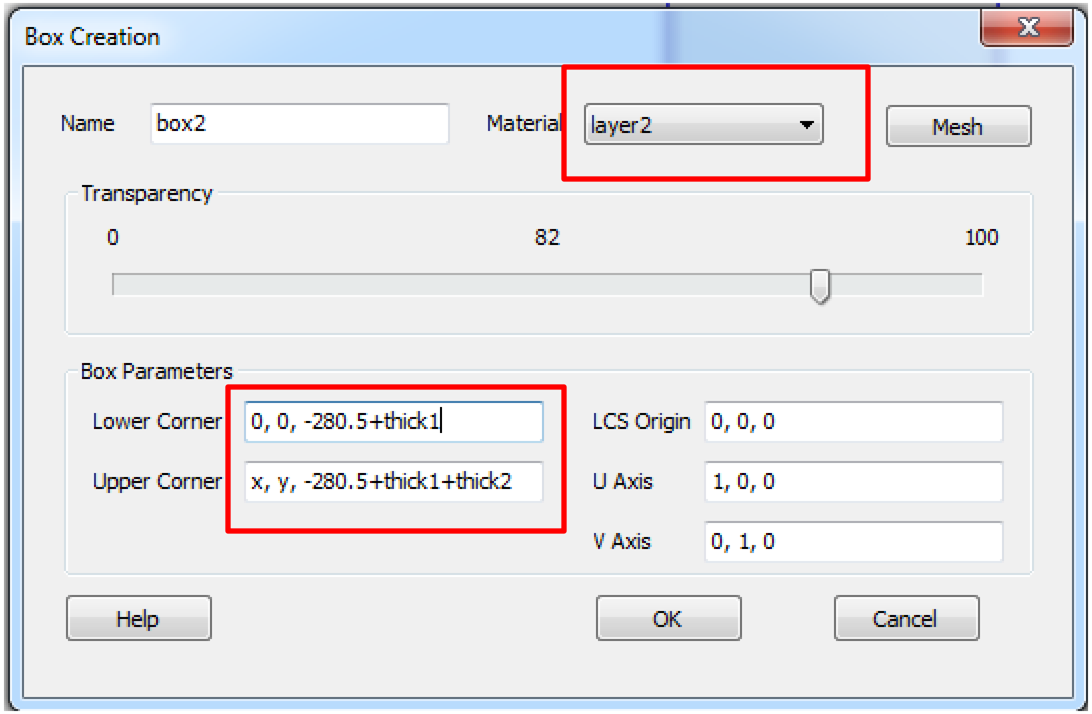
2. Set project size as following



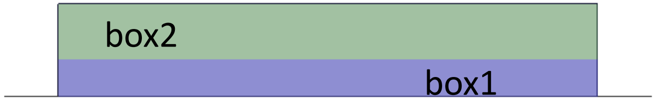
2. Build 1st box as following input



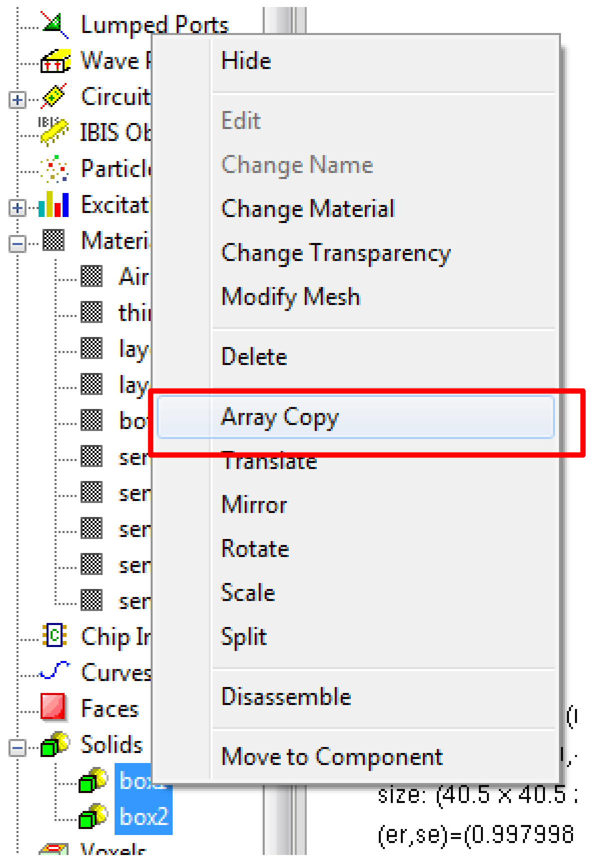
3. Build 2nd box as following input

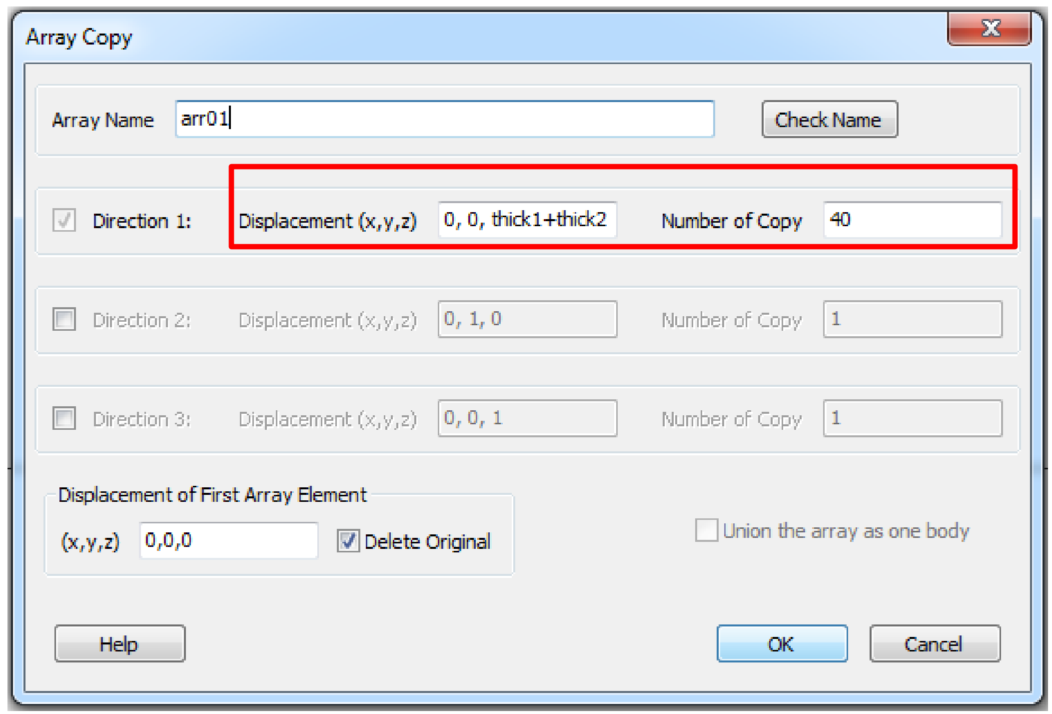


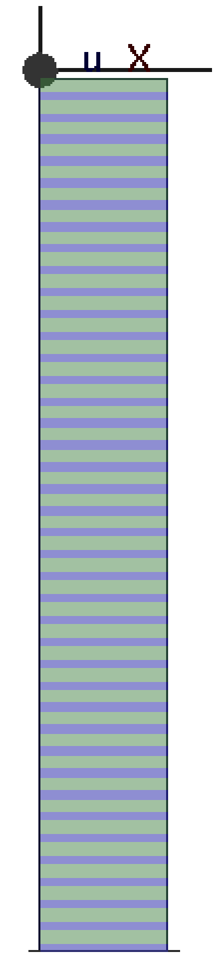
Then, we can see these 2 boxes shown as the right figure.



4. Then, select “box1” & “box2”, making “Array copy”, with following inputs, the 40 bi-layers can be created.



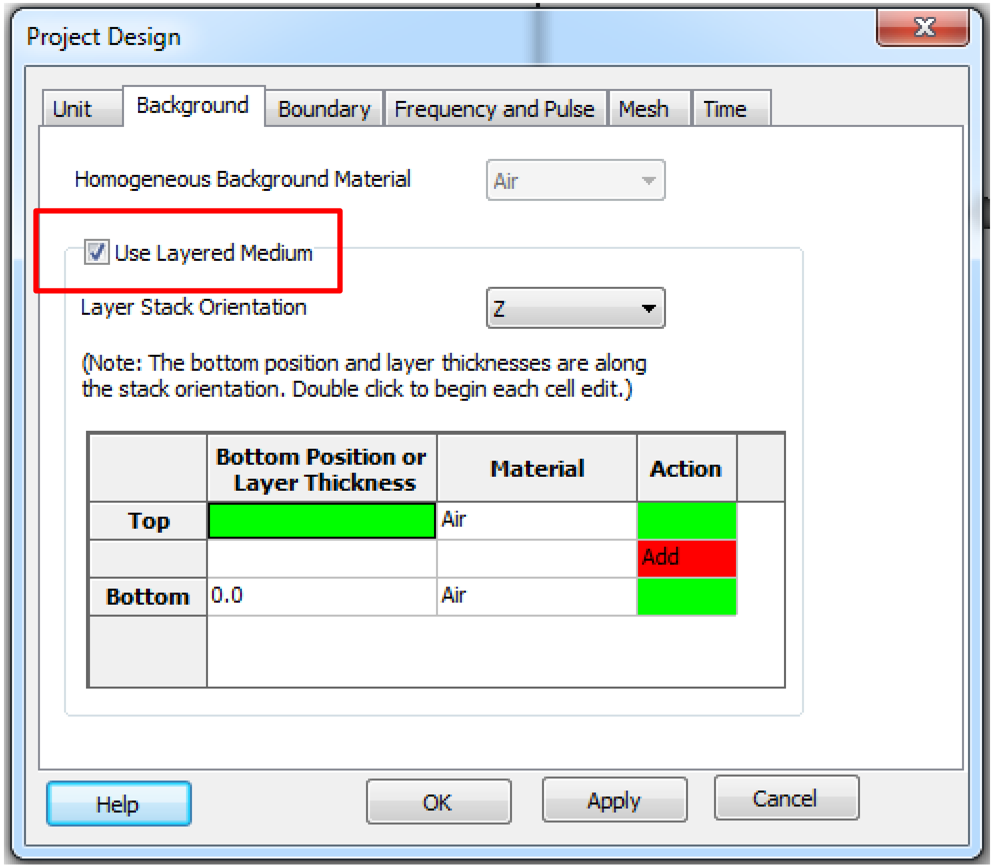




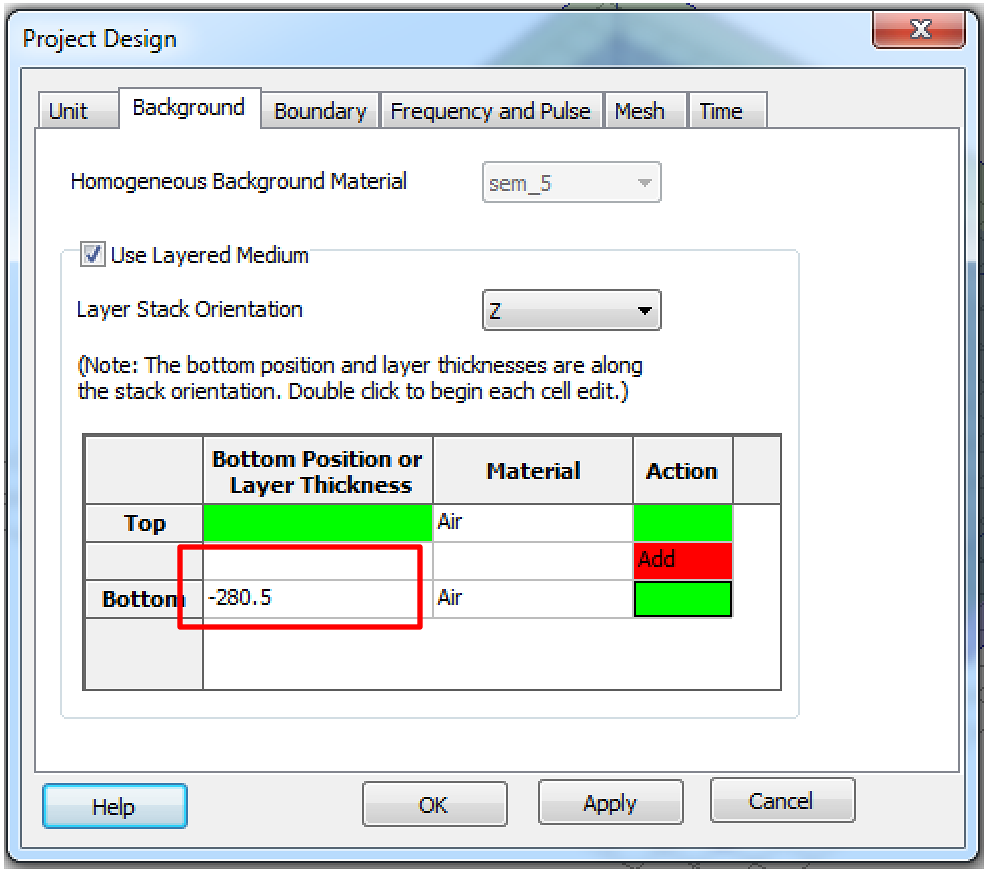
5. After this 40 bi-layers are created, others structures can be built on the top of these layers.

Method (2): Directly building 80 layers one by one

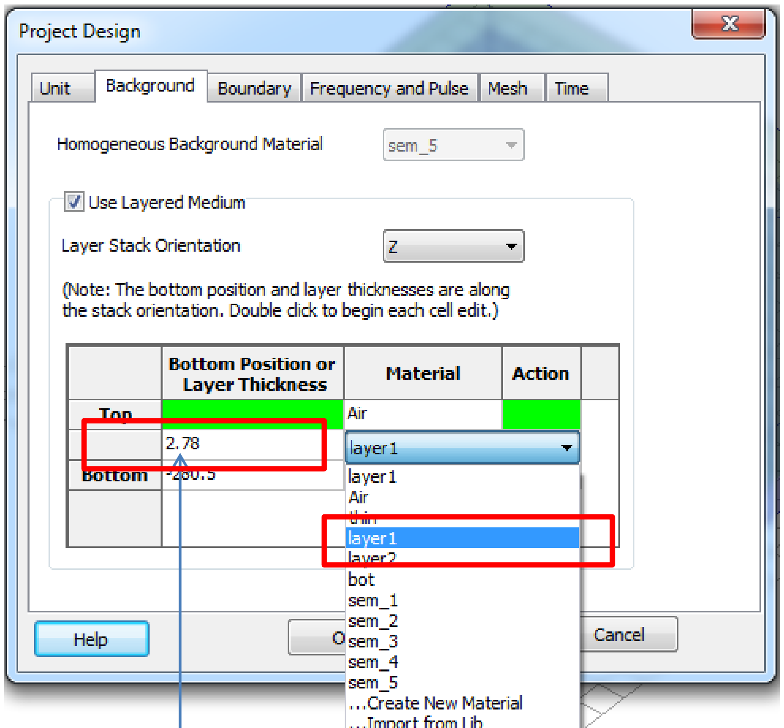
1. Go to the “Project Design” dialog, switch to “Background” page, enable “Use Layered Medium” option

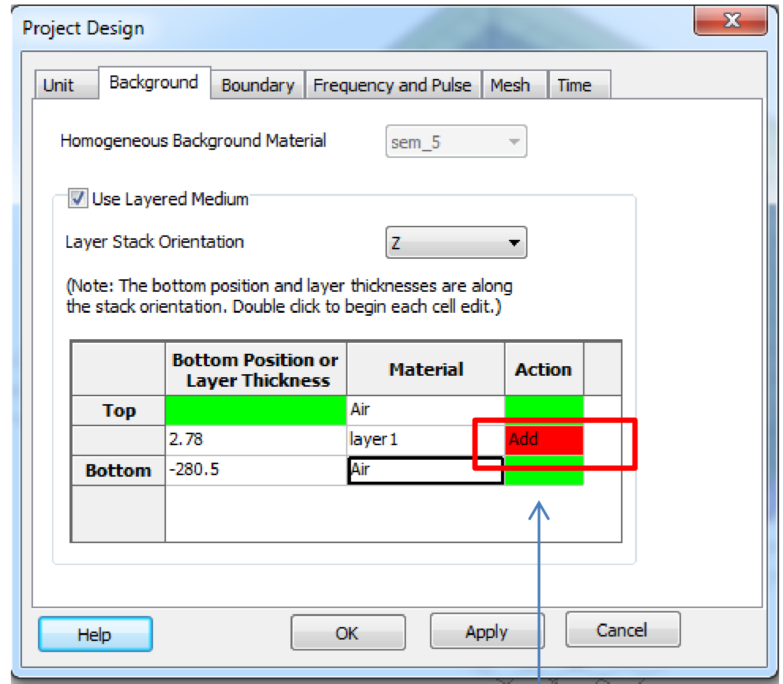


2. Define the bottom interface is “-280.5”, below this interface, the material is “Air”



3. Then add the 1st layer as following operations





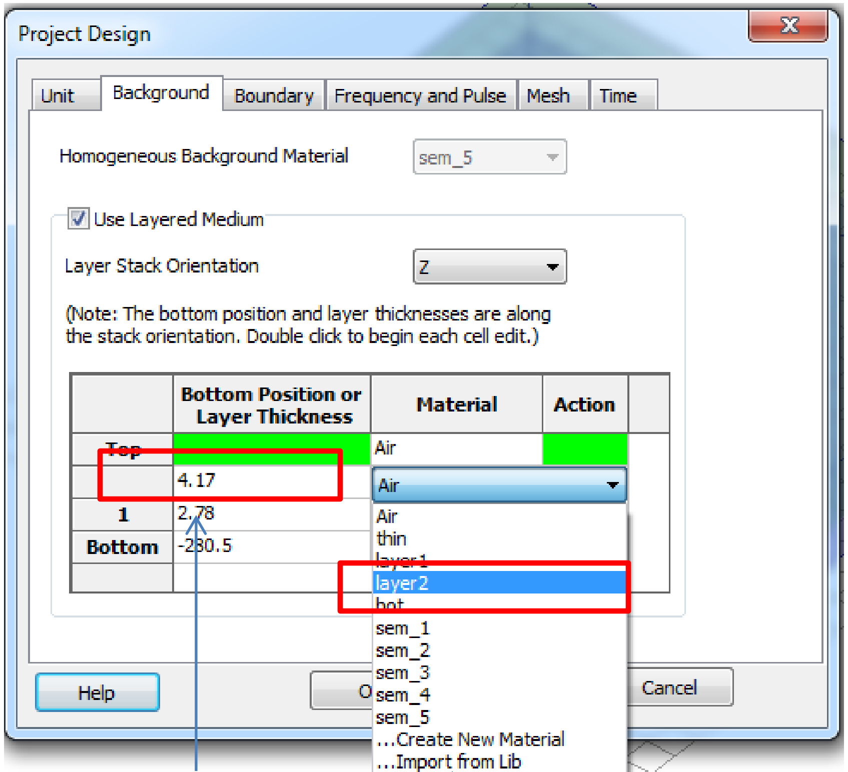
Input the layer thickness as "2.78"

Double click the material box to select the material for this layer as "layer1"

Click "Add" to generate this layer

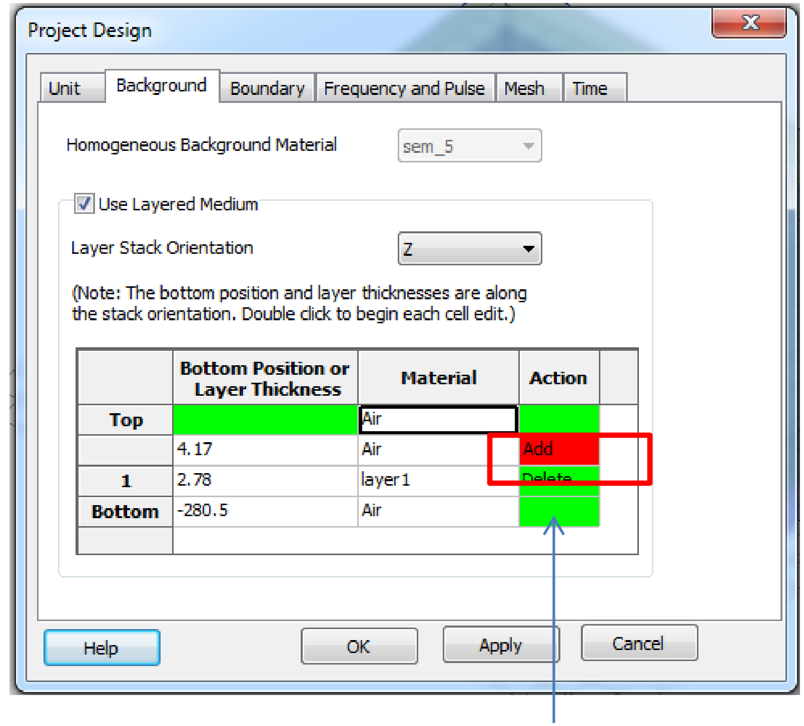
	Bottom Position or Layer Thickness	Material	Action
Top		Air	
			Add
1	2.78	layer1	Delete
Bottom	-280.5	Air	

4. Then add the 2nd layer as following operations



Input the layer thickness as "4.17"

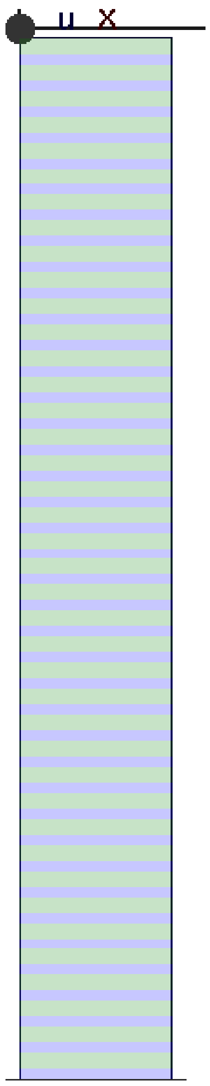
Double click the material box to select the material for this layer as "layer2"



Click "Add" to generate this layer

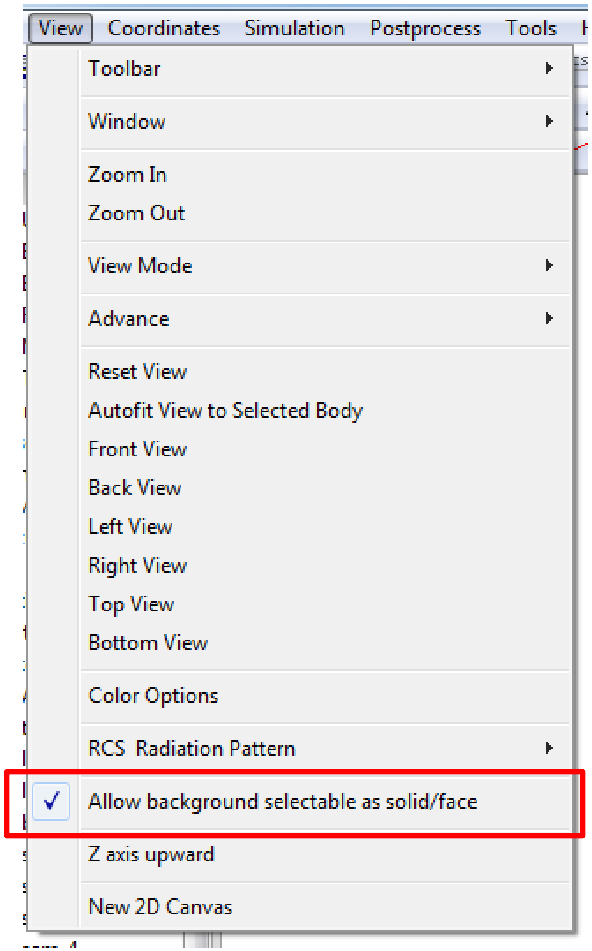
	Bottom Position or Layer Thickness	Material	Action
Top		Air	
			Add
2	4.17	Air	Delete
1	2.78	layer1	Delete
Bottom	-280.5	Air	

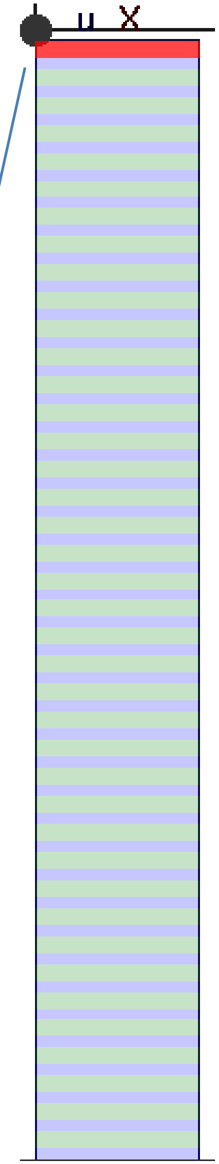
5. Repeat step 3 & 4 to create all 80 layers.



6. After this 40 bi-layers are created, others structures can be built on the top of these layers.

User can use following action to check whether each layer is correct or not.





Hit each layer in the 3D canvas

Check layer's information in the screen

Background / layer2 , Unit: (nm)
bounding box: (0,0,-6.67) , (40.5,40.5,-2.5)
size: (40.5 x 40.5 x 4.17) , center: (20.25,20.25,-4.585)
(er,se)=(0.997998,4492) , (ur,sm)=(1,0)

If user thinks that input 80 layers by hand is too tedious, he can use a simpler way to define this 80 layers by editing the WNT file directly.

- after steps 3 & 4, 2 layers are created.
- close the project & close WCT GUI
- use “Wordpad” or “Notepad” to open the project’s WNT file, user can see the information for these 2 layers

```
Background {
    Layered-Medium {
        Direction   Z
        Bottom {
            Material   Air
            Positoin   -280.5
        }

        Layer { // 1
            Material   layer1
            Positoin   2.78
        }
        Layer { // 2
            Material   layer2
            Positoin   4.17
        }

        Top {
            Material   Air
        }
    }
}
```

Copy & Paste these 2 layers to make it to 80 layers.

Then, save this WNT file and quit “Wordpad”.

Use WCT GUI to open this project again.

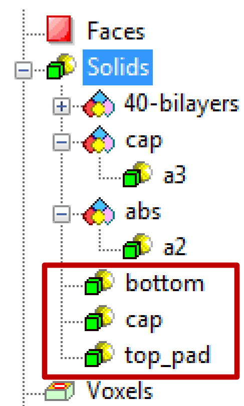
```
Bottom {
    Material   Air
    Positoin   -280.5
}

Layer { // 1
    Material   layer1
    Positoin   2.78
}
Layer { // 2
    Material   layer2
    Positoin   4.17
}
Layer { // 1
    Material   layer1
    Positoin   2.78
}
Layer { // 2
    Material   layer2
    Positoin   4.17
}
Layer { // 1
    Material   layer1
    Positoin   2.78
}
Layer { // 2
    Material   layer2
    Positoin   4.17
}
.....
Top {
    Material   Air
}
```

Demo (3): a Simple way to build a EUV case by modifying existing template

- In the WCT SEM demo package, there are 2 template projects for EUV applications
  - These 2 cases are in the sub-folder: **EUV_templates**

A. For the case using all layers built by boxes

- the project is: .**layer_by_box\case_3.wnt**
- user can modify these data to fit the new setting, then can start the simulation directly

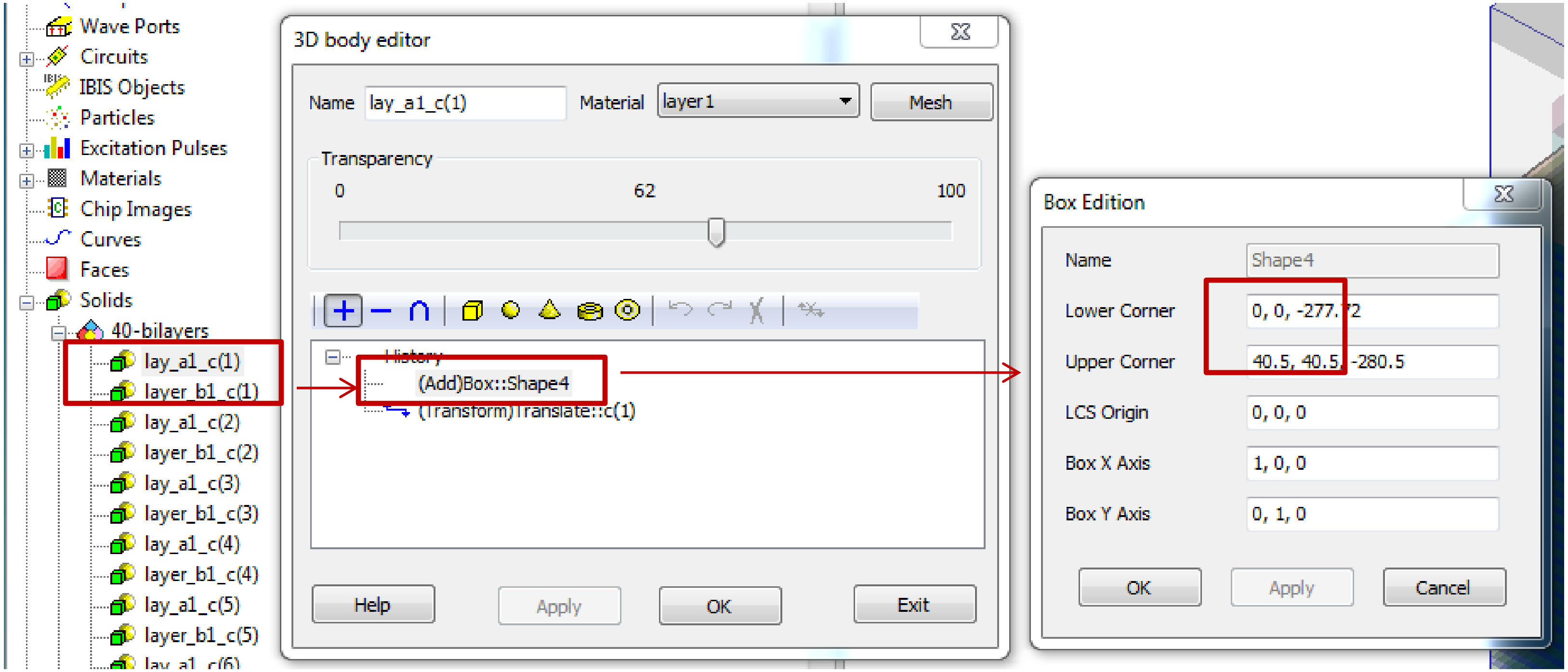


1) The X & Y size of the project boundary

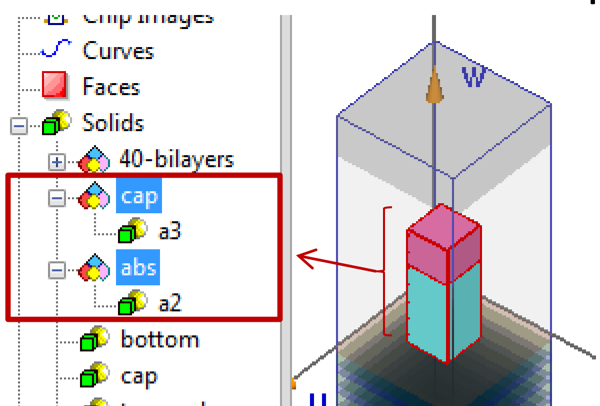
2) The X & Y size of all boxes working as the layers
   - The cap, top_pad, bottom

(continue to the next page)

➢The base box in lay_a1_c(1) & layer_b1_(c1) Cont.



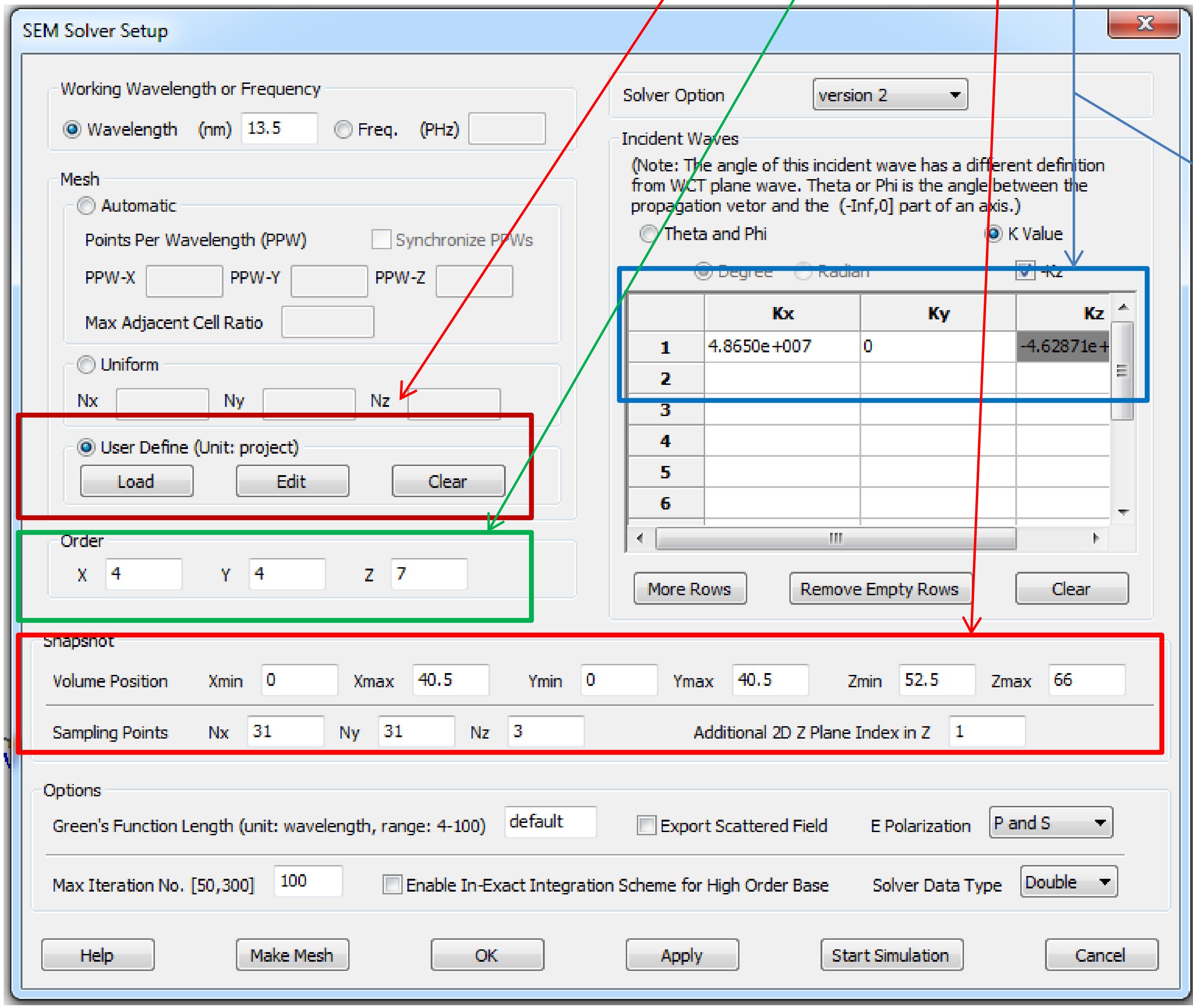
3) Use the Mask editor to make a complicated mask, or generate several boxes for a simple mask

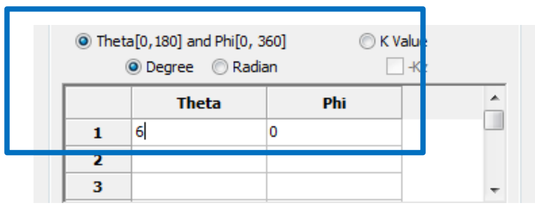


(continue to the next page)

Cont.

4) Define the new mesh grid, plane wave incident angle (or propagation K), order, snapshot range, then user can start the simulation.





Both 2 setup for the incident wave will obtain the same simulation results.

Cont.

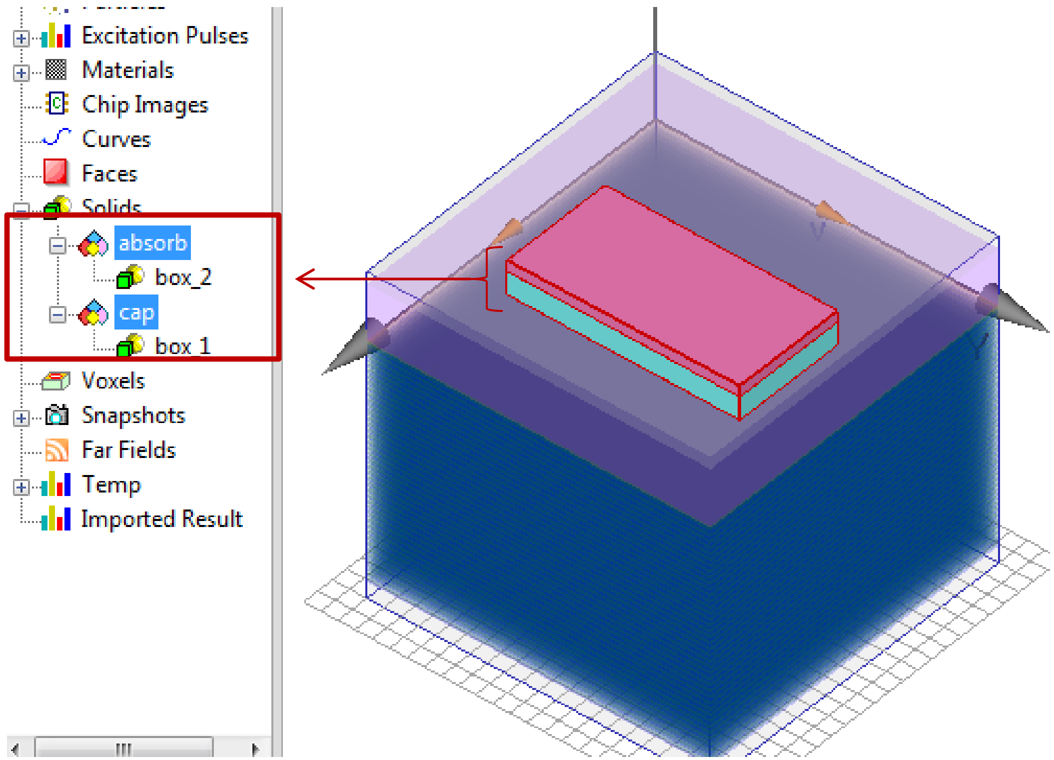
B. For the case defining the background by layered media

➢ the project is: .**pure_layer\case_30_layer.wnt**

➢ user can modify these data to fit the new setting, then can start the simulation directly

1) The X & Y size of the project boundary

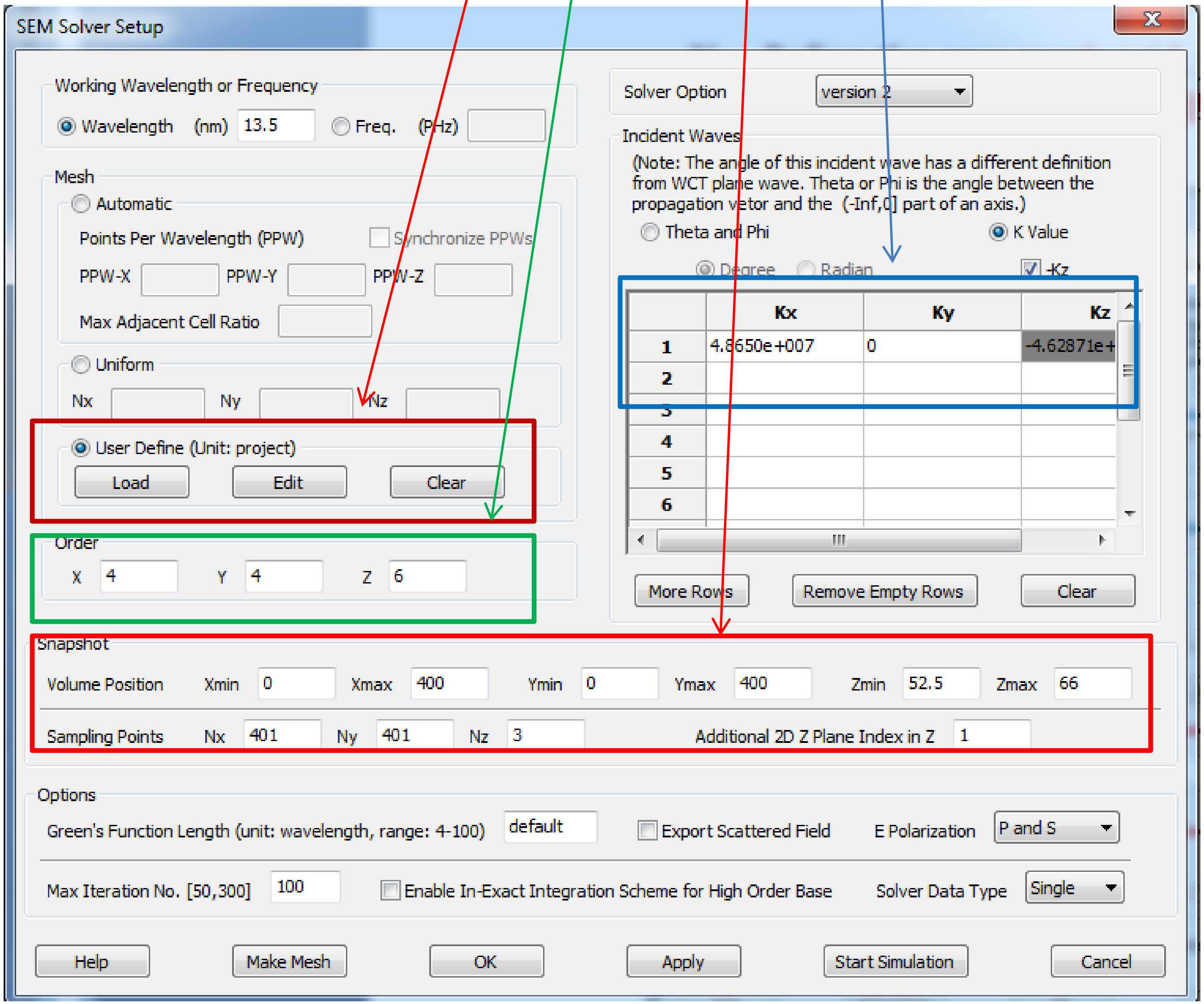
2) Use the Mask editor to make a complicated mask, or generate several boxes for a simple mask



(continue to the next page)

Cont.

3) Define the new mesh grid, plane wave incident angle (or propagation K), order, snapshot range, then user can start the simulation.



Demo (4): Sweeping Frequency/Wavelength

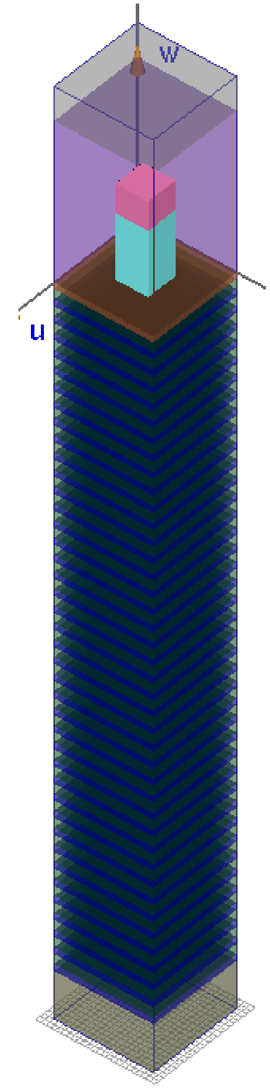
In this demo, we will show how to sweep a range of wavelength.

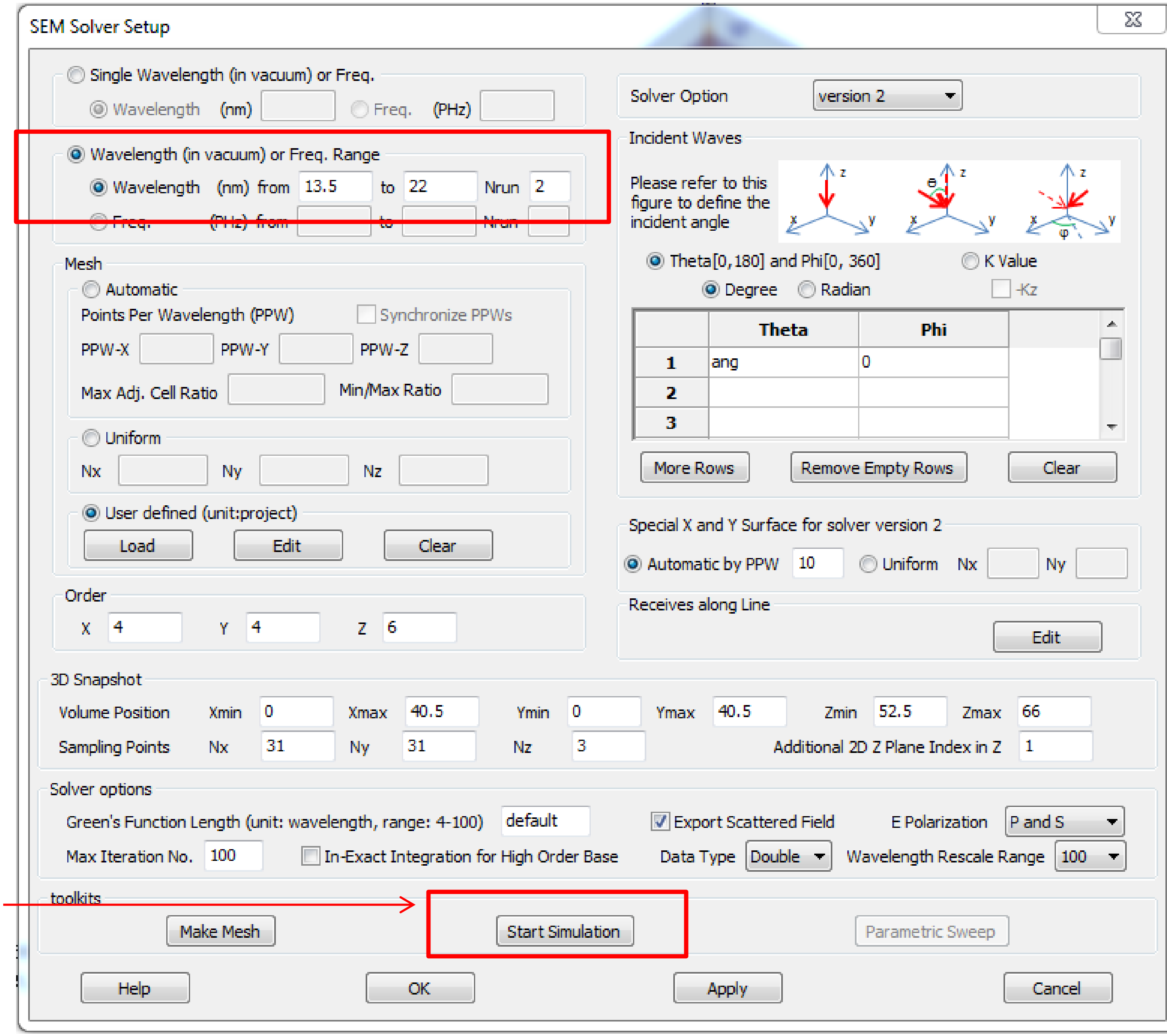
The base case is the one in demo (2), as shown in the right figure. Here, we will sweep the wavelength from 13.5nm to 22nm, by 2 runs, which is equal to:

wl_min=13.5
wl_max=22
Nrun=2
step = (wl_max - wl_min)/(Nrun-1)=8.5

The wavelength for each simulation case is:
[13.5, 13.5+8.5]=[13.5, 22]

The sweep setup is shown in the next page.





After all setup are ready, "Start Simulation"

The simulation data files

Name

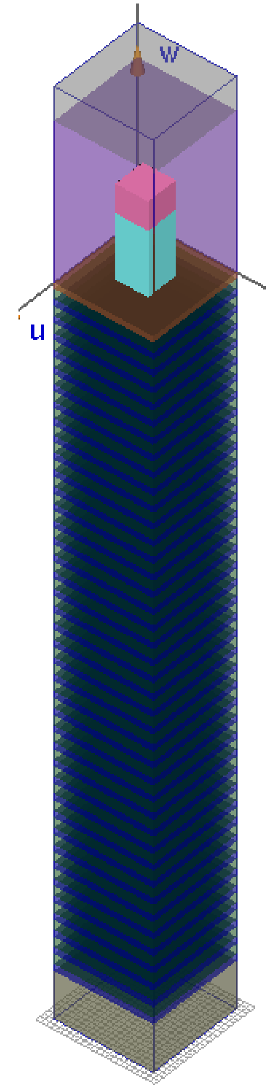
- case_3_eng2_sweep_1_rta_p_sweep.txt
- case_3_eng2_sweep_1_rta_s_sweep.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_file1_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_file1_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_file2_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_file2_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_sct1_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_sct1_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_sct2_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_p_sct2_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_file1_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_file1_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_file2_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_file2_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_sct1_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_sct1_wl_22.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_sct2_wl_13.5.txt
- case_3_eng2_sweep_1_snapshotEUV_k1_s_sct2_wl_22.txt

The working wavelength for each case in the sweep is shown in the file name.

Demo (5): Parametric Sweeping

In this demo, we will show how to sweep parameters in the project.

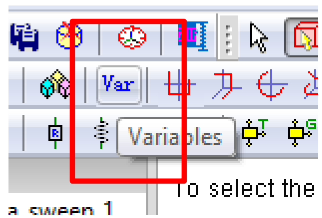
The base case is the one in demo (2), as shown in the right figure. However, we use variable “freq” to define the SEM solver working frequency, and use variable “ang” to define the plane wave source incident angle.



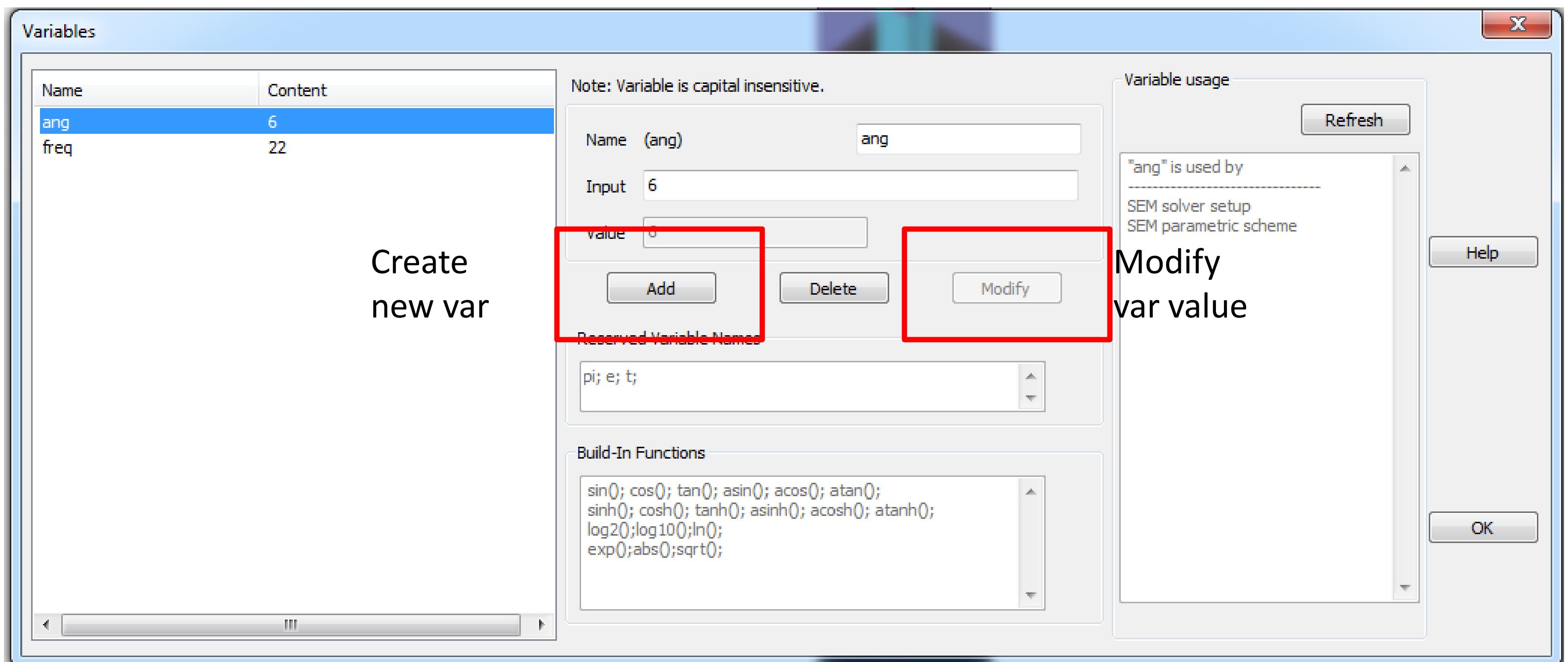
Here, we assume the base case in the demo (2) is built.

Then, we will define variables and configure them as the working frequency and the incident angle.

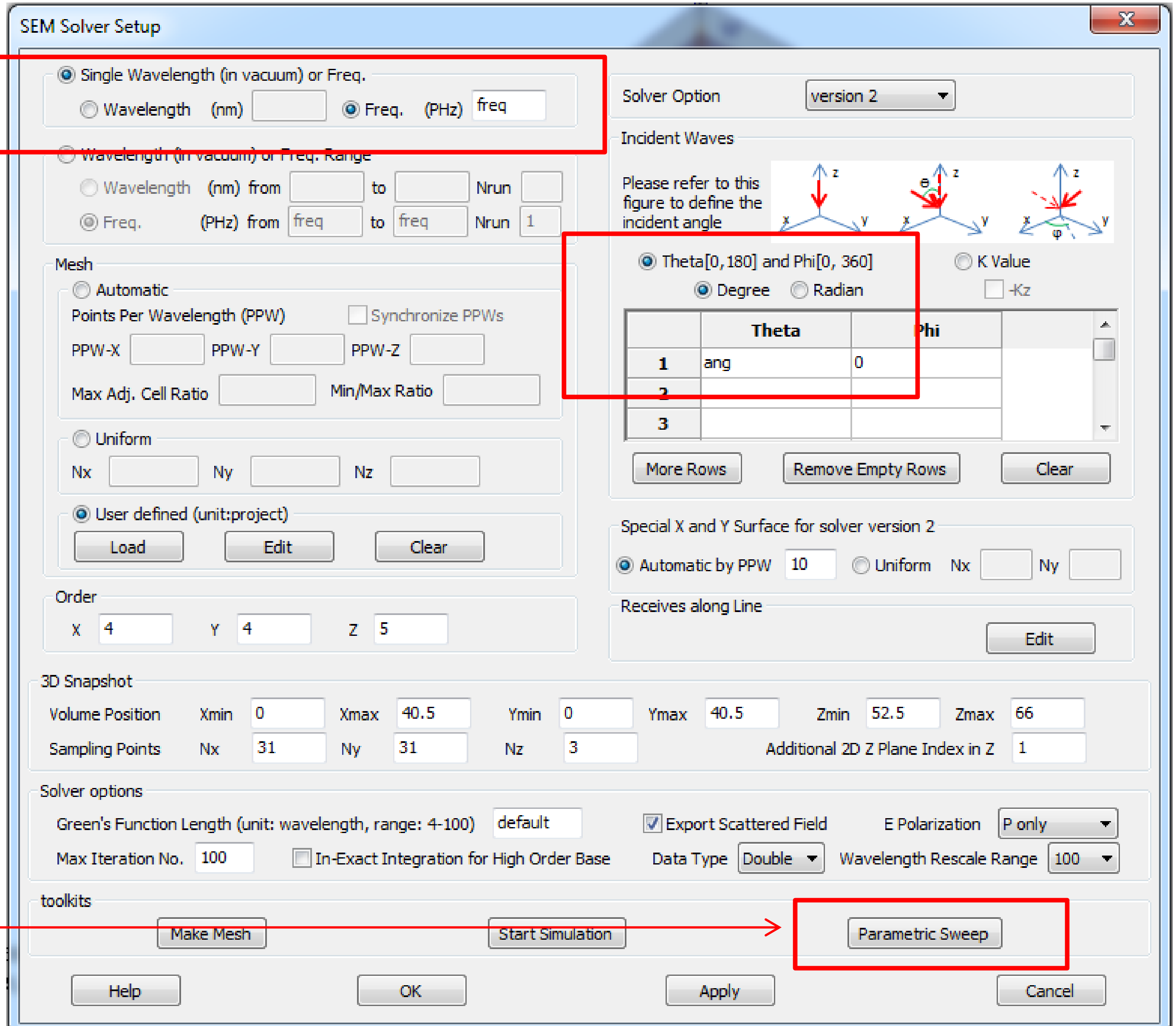
1) Define variables



2) Add variable “freq” & “ang”, the init values for them are “22” & “6”, respectively.

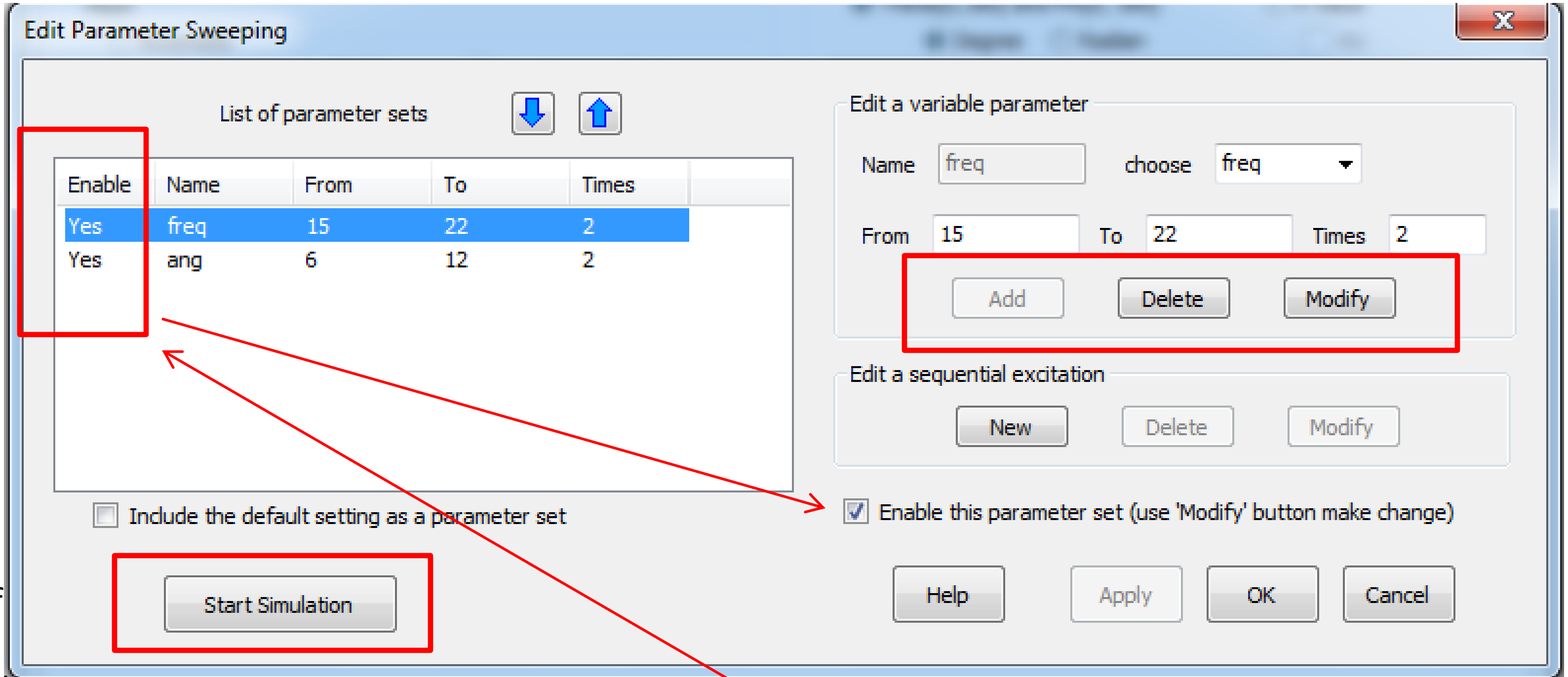


(3) In the SEM solver setup dialog, set working freq. as “*freq*”, soucre incident angle as “*ang*”



After all setup are ready, configure how to sweep

In the parameter sweep dialog, define which variable will be sweep and the sweep range, steps.



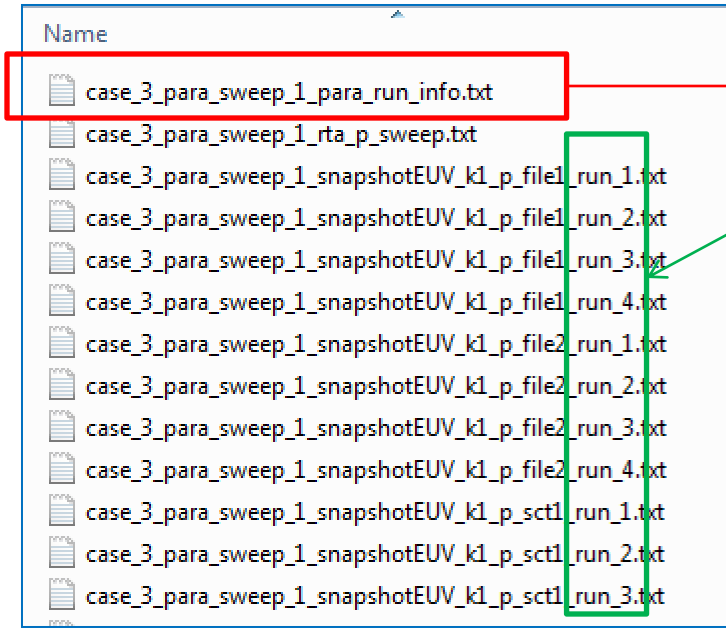
Start sweep simulation if all variable sets are ready

Note:

1) if a variable is not defined to be sweep, this variable will use the initial value as defined in the variable setup dialog.
2) The sweep will include the variable set with enable-flag "**Yes**" only. The variable set without "Yes" flag will be skipped in simulation.

The SEM parametric simulation results will stored in the folder:
Project_folder\project_res\sem\para_sweep

Following are the simulation data files for parametric sweep



Run=1, Paramaters: freq = 15; ang = 6
Run=2, Paramaters: freq = 15; ang = 12
Run=3, Paramaters: freq = 22; ang = 6
Run=4, Paramaters: freq = 22; ang = 12

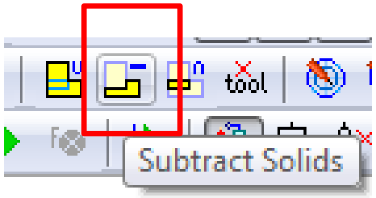
The “info.txt” has the parameter value in each simulation.

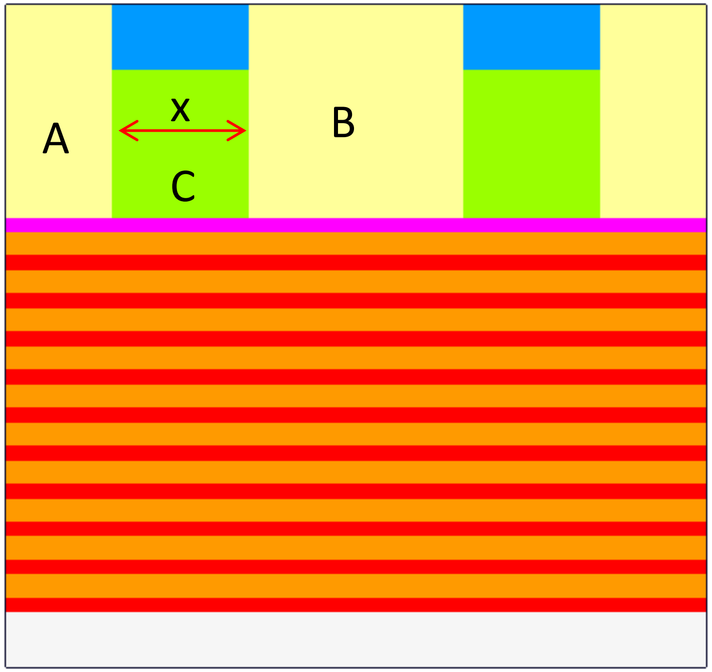
Note for the parametric sweep

For the project define in GUI, almost all inputs can be defined by variables, for example, the solid's size. Therefore, the parametric sweep can sweep the solid size also.

As the case shown in the figure, the width of solid C is defined by "X" (X=10 as initial value). In the sweep, we will sweep X=[10, 20]

As can be seen, for X=20, the solid C may clash with adjacent solid A or B. In this case, before the simulation, user need to set A=A-C and B=B-C by 3D boolean operation.



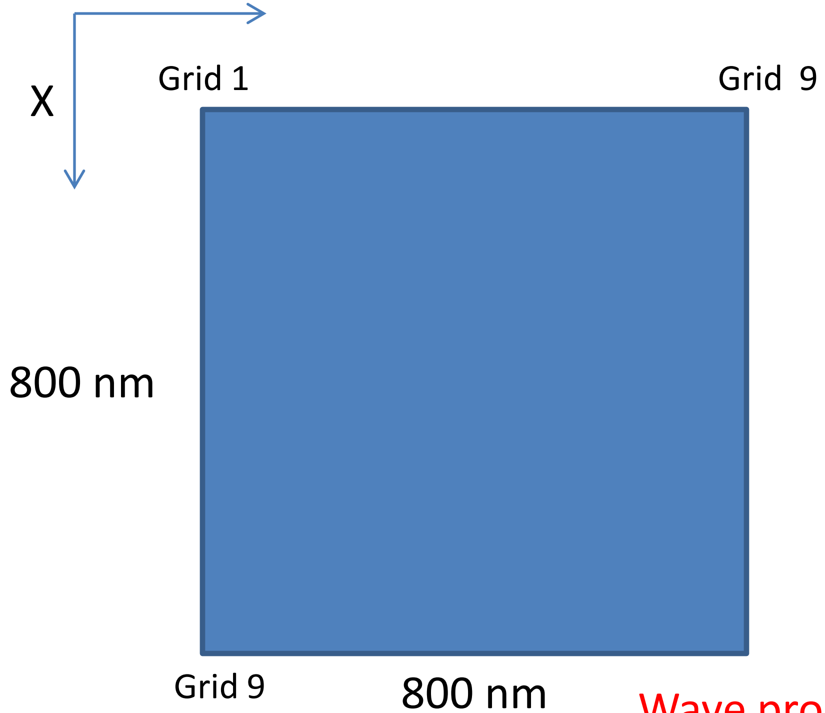


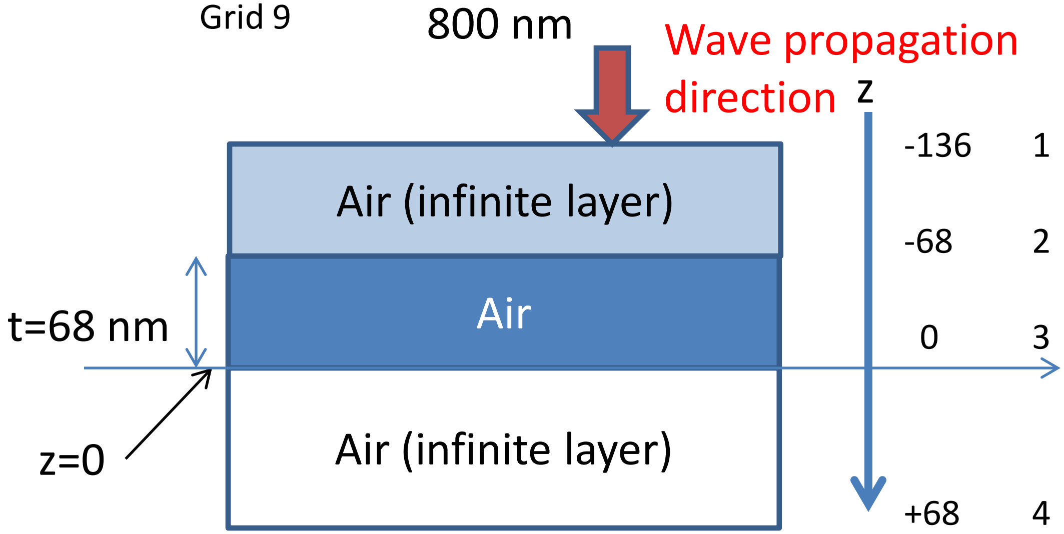
Even in the beginning, for the default X=10, solid C does not clash with A and B.

Benchmarks

- In this section, we will show
  - the simulation accuracy between
    - WCT SEM solver vs. Analytical solution
    - WCT SEM solver vs. FDTD solver
    - WCT SEM solver vs. other FEM solver
  - The simulation performance between the WCT SEM solver ver 1 vs. ver 2
    - Accuracy
    - Memory requirements
    - Simulation time
  - We also show the performance of the solver ver 2 for a large case - 400x400 nm^2 in X & Y.
  - A freq. sweep for a filter composed by thin Au film on S_iO_2 and VO_2 substrate
  - A freq. sweep for an VO_2 filter

Benchmark Test I: Homogenous Air





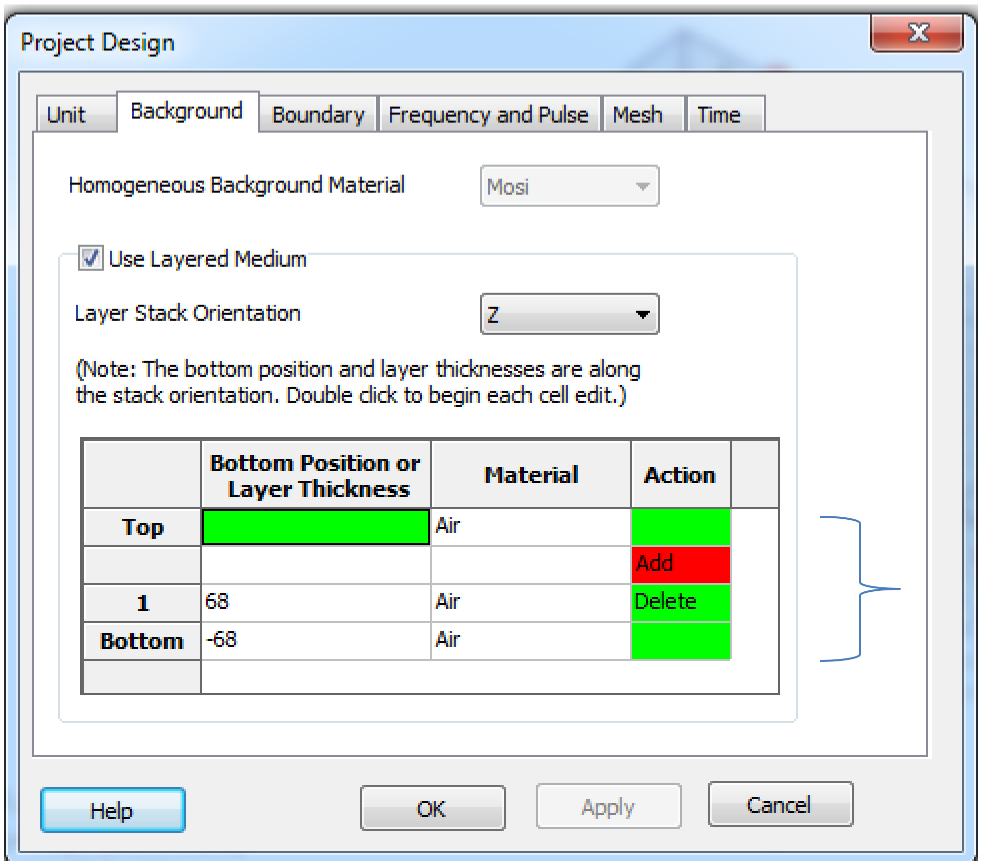
Δx= Δy=800/8=100
Δz=68

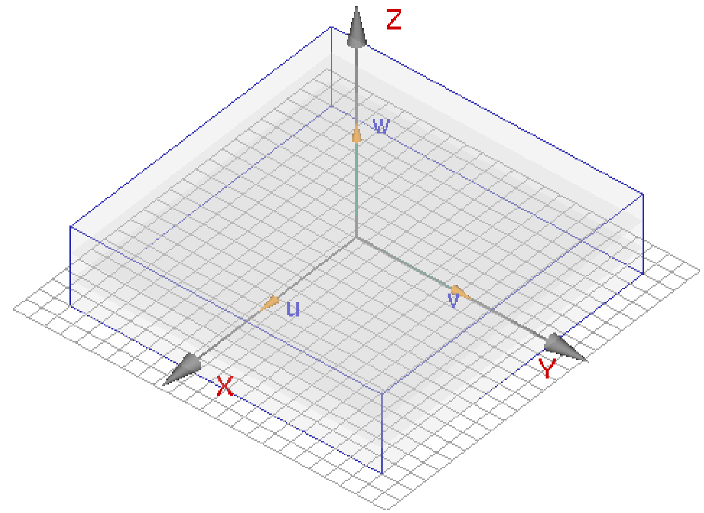
In order to make it easy to be modified to a 3 layers case, we setup this case as 3 air layers

Polarization

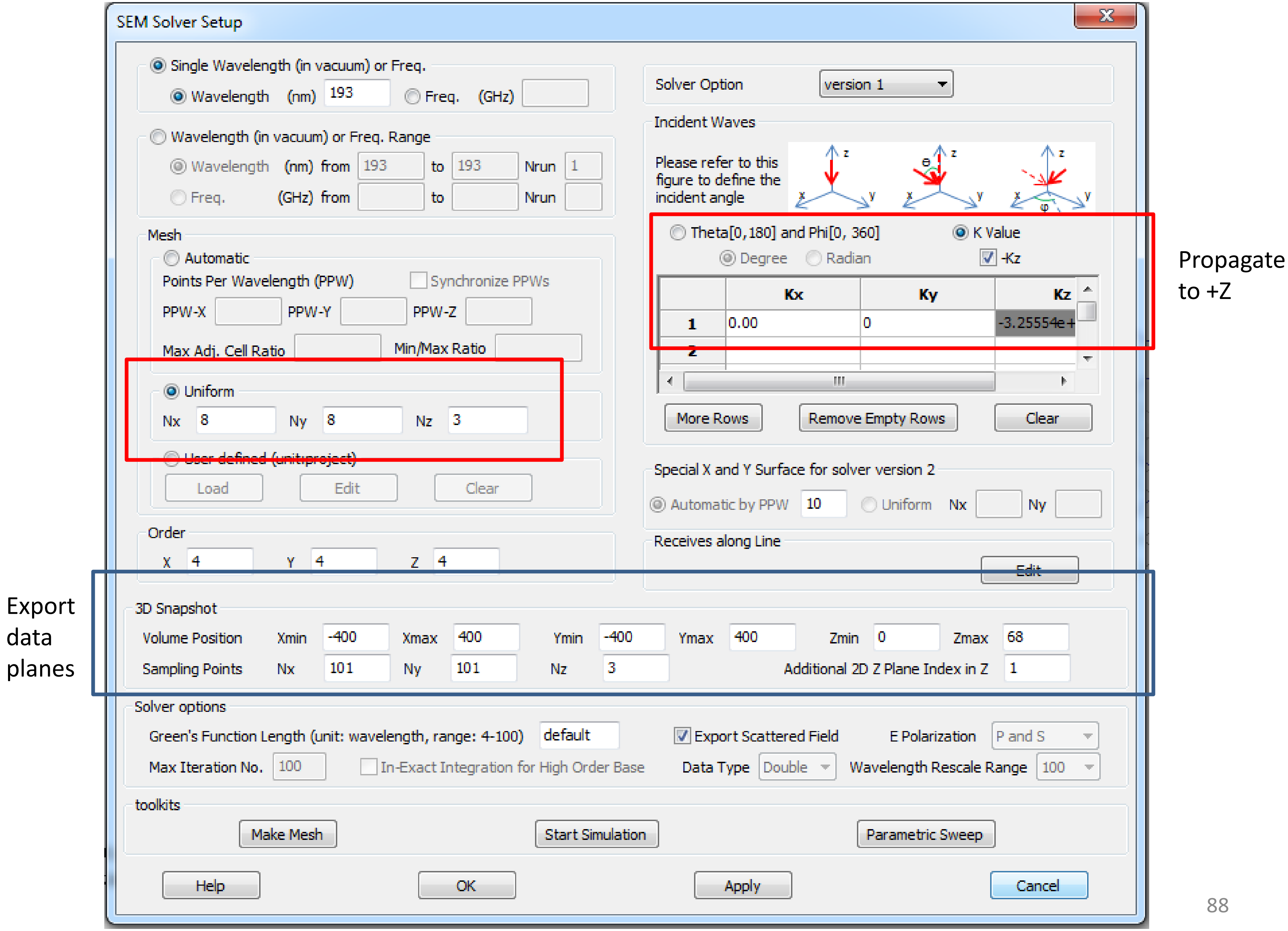
$\Theta=180^o$, $\Phi=0\ ^o \rightarrow$
P=(-1, 0, 0) = X polarization
S=(0, -1, 0) = Y polarization

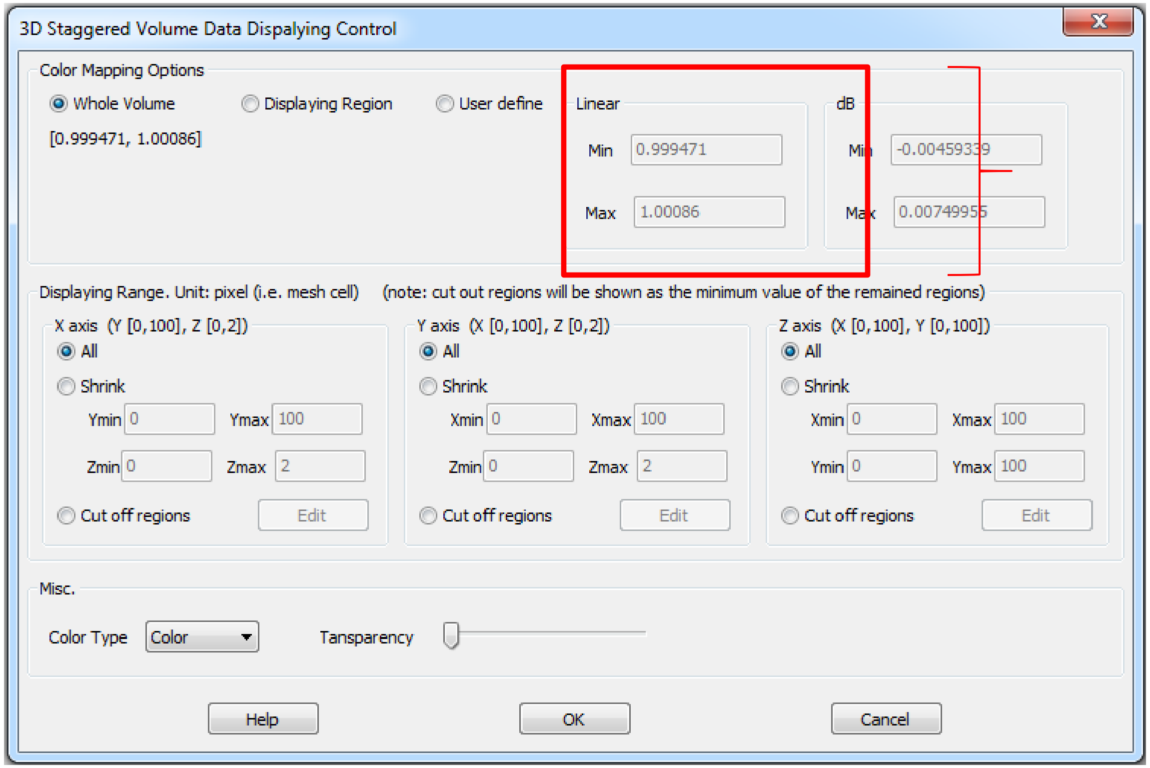
WCT case setup in GUI





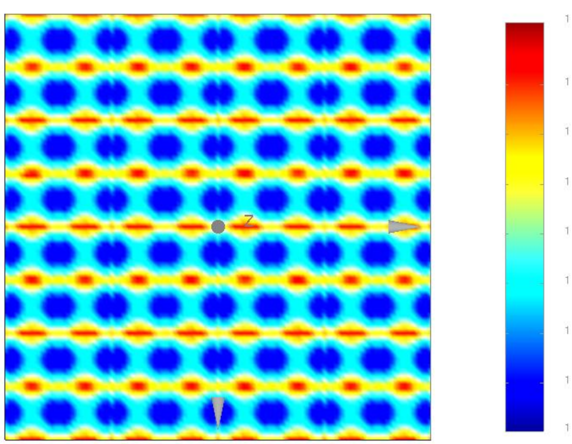
3 layers air


SEM Solver Setup
Single Wavelength (in vacuum) or Freq.
Wavelength (nm) 193 Freq. (GHz)
Wavelength (in vacuum) or Freq. Range
Wavelength (nm) from 193 to 193 Nrun 1
Freq. (GHz) from to Nrun
Mesh
Automatic
Points Per Wavelength (PPW) Synchronize PPWs
PPW-X PPW-Y PPW-Z
Max Adj. Cell Ratio Min/Max Ratio
Uniform
Nx 8 Ny 8 Nz 3
User defined (unit:project)
Load Edit Clear
Order
X 4 Y 4 Z 4
Solver Option version 1
Incident Waves
Please refer to this figure to define the incident angle
Theta[0,180] and Phi[0, 360] K Value
Degree Radian -Kz
Kx Ky Kz
1 0.00 0 -3.25554e+
2
More Rows Remove Empty Rows Clear
Special X and Y Surface for solver version 2
Automatic by PPW 10 Uniform Nx Ny
Receives along Line
Edit
3D Snapshot
Volume Position Xmin -400 Xmax 400 Ymin -400 Ymax 400 Zmin 0 Zmax 68
Sampling Points Nx 101 Ny 101 Nz 3 Additional 2D Z Plane Index in Z 1
Solver options
Green's Function Length (unit: wavelength, range: 4-100) default
Export Scattered Field
E Polarization P and S
Max Iteration No. 100
In-Exact Integration for High Order Base
Data Type Double
Wavelength Rescale Range 100
toolkits
Make Mesh Start Simulation Parametric Sweep
Help OK Apply Cancel
Propagate to +Z
Export data planes

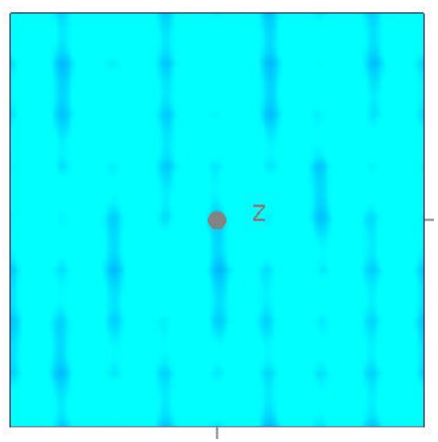


The magnitude of field at Z=0, 34, 68 nm plane are all almost eq. to 1. The variation is smaller than 0.1%.

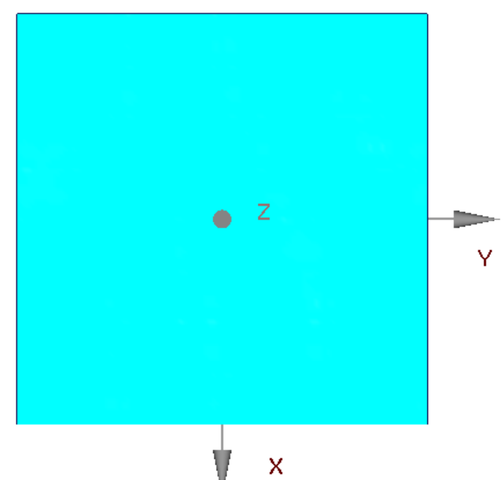
Ex in P polarization



Z=0

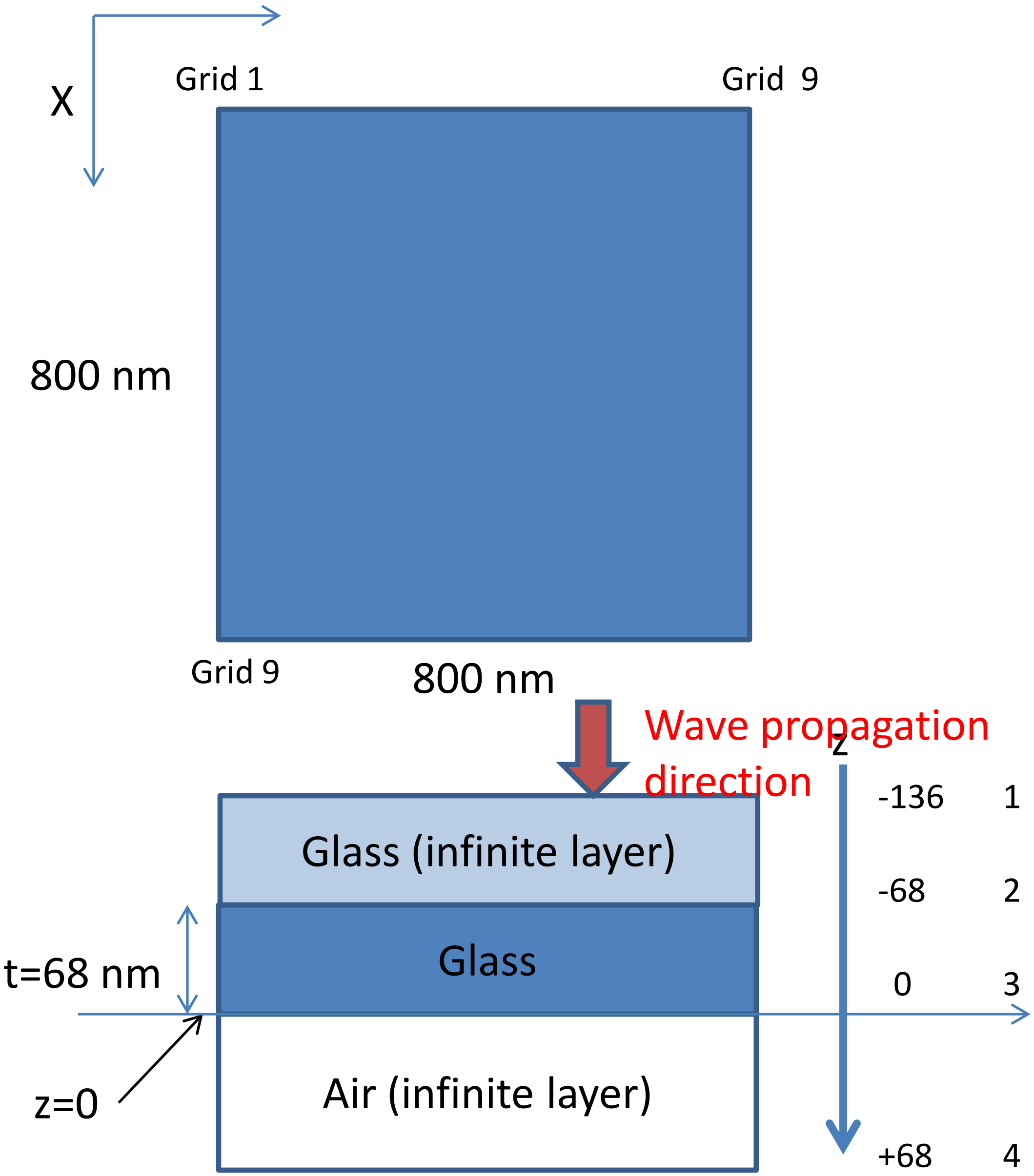


Z=34



Z=68

Benchmark Test II: Two layers Media



$\Delta x = \Delta y = 800/8 = 100$

$\Delta z = 68$

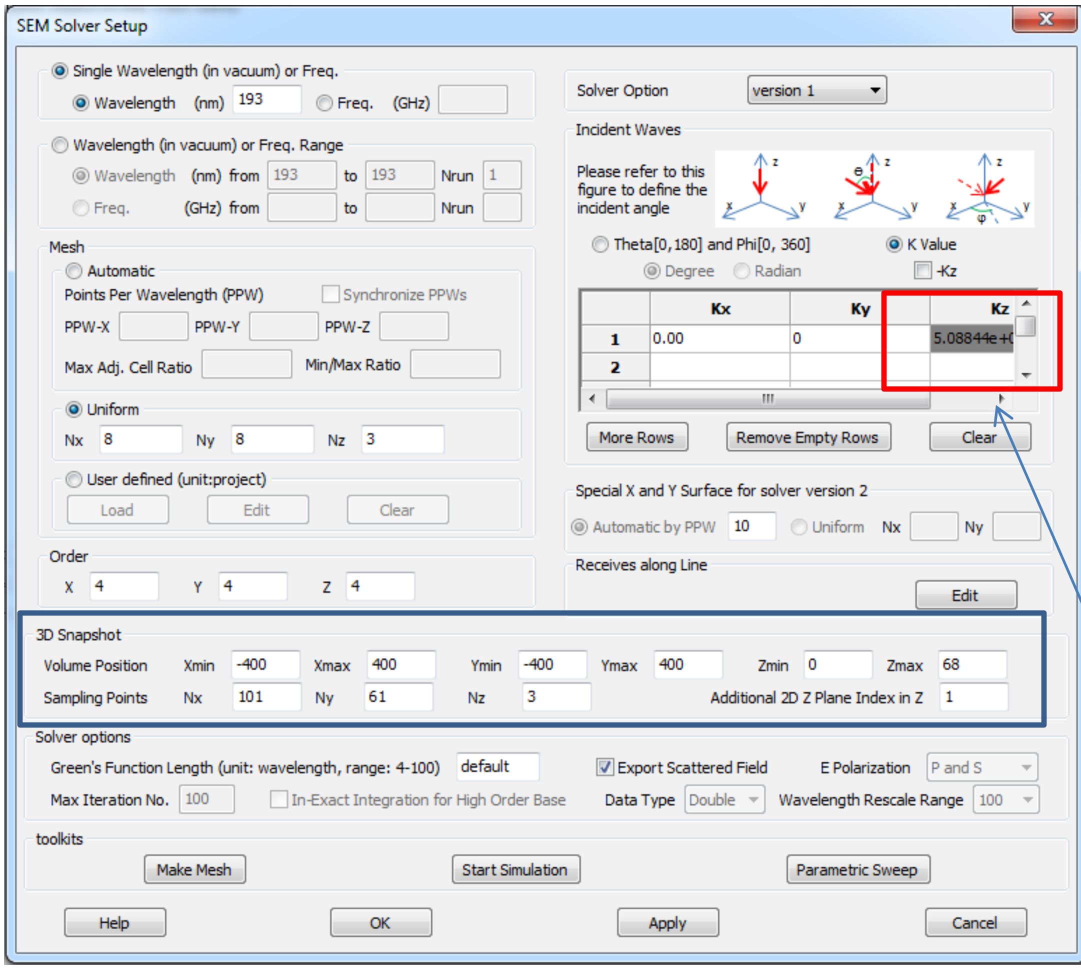
Polarization

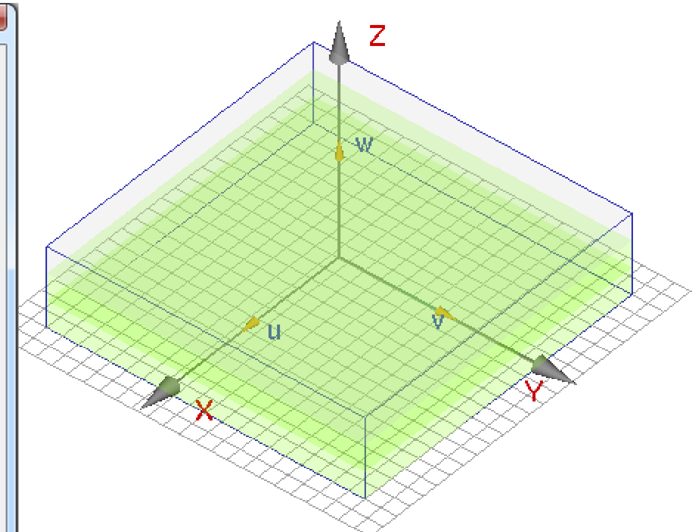
$\Theta = 180^{o}$, $\Phi = 0\ ^{o} \rightarrow$

P=(-1, 0, 0) = X polarization

S=(0, -1, 0) = Y polarization

WCT case setup in GUI





Maybe in the beginning this Kz is not correct, it is due to the system has not made the final calculation. After press “OK” or “Simulation”. This part will become correct.

The calculation for the ideal transmission

$$f = \frac{c}{\lambda_0} = \frac{299792458}{193e^{-9}} = 1.5533\mathrm{e}^{15}$$

$$K_{z0} = \varpi\sqrt{\varepsilon_0\mu_0} = 2\pi f\sqrt{\varepsilon_0\mu_0}$$

$$= 2\pi \times 1.5533e^{15} \times \sqrt{8.85419e^{-12} \times 4\pi e^{-7}}$$

$$= 2\pi \times 1.5533e^{15} \times 3.3356\mathrm{e}^{-9}$$

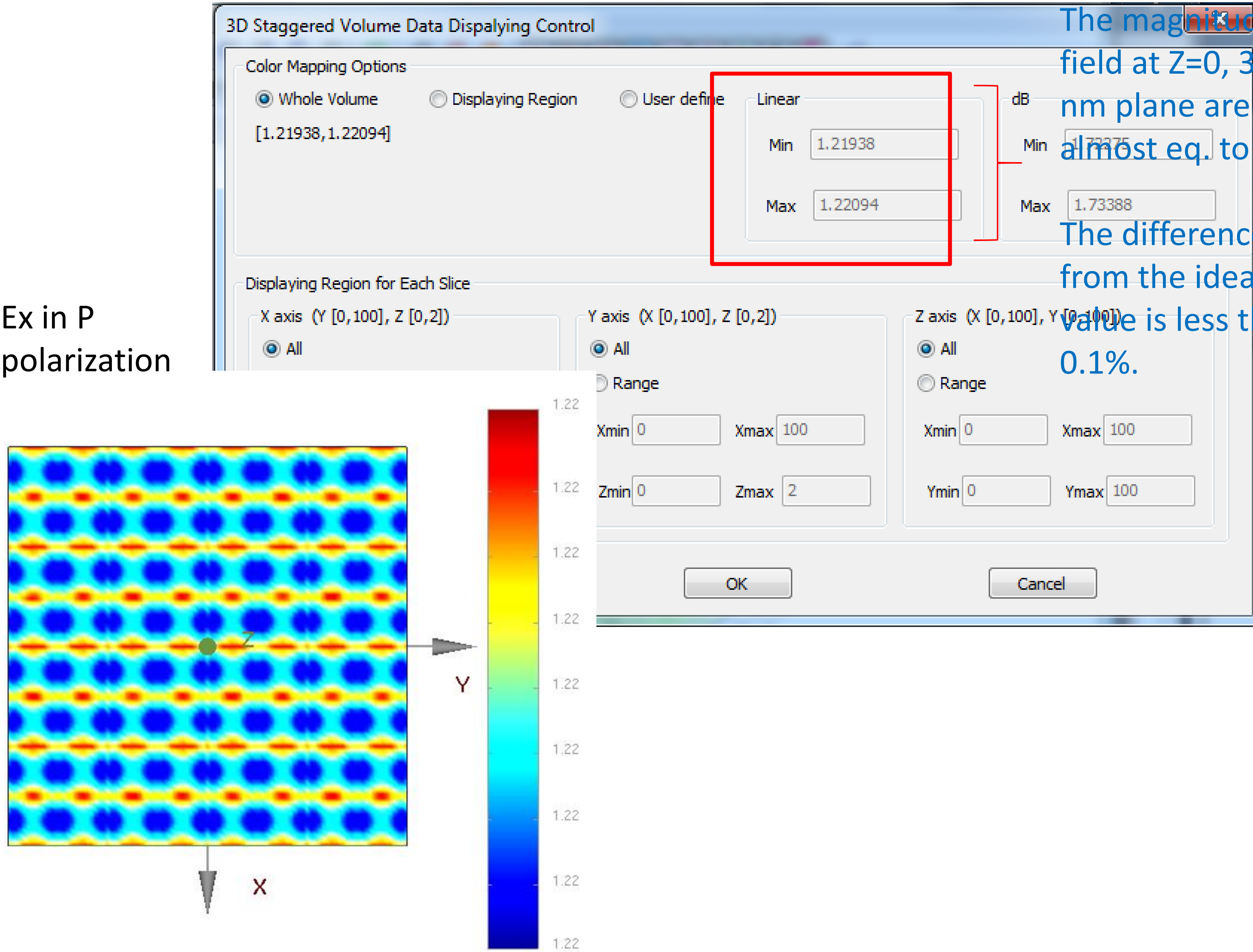
$$= 32.5544e^{6}$$

$$K_z = K_{z0}\sqrt{\varepsilon_r} = 3.25544e^{7}\sqrt{2.443} = 5.0883e^{7}$$

Ideal transmission:

$$\frac{2n_2}{n_1 + n_2} = \frac{2\sqrt{2.443}}{1 + \sqrt{2.443}} = 1.2197$$

Ex in P polarization

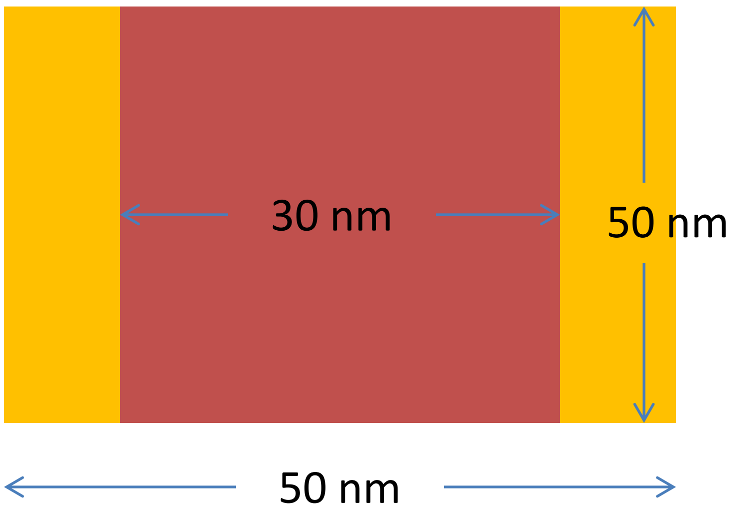


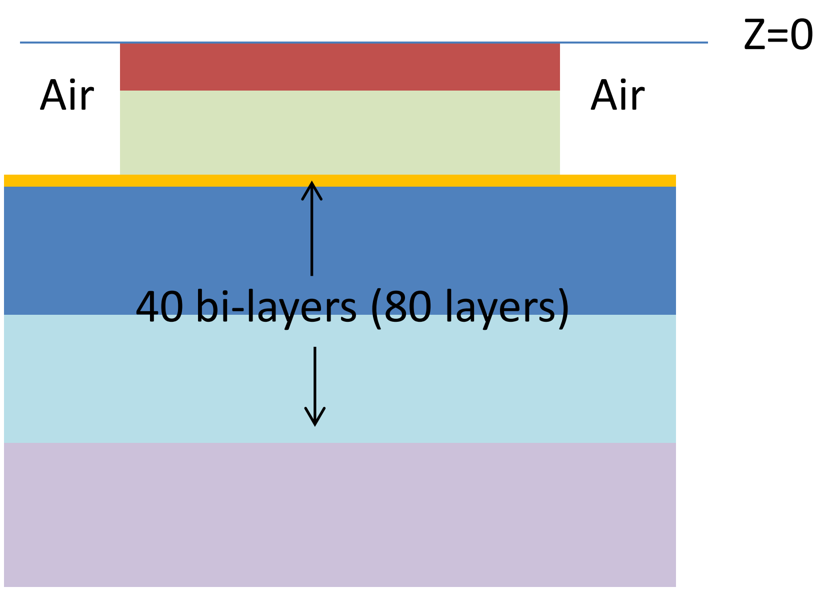
The magnitude of field at Z=0, 34, 68 nm plane are all almost eq. to 1.22.

The difference from the ideal value is less than 0.1%.

Benchmark Test III

ε_r	J	σ
0.913	0.044	5.435e4
0.9	0.057	7.041e4
0.785	0.03	3.706e4
0.999	0.004	4.94e3
0.848	0.012	1.482e4
0.954	0.021	2.594e4





$\epsilon = 0.913 + 0.044j$
Thickness = 14 nm

$\epsilon = 0.9 + 0.057j$
Thickness = 56 nm

$\epsilon = 0.785 + 0.03j$
Thickness = 2.5 nm

Top Layer:
$\epsilon = 0.999 + 0.004j$
Thickness = 4 nm

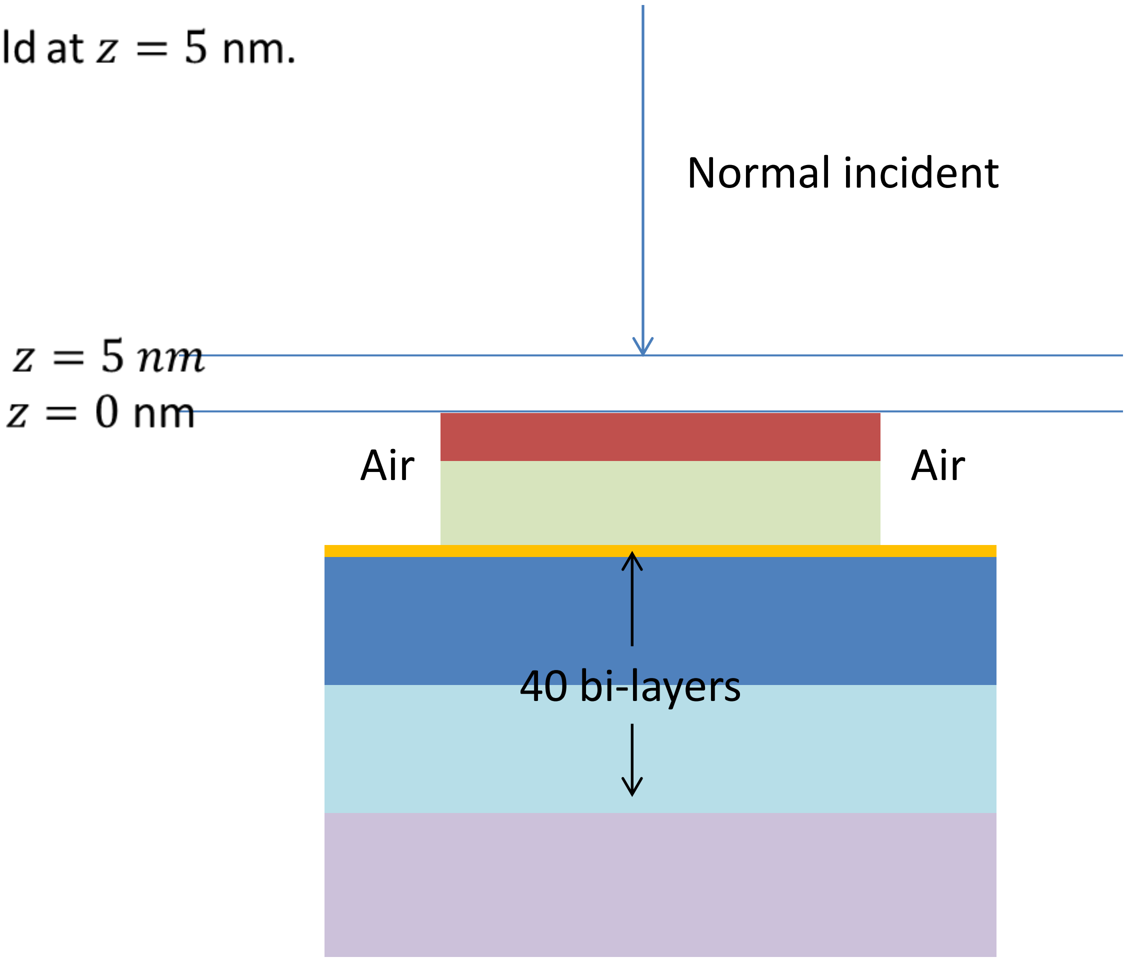
Bottom Layer:
$\epsilon = 0.848 + 0.012j$
Thickness = 3 nm

$\epsilon = 0.954 + 0.021j$
Thickness = half space

In this case, we will compare the results from the WCT FDTD transient solver and the WCT SEM spectrum solver.

$\lambda = 13.5$ nm

Output field at $z = 5$ nm.



$$f=\frac{c}{\lambda_0}=\frac{299792458}{13.5e^{-9}}=22.207\mathrm{e}^{15}$$

$$Kz=\varpi\sqrt{\varepsilon\mu}=2\pi f\sqrt{\varepsilon_0\mu_0}$$

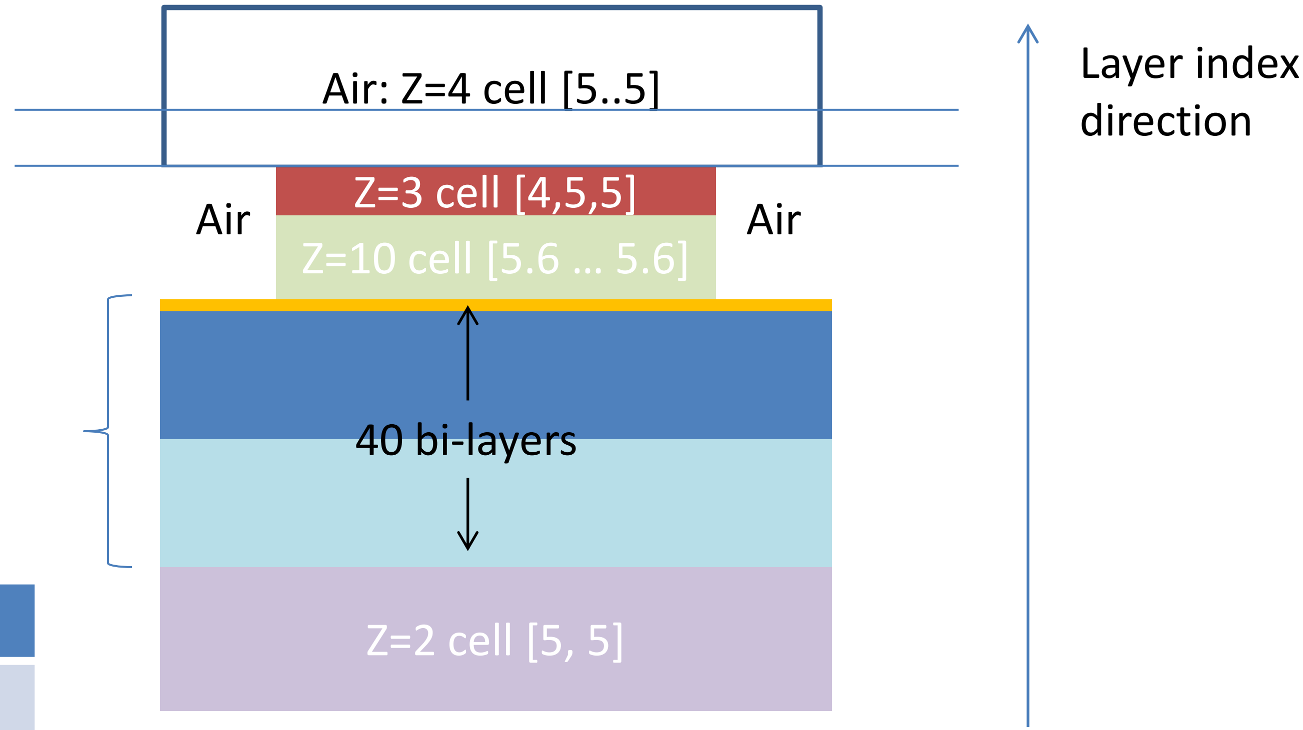
$$=2\pi\times 22.207e^{15}\times\sqrt{8.85419e^{-12}\times 4\pi e^{-7}}$$

$$=4.6542e^{8}$$

$$\tilde{\varepsilon}_r=\varepsilon_r-j\frac{\sigma}{\varepsilon_0\varpi}\Rightarrow$$

$$\frac{\sigma}{\varepsilon_0\varpi}=\frac{\sigma}{8.854187817\mathrm{e}^{-12}\cdot 2\pi\cdot 22.207\mathrm{e}^{15}}$$

ε_r	J	σ
0.913	0.044	5.435e4
0.9	0.057	7.041e4
0.785	0.03	3.706e4
0.999	0.004	4.94e3
0.848	0.012	1.482e4
0.954	0.021	2.594e4



ε_r	J	σ
0.913	0.044	5.435e4
0.9	0.057	7.041e4
0.785	0.03	3.706e4
0.999	0.004	4.94e3
0.848	0.012	1.482e4
0.954	0.021	2.594e4

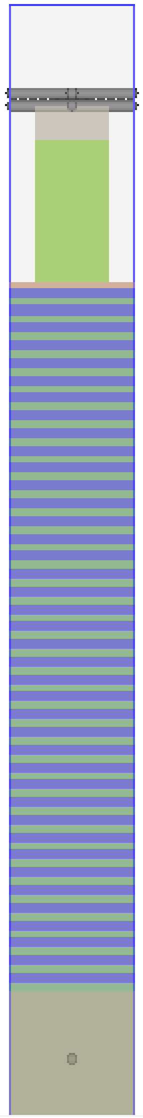
Total Z layers: 4+3+10+1+40x2+2=100

SEM solver setting
Cell number: (5, 5, 100)
Order: (5, 5, 3)

FDTD Solver

For total field Test

WCT



4 1D receiver arrays

Materials

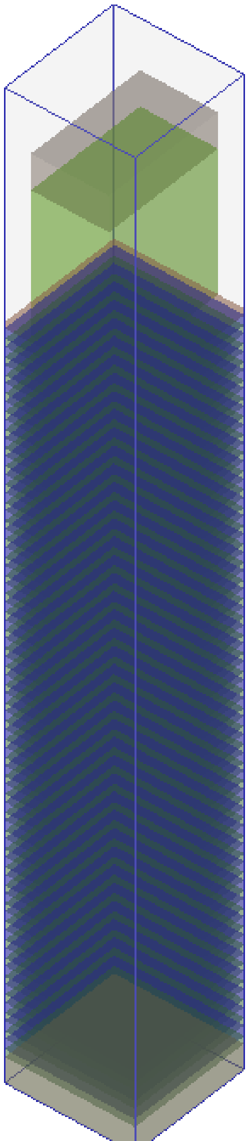
1.0 0.0 1.0 0.0
0.954 0.021 1.0 0.0
0.913 0.044 1.0 0.0
0.9 0.057 1.0 0.0
0.785 0.03 1.0 0.0
0.999 0.004 1.0 0.0
0.848 0.012 1.0 0.0

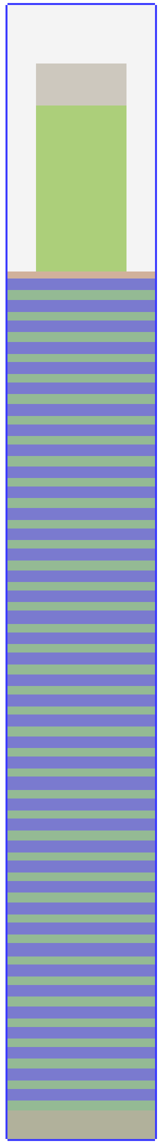
SEM

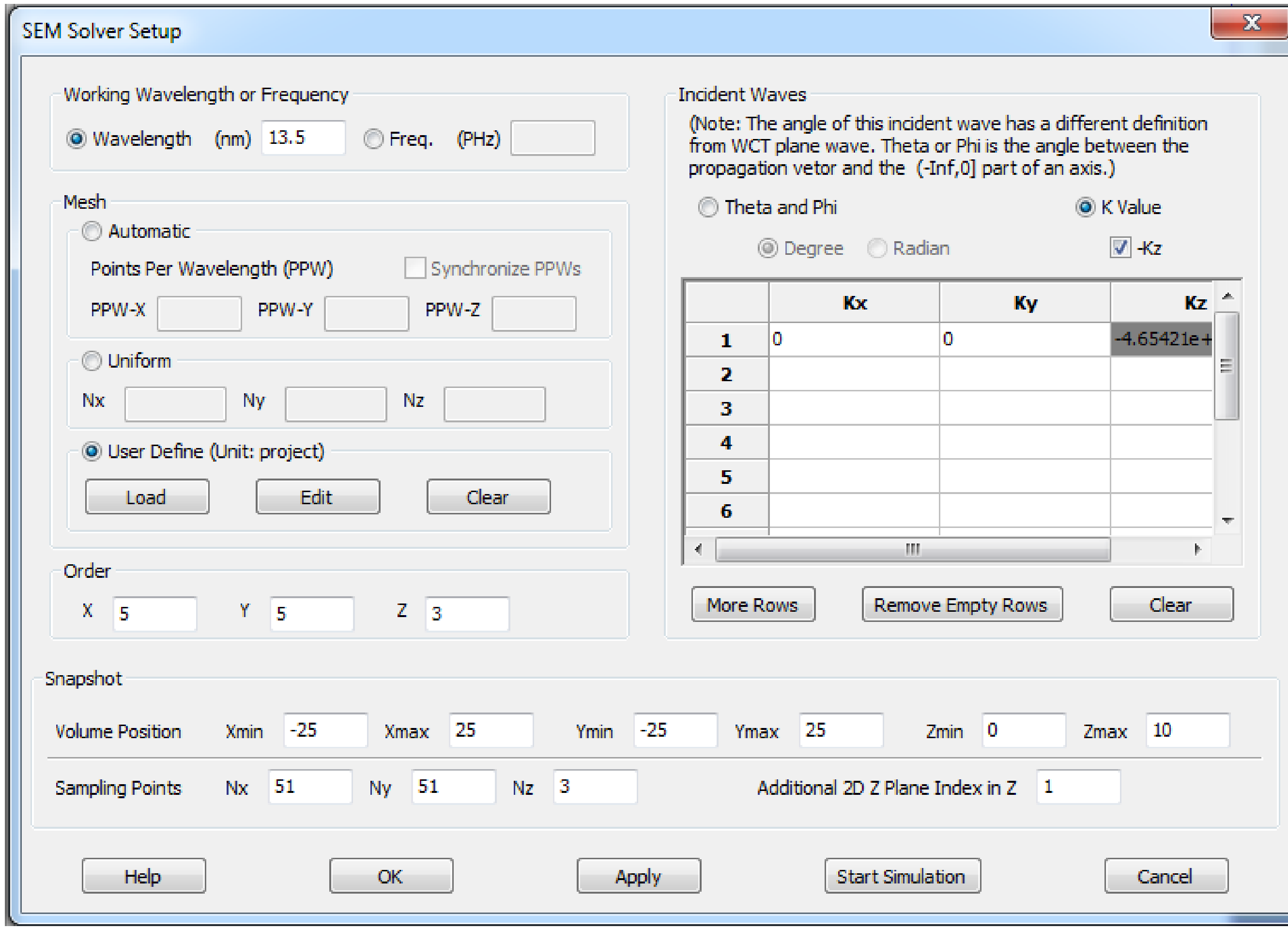
Geometry

6
6
101
1 5 1 5 1 100 1
1 5 1 5 1 2 2
1 5 1 5 3 3 7
…
1 5 1 5 82 82 6
1 5 1 5 83 83 5
1 5 2 4 84 93 4
1 5 2 4 94 96 3

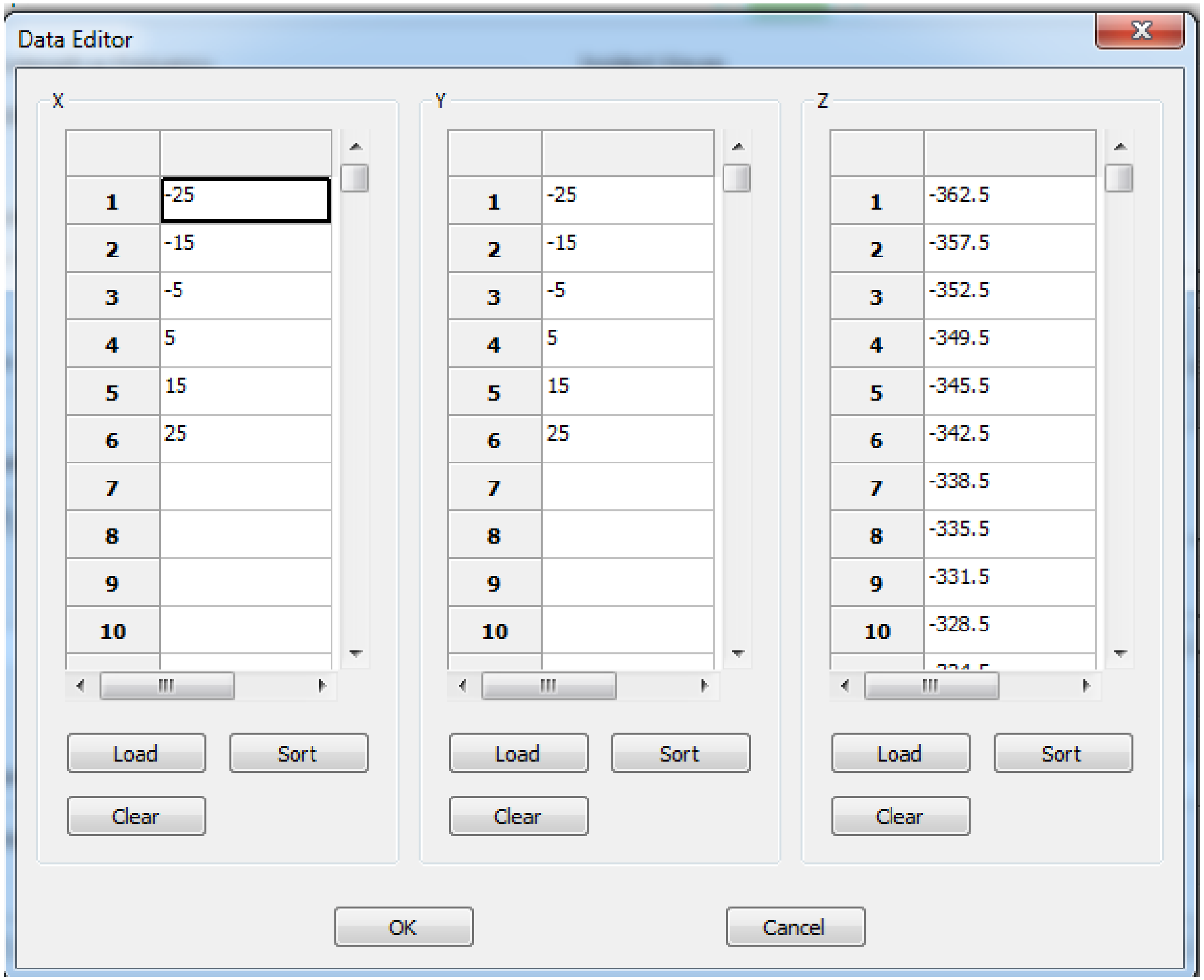
SEM Solver





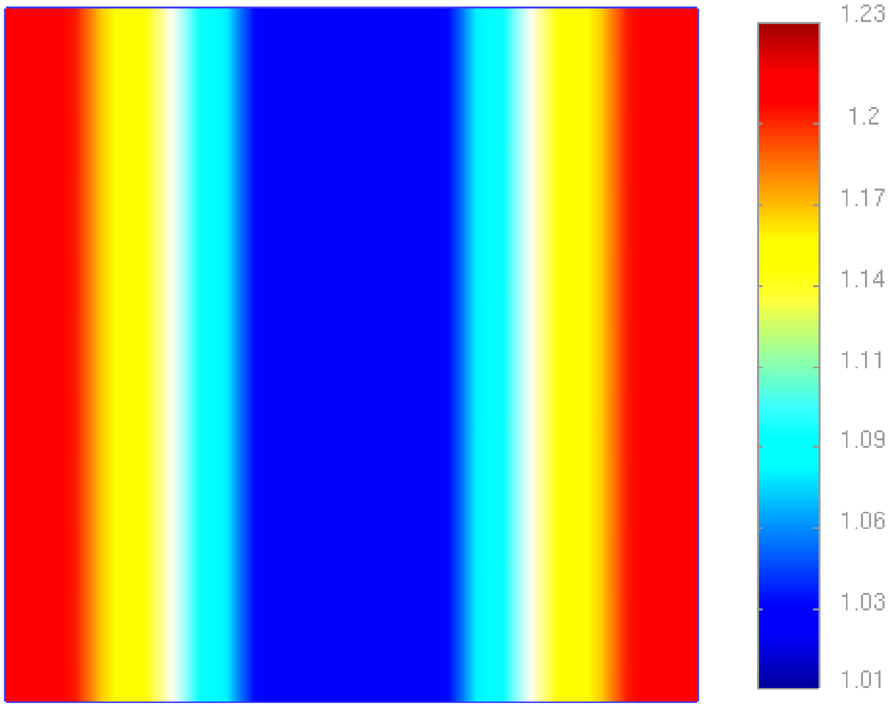

SEM Solver Setup
Working Wavelength or Frequency
Wavelength (nm) 13.5
Freq. (PHz)
Mesh
Automatic
Points Per Wavelength (PPW)
Synchronize PPWs
PPW-X
PPW-Y
PPW-Z
Uniform
Nx
Ny
Nz
User Define (Unit: project)
Load
Edit
Clear
Order
X 5
Y 5
Z 3
Incident Waves
(Note: The angle of this incident wave has a different definition from WCT plane wave. Theta or Phi is the angle between the propagation vetor and the (-Inf,0] part of an axis.)
Theta and Phi
K Value
Degree
Radian
-Kz
Kx
Ky
Kz
1
0
0
-4.65421e+
2
3
4
5
6
More Rows
Remove Empty Rows
Clear
Snapshot
Volume Position
Xmin -25
Xmax 25
Ymin -25
Ymax 25
Zmin 0
Zmax 10
Sampling Points
Nx 51
Ny 51
Nz 3
Additional 2D Z Plane Index in Z 1
Help
OK
Apply
Start Simulation
Cancel

In this case, we use user defined mesh as following

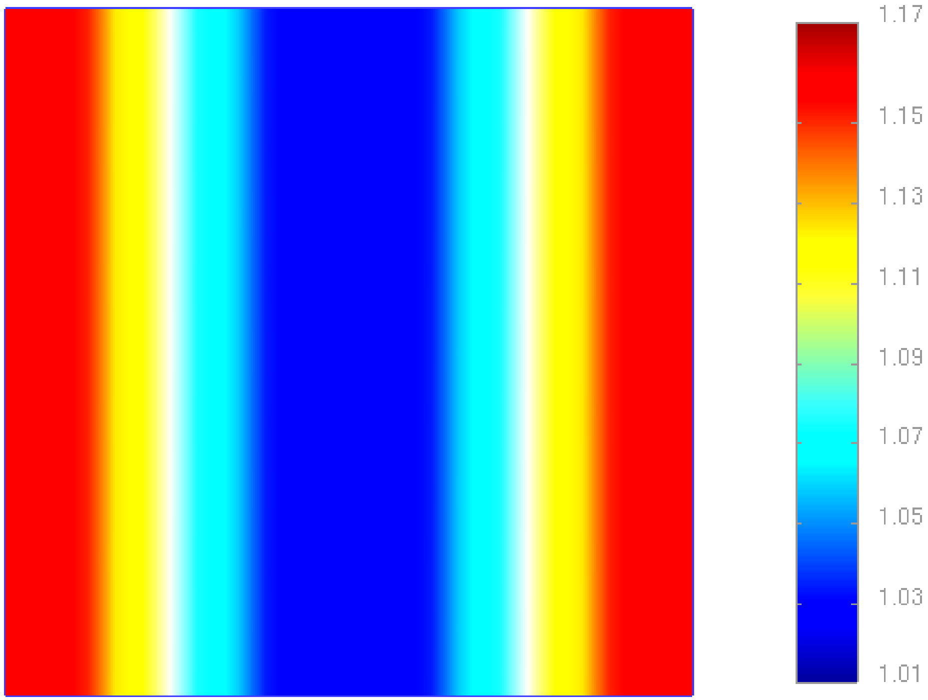


SEM solver Result

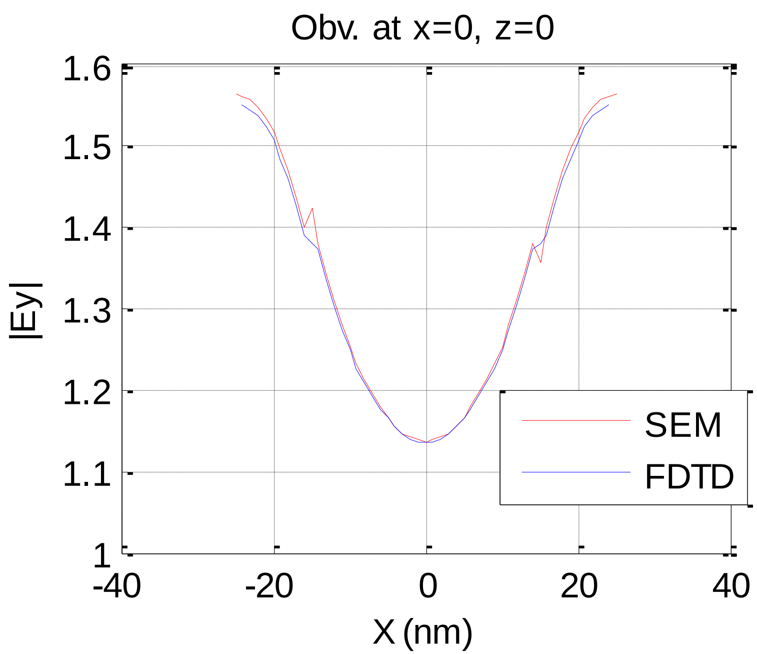
Ex in P polarization

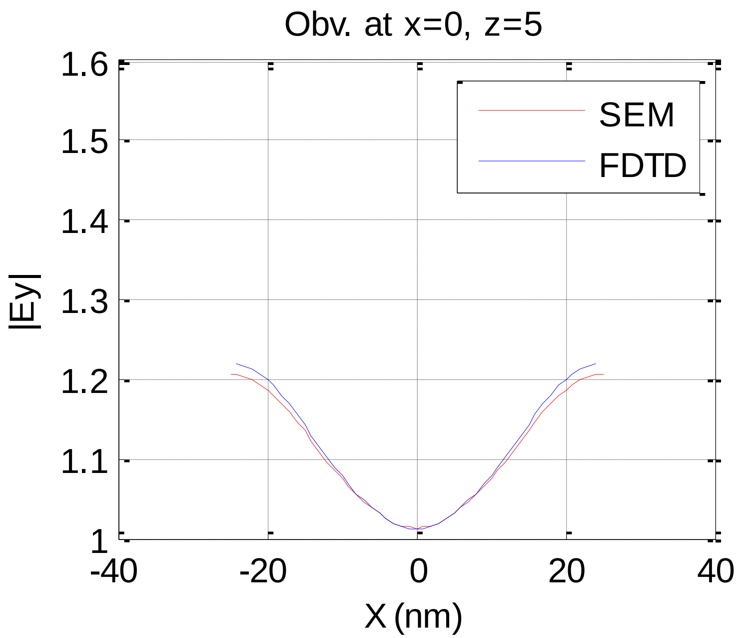


Ey in S polarization



Ey total field on the receiver array (the array is shown in page #44)

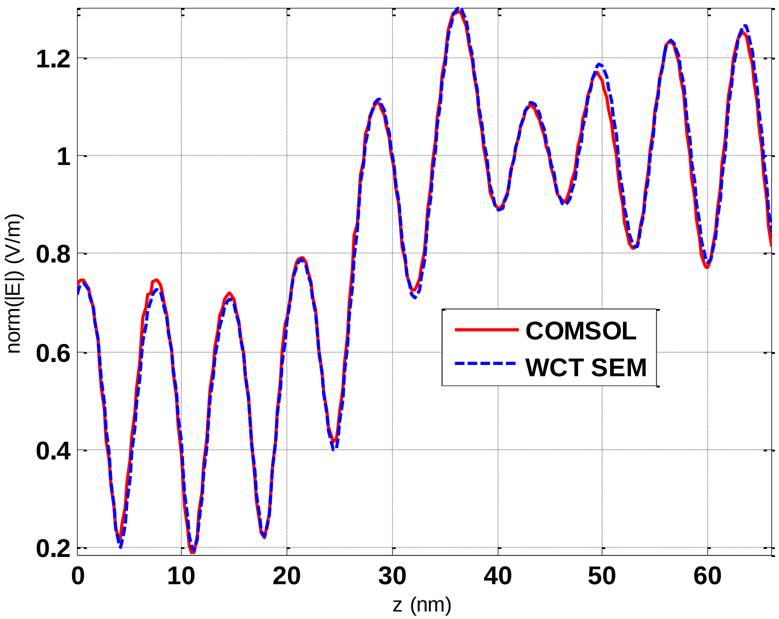


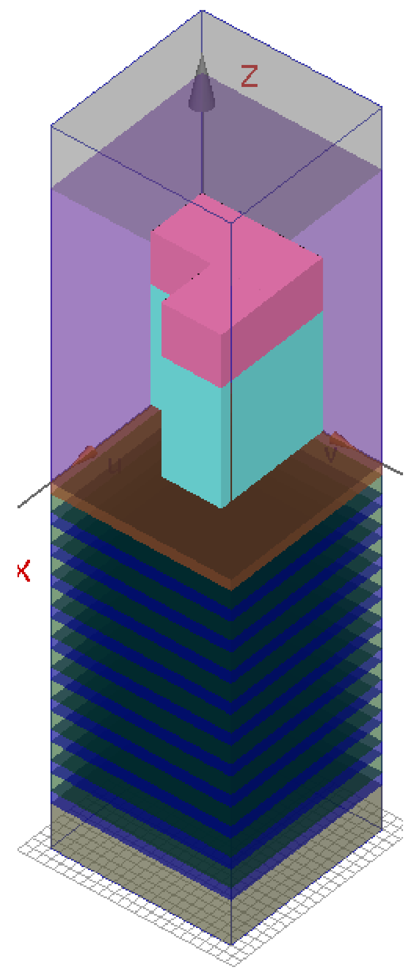


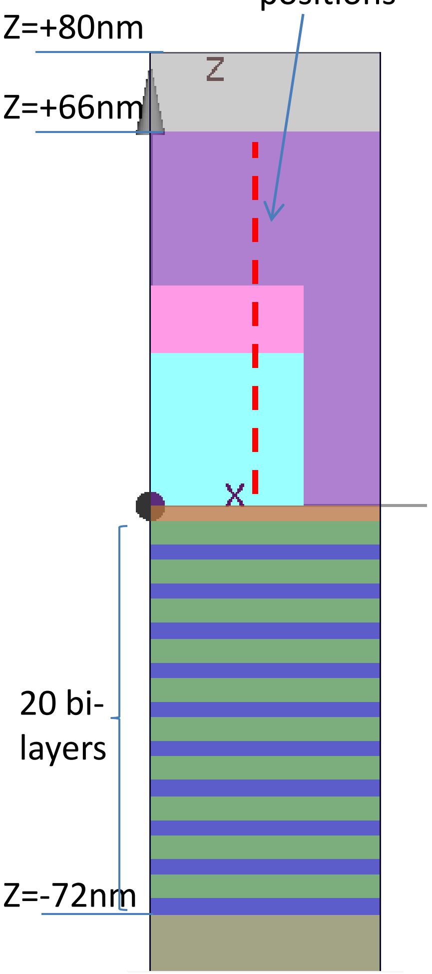
Benchmark Test IV

40.5x40.5 nm^2 case
K=(4.865e7,0,-4.629e8), P polarization

Receiver sampling positions:
X=20 nm
Y=20 nm
Z=0:1.3:66 nm



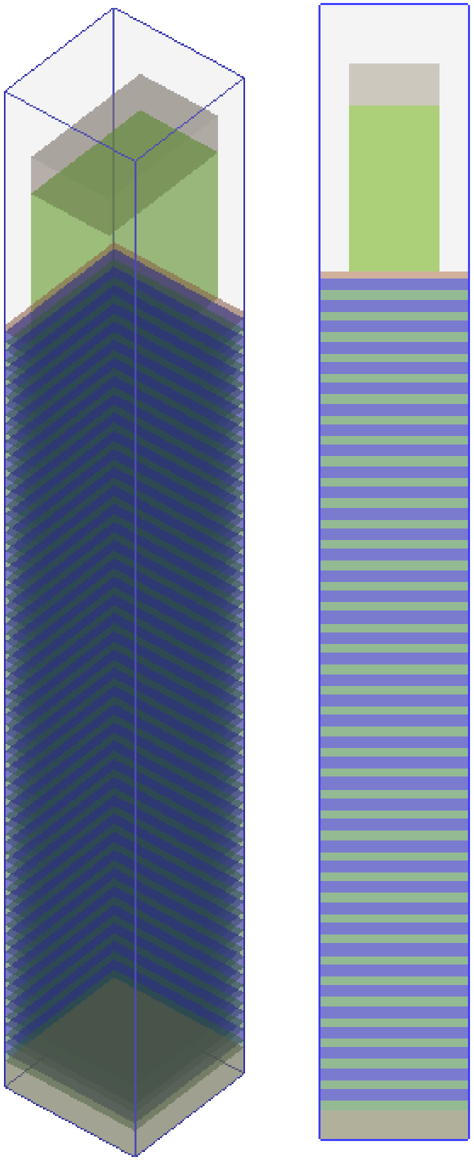




Benchmark Test V

Solver v1 vs. v2

50x50 nm^2 case
Simulate P & S polarization in one run



The accuracy of SEM solver has been shown in the previous page, here, we will compare the difference in solver 1 & solver 2

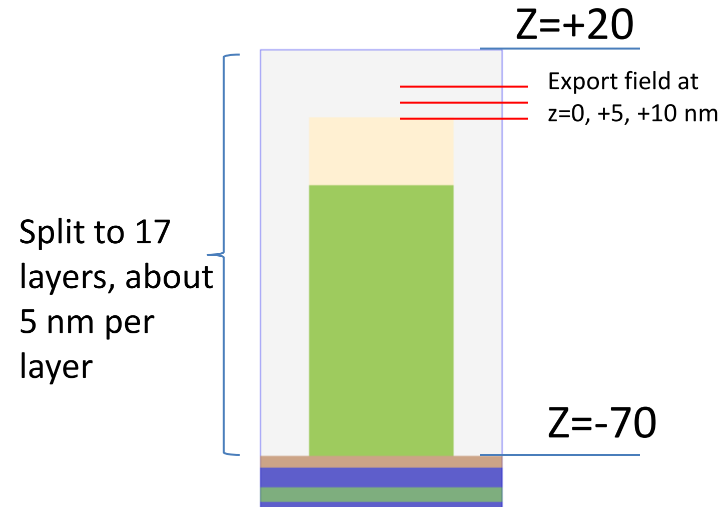
- Project settings
- SEM solver setting
- Simulation time
- result

(Due to this is a small case, we don't shown the memory comparison)

Setting Difference

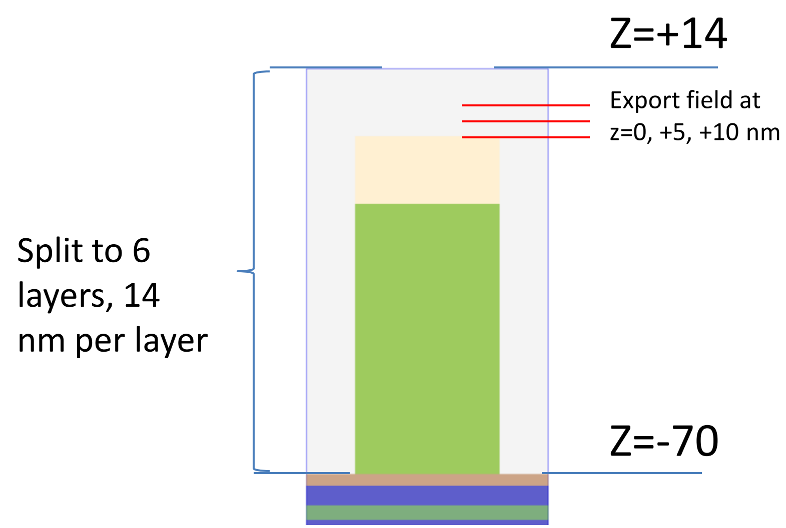
➢ **solver 1**: due to all layers in Z should be calculated, in order to make all cells in Z has a similar Z size, we spilt the top region into 17 cells, as shown in the right figure. And we set the order in Z as 4, for 5 nm cell.

- order for whole system: (4,4,4)
- cell size in X & Y both are 10 nm



➢ **solver 2**: we will only calculate the not-layered region, as shown in the right figure, we split this region into 5 cells, 14 nm per cell, about 1 λ. And set the order in Z as 6.

- order for whole system: (4,4,6)
- cell size in X & Y both are 10 nm



Simulation Time: by a Intel i7-3770 CPU

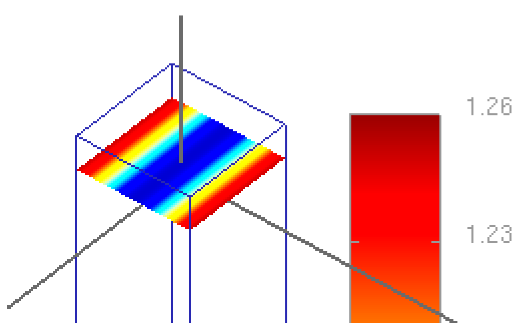
- **solver 1**: 73s
- **solver 2**
  - double precision – 69s
  - single precision – 62s

Therefore, for a small case, 2 solver has a similar simulation time

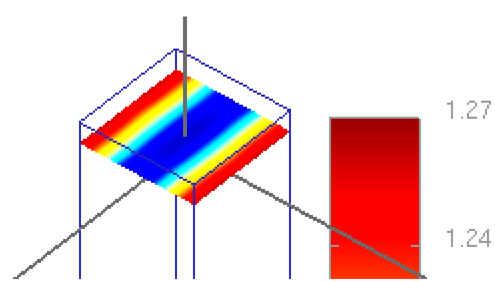
Simulation Results

We show the 2D plot figure as following

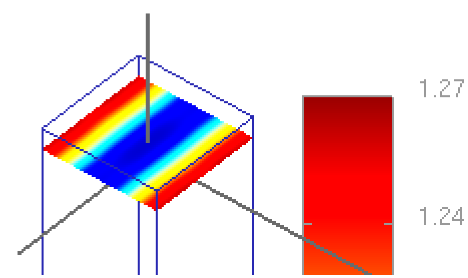
Solver 1: Ex at Z=+5nm, in P polarization



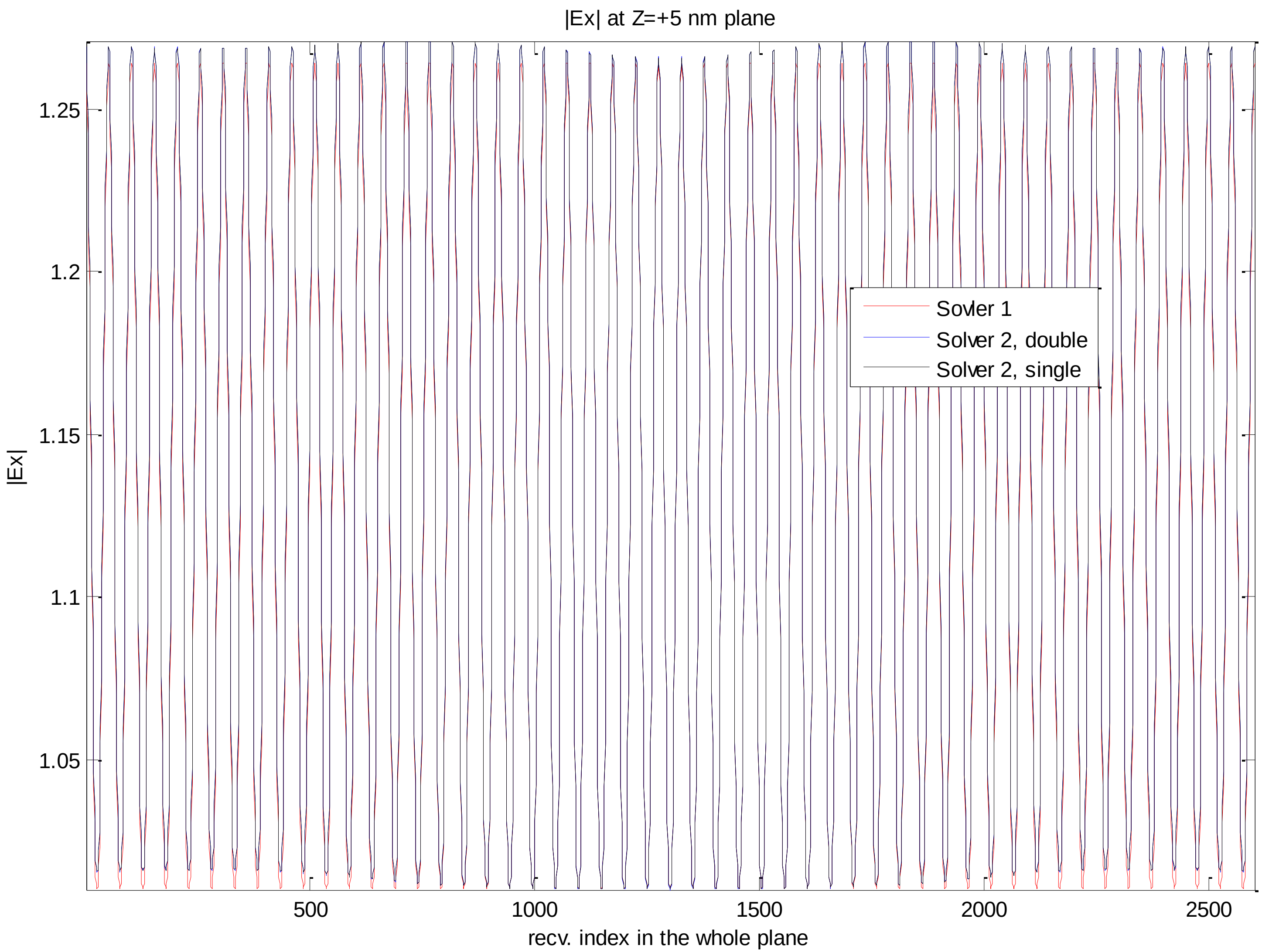
Solver 2: Ex at Z=+5nm, in P polarization, double precision



Solver 2: Ex at Z=+5nm, in P polarization, single precision



Following is the |Ex| in the Z=+5 nm plane, we can see they are very close



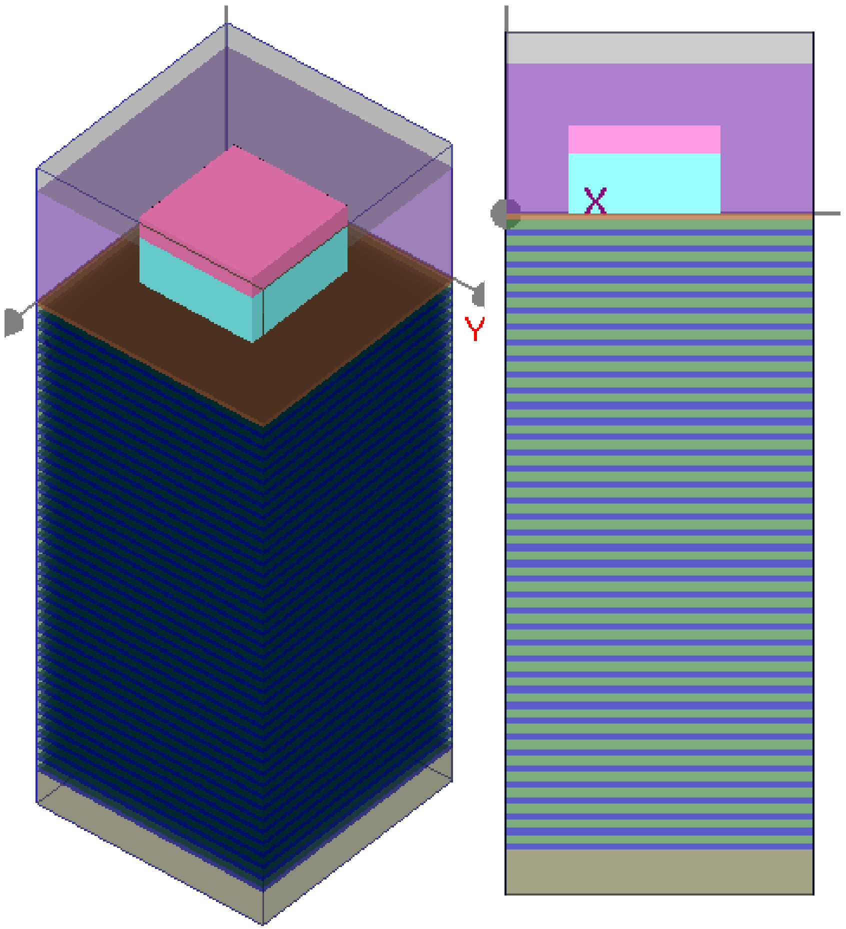
Benchmark Test VI

Solver v1 vs. v2

135x135 nm^2 case
Simulate P & S polarization in one run

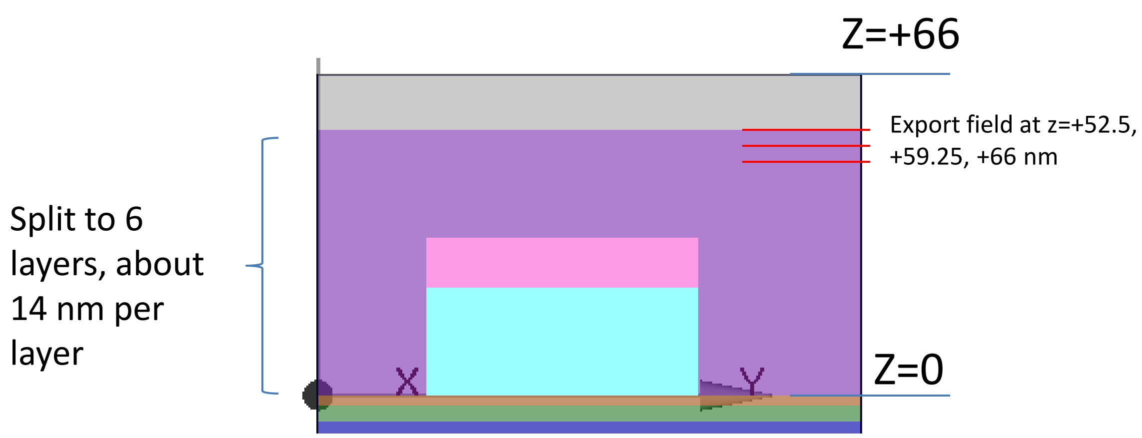
Here, we will compare the difference in solver 1 & solver 2

- Project settings
- Memory requirement
- Simulation time
- result



Setting

- **solver 1** & **solver 2**
  - in this case, for the region with the structure- Z=[0, +66] nm, we split the space into 6 cells, about 14 nm per cell, as shown in the following figure
  - the order both are: (4, 4, 5)
  - cell size in X & Y both are 13.5 nm
  - the exporting field is at Z= +52.5, +59.25, +66 nm, 3 planes



Simulation Time: by a Intel i7-5820k CPU

- **solver 1**: 22min
- **solver 2**
  - double precision – 170s
  - single precision – 180s

Therefore, for this case, solver 2 is about **8** times faster than solver 1

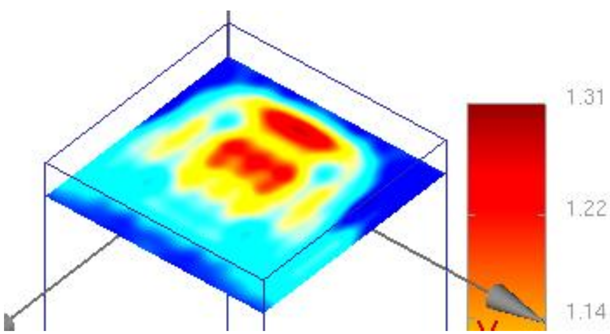
Memory Requirement

- **solver 1**: don't require hard drive swap storage, 30 GB
- **solver 2**
  - double precision – 10 GB
  - single precision – 6.5 GB

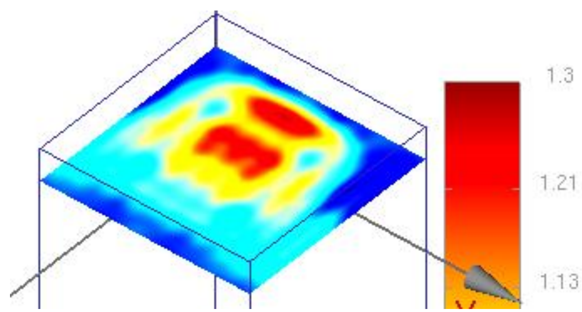
Simulation Results

We show the 2D plot figure as following

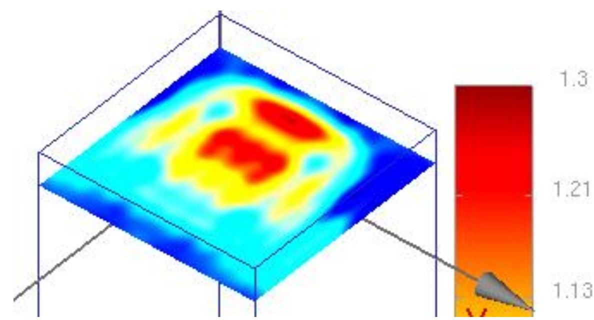
Solver 1: Ex at Z=+59.25 nm, in P polarization



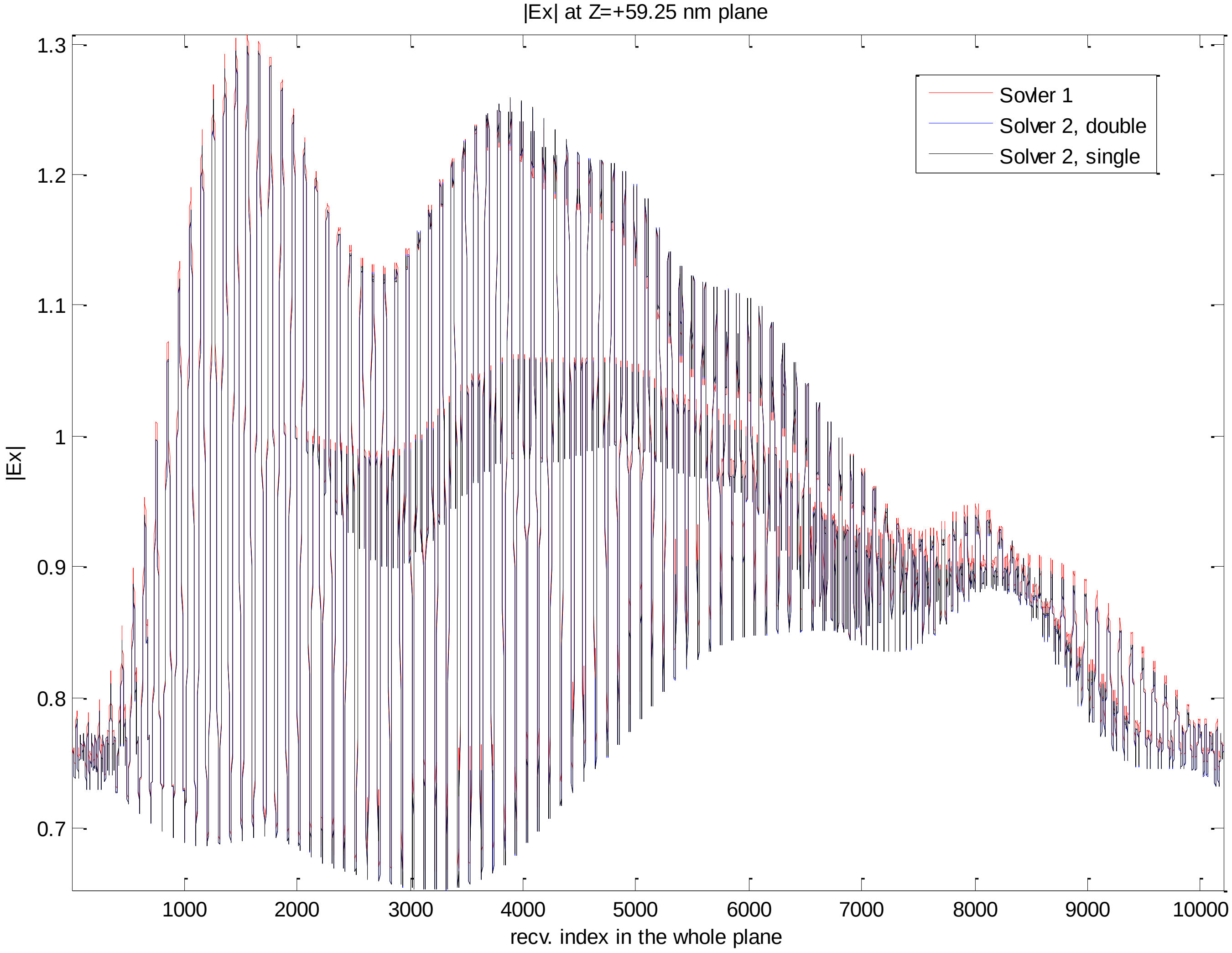
Solver 2: Ex at Z=+59.25nm, in P polarization, double precision



Solver 2: Ex at Z=+59.25nm, in P polarization, single precision



Following is the |Ex| in the Z=+59.25 nm plane, we can see they are very close



Benchmark Test VII

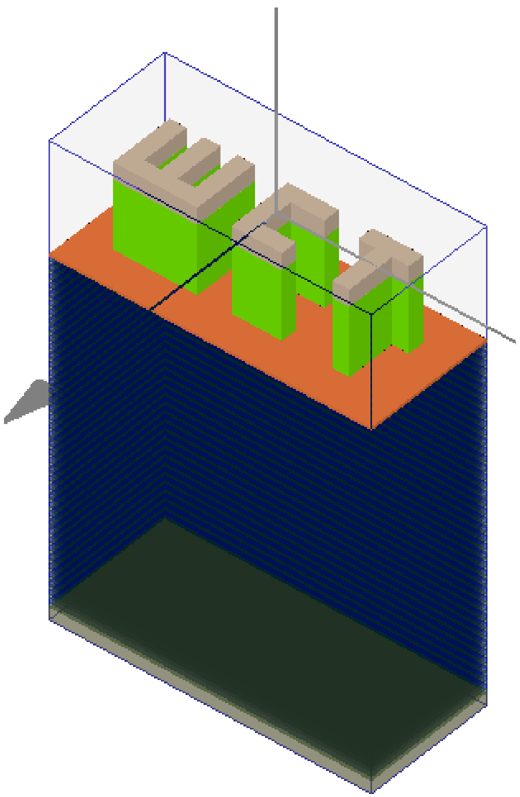
Solver v1 vs. v2

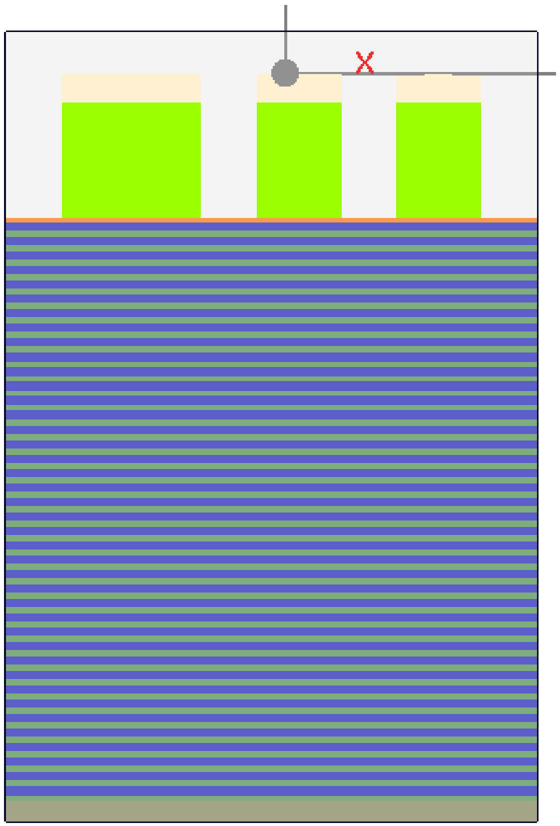
110x257.5 nm^2 case (9λx19λ)

Simulate P & S polarization in one run

Here, we will compare the difference in solver 1 & solver 2

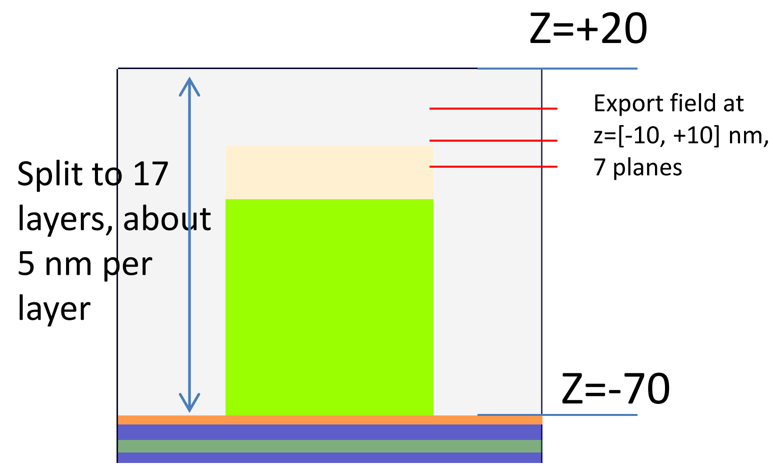
- Project setting
- Memory requirement
- Simulation time
- Results



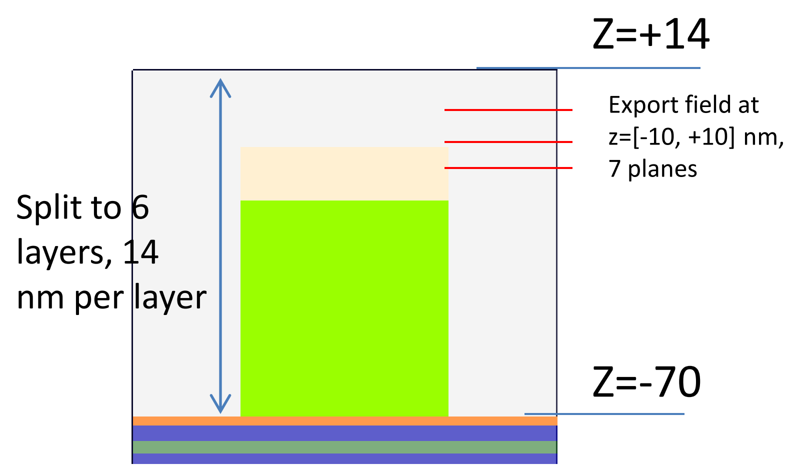


Setting Difference

- **solver 1**: due to all layers in Z should be calculated, in order to make all cells in Z has a similar Z size, we spilt the top region into 17 cells, as shown in the right figure. And we set the order in Z as 4, for 5 nm cell.
  - order for whole system: (4,4,4)
  - cell number: [8,9,100] for whole domain
  - cell size in X & Y both are around 13.5 nm



- **solver 2**: we will only calculate the not-layered region, as shown in the right figure, we split this region into 6 cells, 14 nm per cell, about 1 λ. And set the order in Z as 6.
  - order for SEM region: (4,4,6)
  - cell number: [8,9,6] for SEM domain
  - cell size in X & Y both are around 13.5 nm



Simulation Time: by a Intel i7-5820k CPU

- **solver 1**: 64 min
- **solver 2**
  - double precision – 343s
  - single precision – 370s

Therefore, for this case, solver 2 is about **11** times faster than solver 1

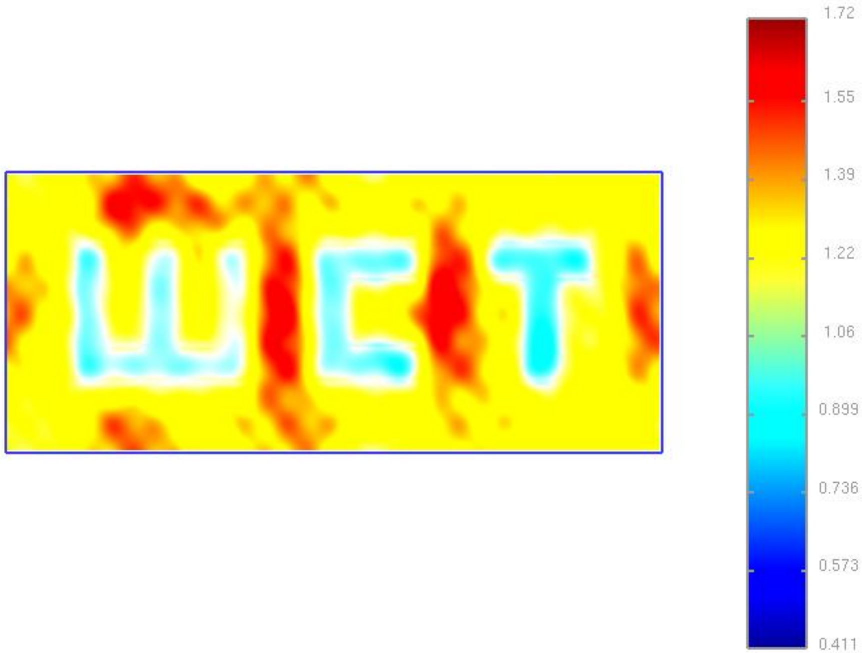
Memory Requirement

- **solver 1**: max memory usage – 37 GB, with hard drive swap storage - 59 GB
- **solver 2**
  - double precision – 26 GB
  - single precision – 17 GB

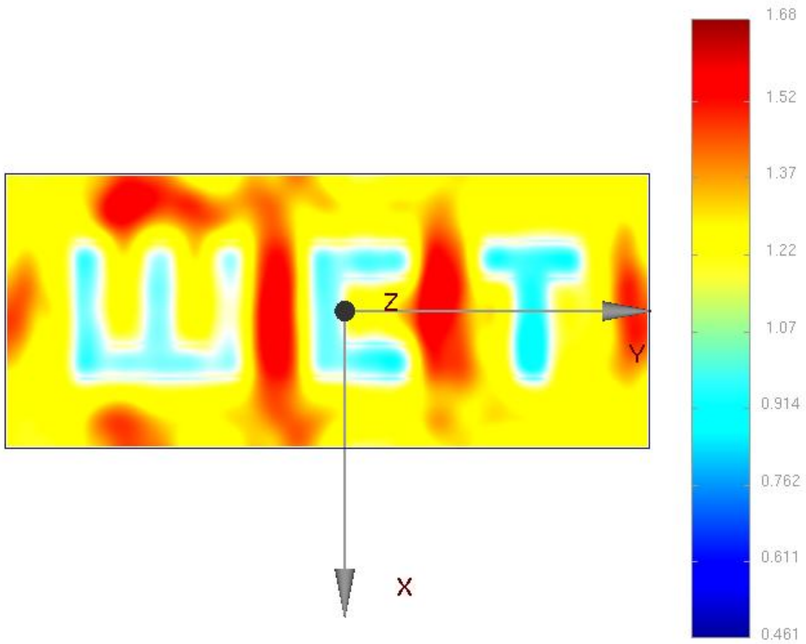
Simulation Results

We show the 2D plot figure as following

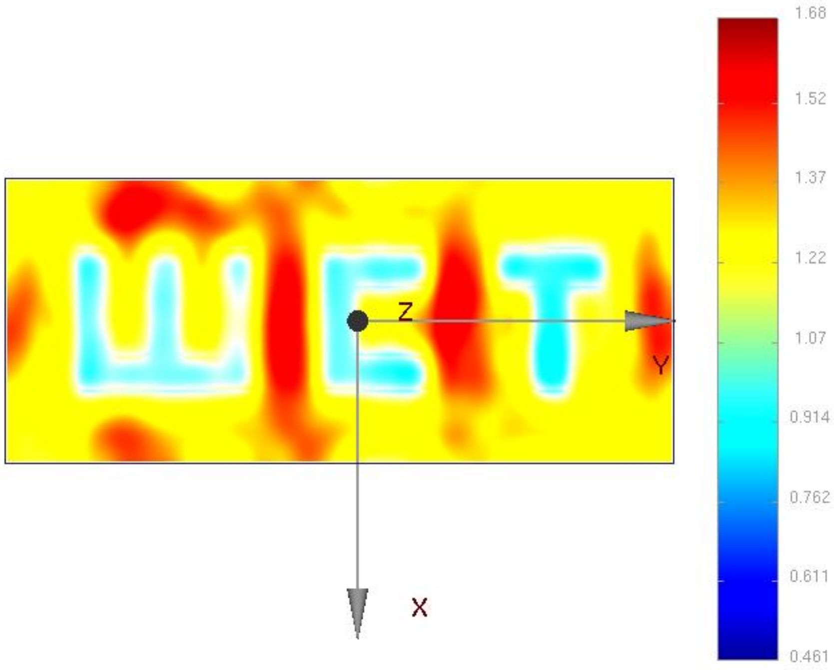
Solver 1: Ex at Z=-6.67 nm, in P polarization



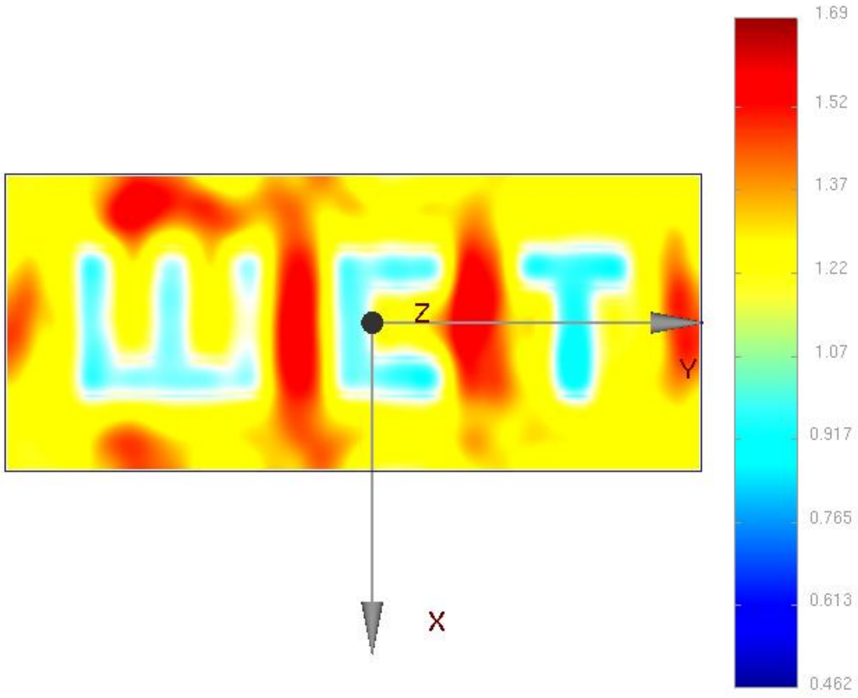
Solver 2: Ex at Z=-6.67 nm, in P polarization, double precision



Solver 2: Ex at Z=-6.67 nm, in P polarization, double precision



Solver 2: Ex at Z=-6.67 nm, in P polarization, single precision

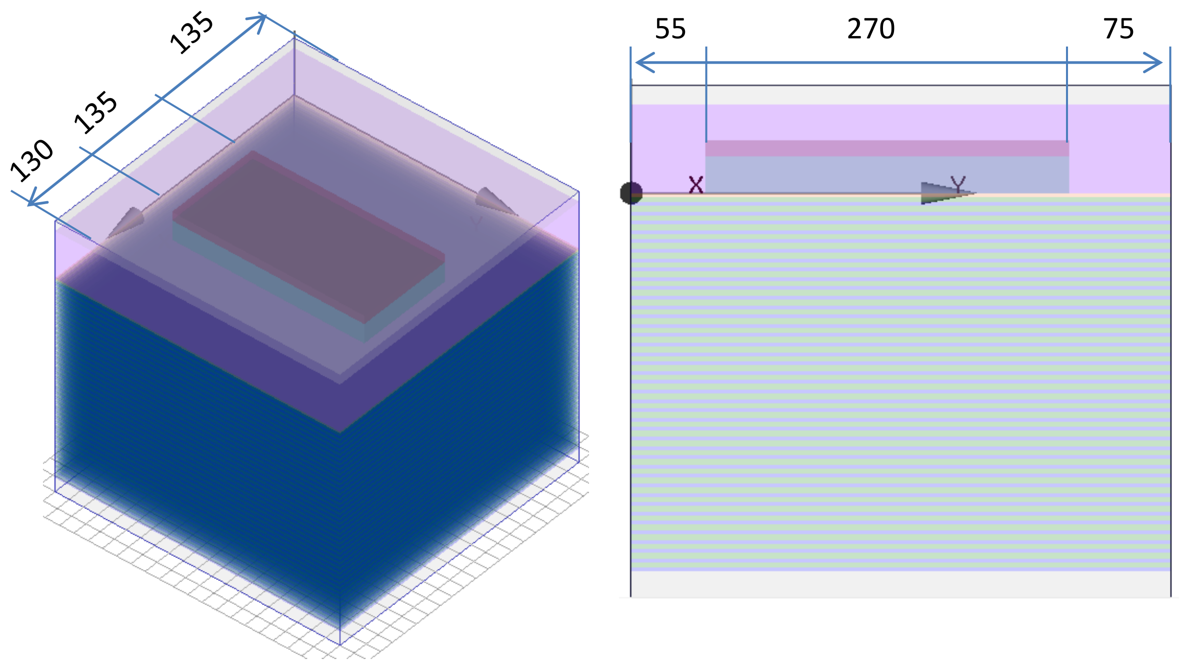


Benchmark Test VIII

Solver v2

400x400 nm^2 EUV case (30λx30λ)
Simulate P & S polarization in one run

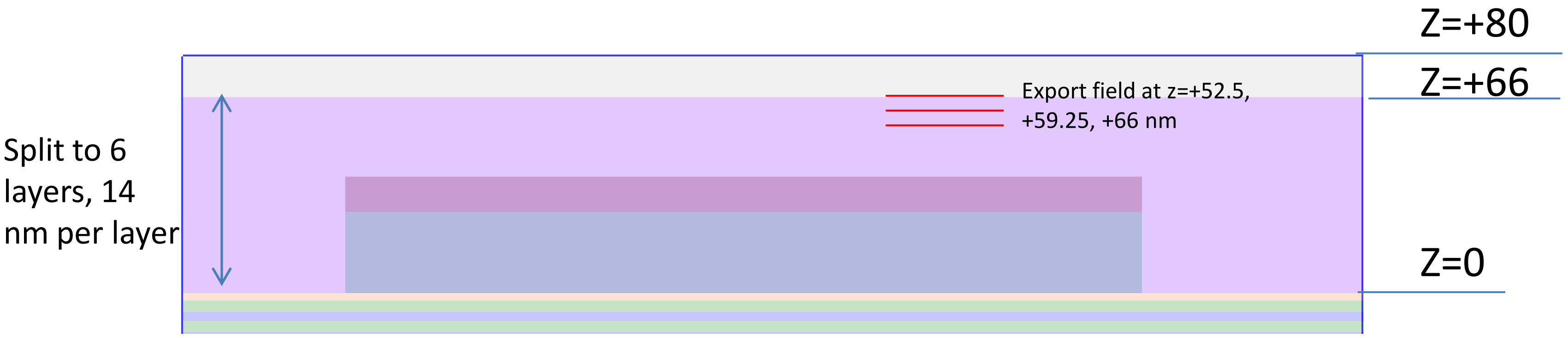
Here, we will show the simulation by solver v2 only, because the memory requirement for solver v1 is excessive for most servers.



Settings

➢ **solver 2**: we will only calculate the not-layered region, as shown in the following figure, we split this region into 6 cells, 14 nm per cell, about 1 λ. There are following 3 settings

1) Double precision, integration by exact matched nodal points
   - ❑ order for SEM region: (4,4,5)
   - ❑ cell number: [30,30,6] for SEM domain
   - ❑ cell size in X & Y both are around 13.5 nm
2) Double precision, integration by in-exact matched nodal points
   - ❑ order for SEM region: (5,5,5)
   - ❑ cell number: [21,21,6] for SEM domain
   - ❑ cell size in X & Y both are around 20 nm
3) Double precision, integration by in-exact matched nodal points
   - ❑ order for SEM region: (5,5,6)
   - ❑ cell number: [21,21,6] for SEM domain
   - ❑ cell size in X & Y both are around 20 nm



Simulation Time: by a Intel i7-5820k CPU

- **solver 2**
  - ❑ double precision, order(4,4,5), cells number (30,30,6), integration by exact matched nodal points
    - 35 min
  - ❑ double precision, order(5,5,5), cells number (21,21,6), , integration by in-exact matched nodal points
    - 23 min
  - ❑ double precision, order(5,5,6), cells number (21,21,6), , integration by exact matched nodal points
    - 32.5 min

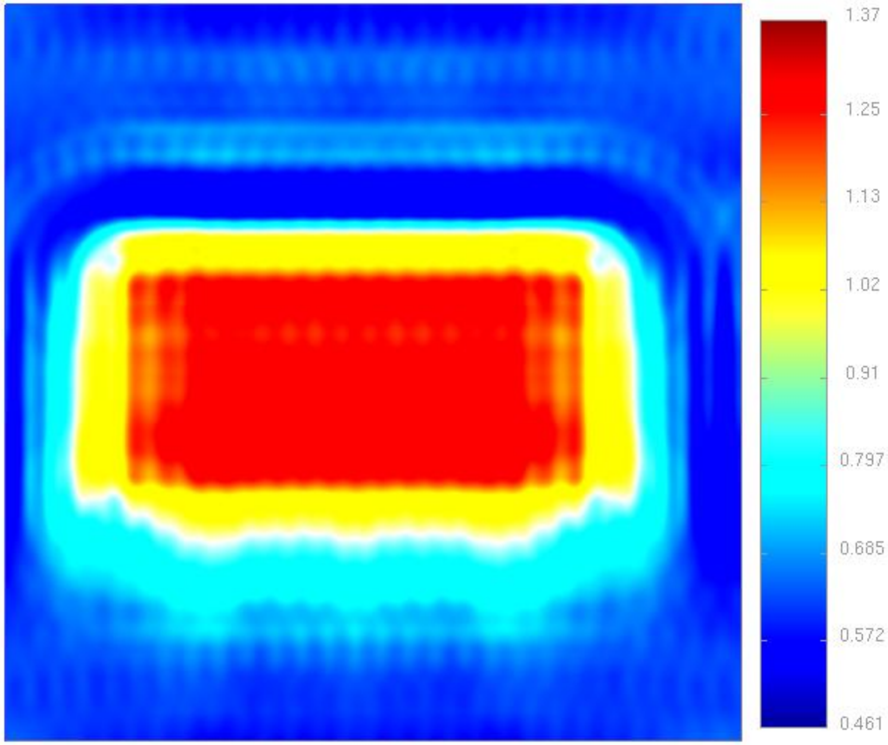
Memory Consumption

- **solver 2**
  - ❑ double precision, order(4,4,5), cells number (30,30,6), integration by exact matched nodal points
    - 110 GB
  - ❑ double precision, order(5,5,5), cells number (21,21,6), integration by in-exact matched nodal points
    - 56 GB
  - ❑ double precision, order(5,5,5), cells number (21,21,6), integration by exact matched nodal points
    - 73 GB

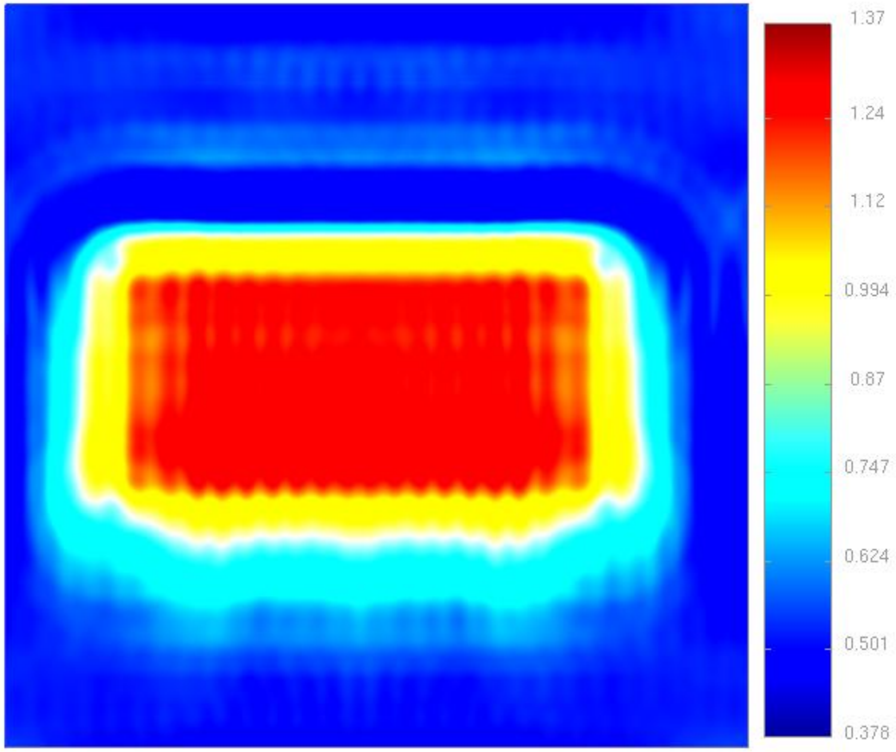
Simulation Results

We show the 2D plot figure as following

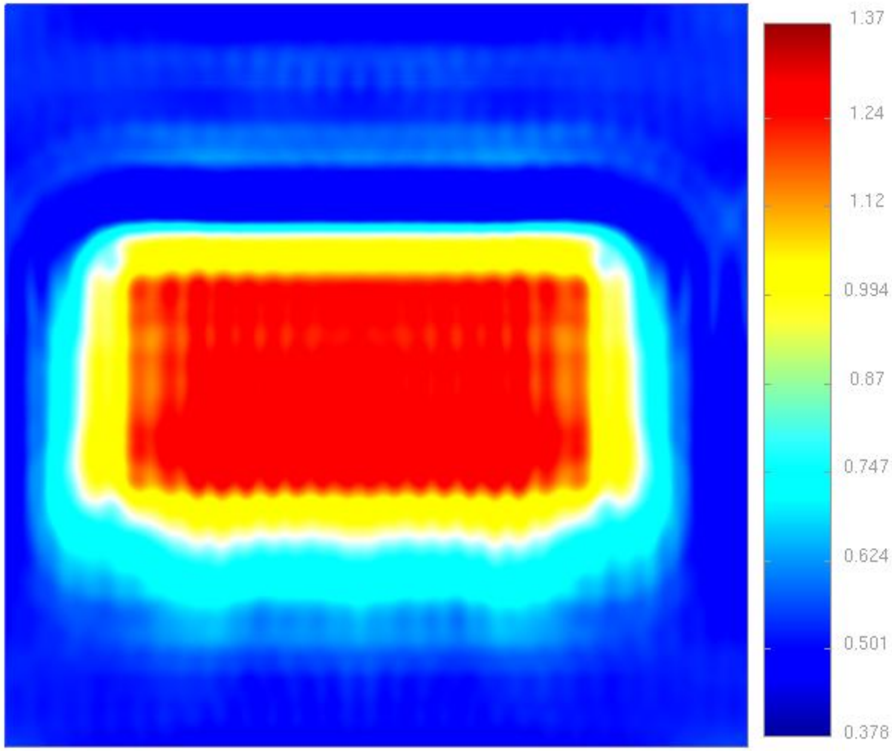
Solver 2: Ex at Z=52.5 nm, in P polarization, order (4,4,5), cells number (30,30,6), integration by exact matched nodal points



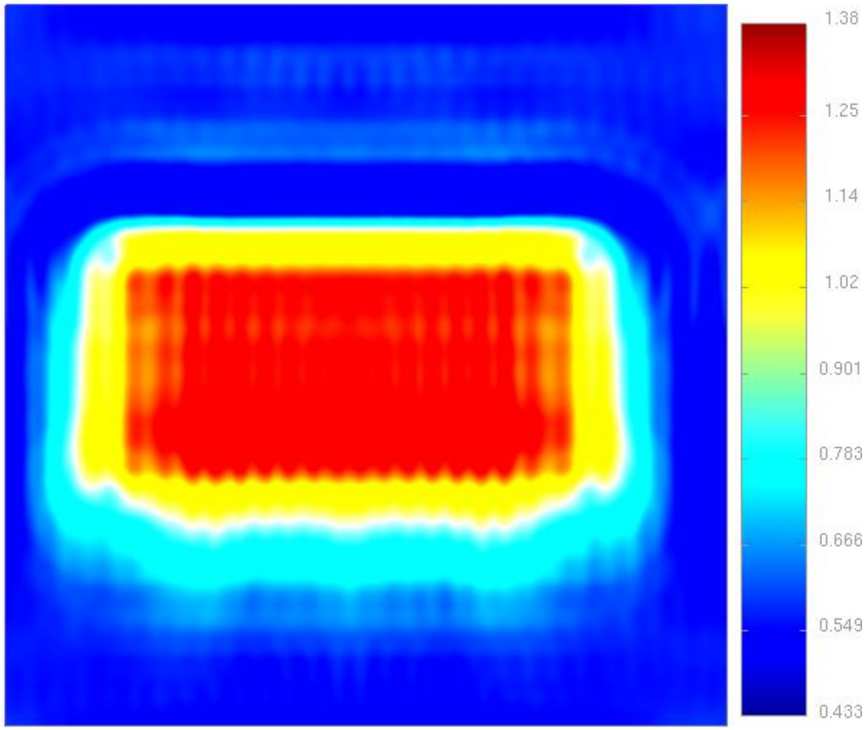
Solver 2: Ex at Z=52.5 nm, in P polarization, order (5,5,5), cells number (21,21,6), integration by in-exact matched nodal points



Solver 2: Ex at Z=52.5 nm, in P polarization, order (5,5,5), cells number (21,21,6), integration by in-exact matched nodal points



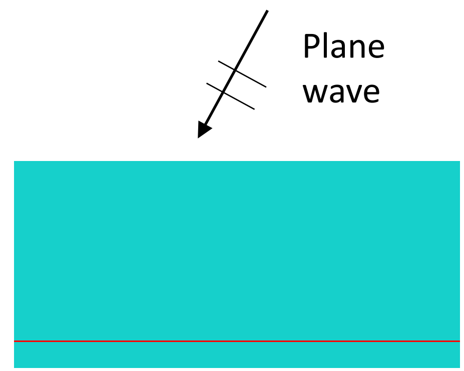
Solver 2: Ex at Z=52.5 nm, in P polarization, order (5,5,6), cells number (21,21,6), integration by in-exact matched nodal points



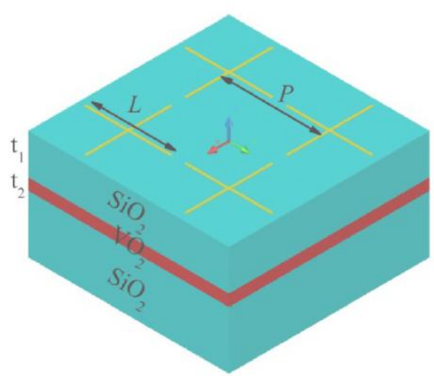
Benchmark Test IX

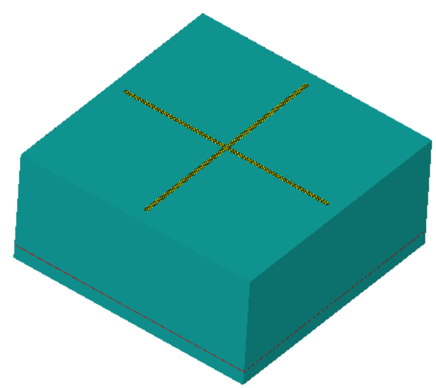
Freq. sweep on a thin Au film on S_iO_2 and VO_2 substrate

Application in THz



This case comes from the simulation model in the paper “Broadband tunable terahertz absorber based on vanadium dioxide metamaterials”, ZHENGYONG SONG, KAI WANG, JIAWEN LI, QING HUO LIU, *Vol. 26, No. 6 | 19 Mar 2018 | OPTICS EXPRESS 7148*.



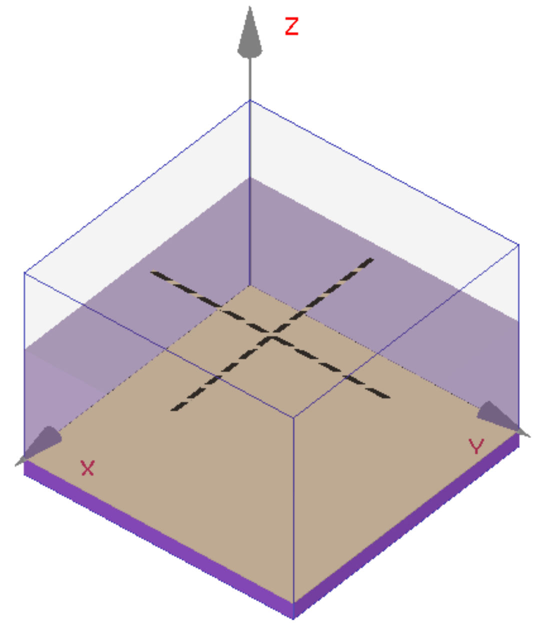


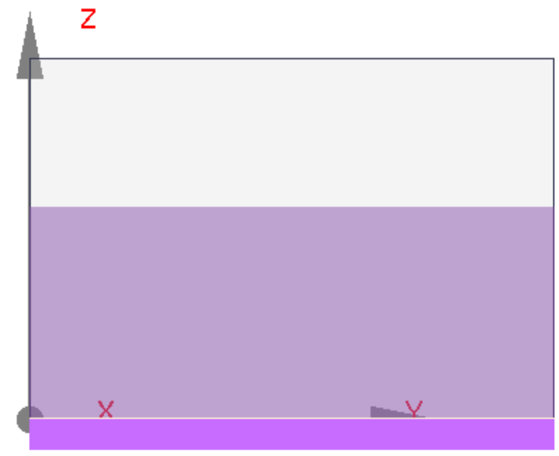
This case is built in the demo package:
sweep_freq_dispersive_material\filter_1\VO2 absorber_sig_2000_sw.wnt

The structure has a filtering effect in a specified freq. range. The principle of this device can be referred to the paper.

The whole device is composed by filter array with periodic boundary. Therefore, in the simulation, we can use a single filter to simulate the whole device.

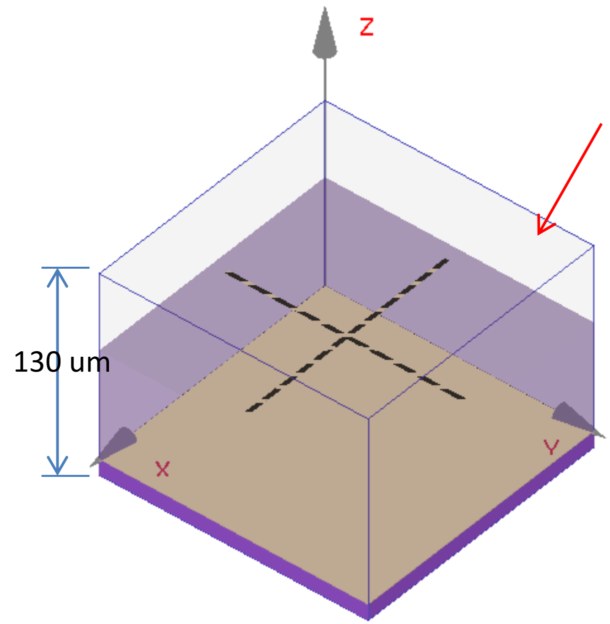
In this case, we will investigate the performance of the filter in the freq. range [0.3, 0.8] THz. The evaluation data are the reflectance, transmittance and absorptance.





There are several key points in the project design

1) There are 2 dispersive materials, Au & VO_2, used in the project, especially, VO_2 uses a variable in defining the material property.
2) There is extreme thin Au structures in the project, in order to capture the structure correctly, this case use a very special automatic mesh.



The cross shaped Au has a thickness of 0.02 um.

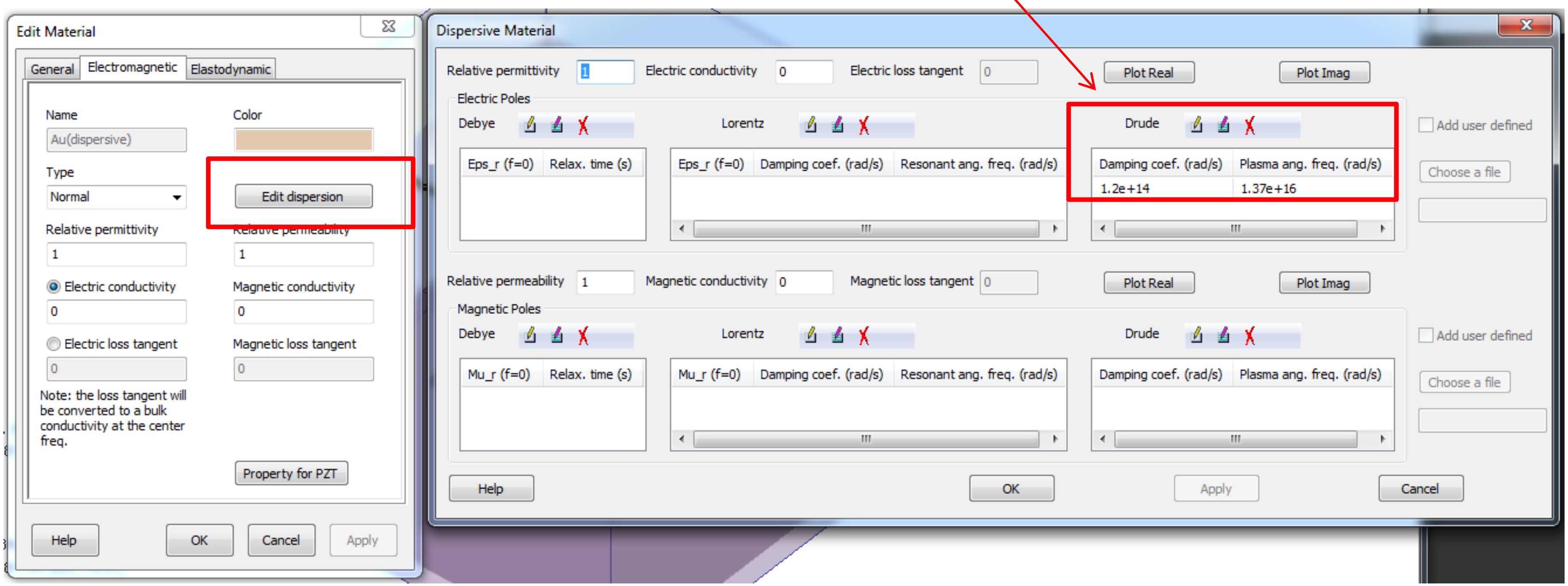
For the other parts, the project is very simple, user can build several boxes to setup the basic structure. The detail parameters can be referred to the demo project.

- Dispersive material Au.

Drude model $\varepsilon_{Au} = 1 - \omega_p^2 / \omega(\omega + i\Gamma)$

with plasma frequency $\omega_p = 1.37\times10^{16}\ rad/s$

collision frequency $\Gamma = 1.2\times10^{14}\ rad/s$



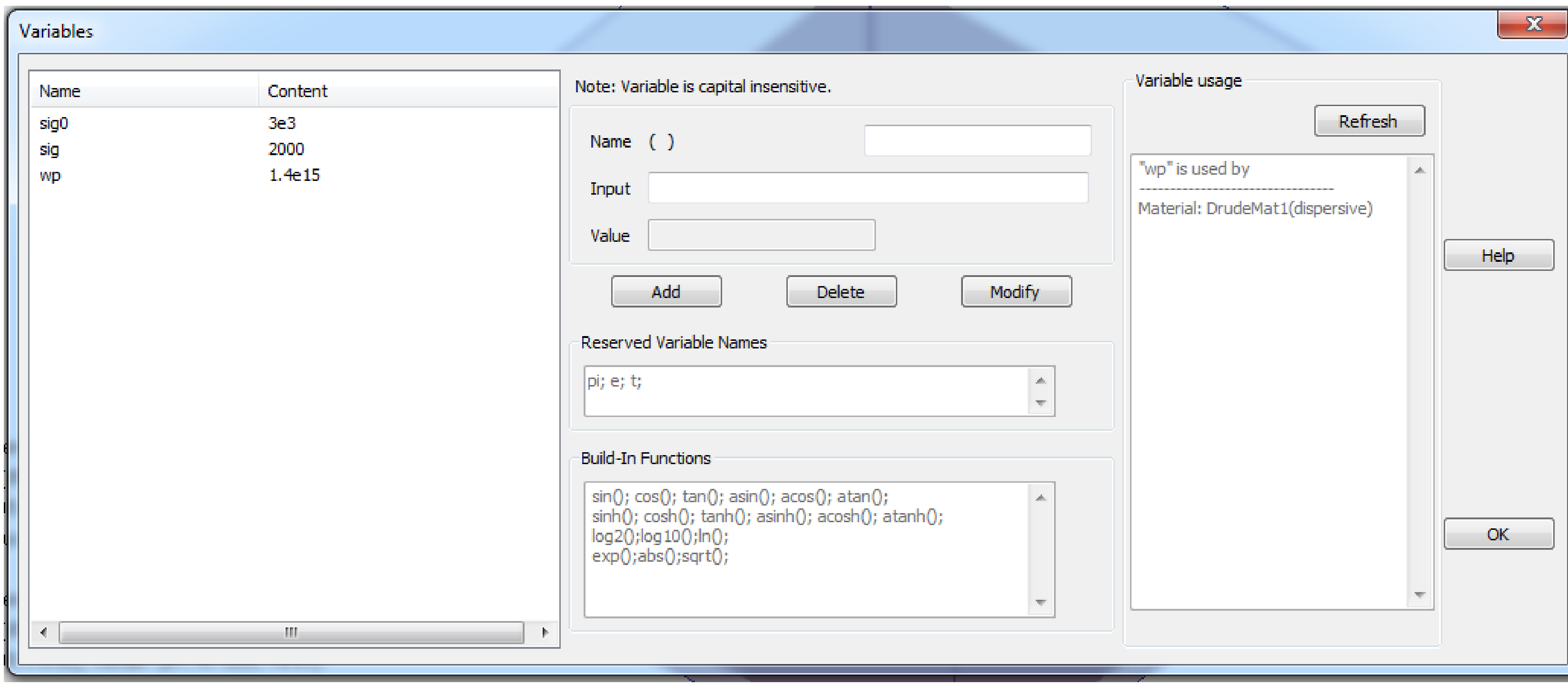
➢ Dispersive material VO_2

Drude model $$\varepsilon(\omega)=\varepsilon_{\infty}-\frac{\omega_p^2(\sigma)}{\omega^2+i\gamma\omega}$$ where $\varepsilon_{\infty}=12$

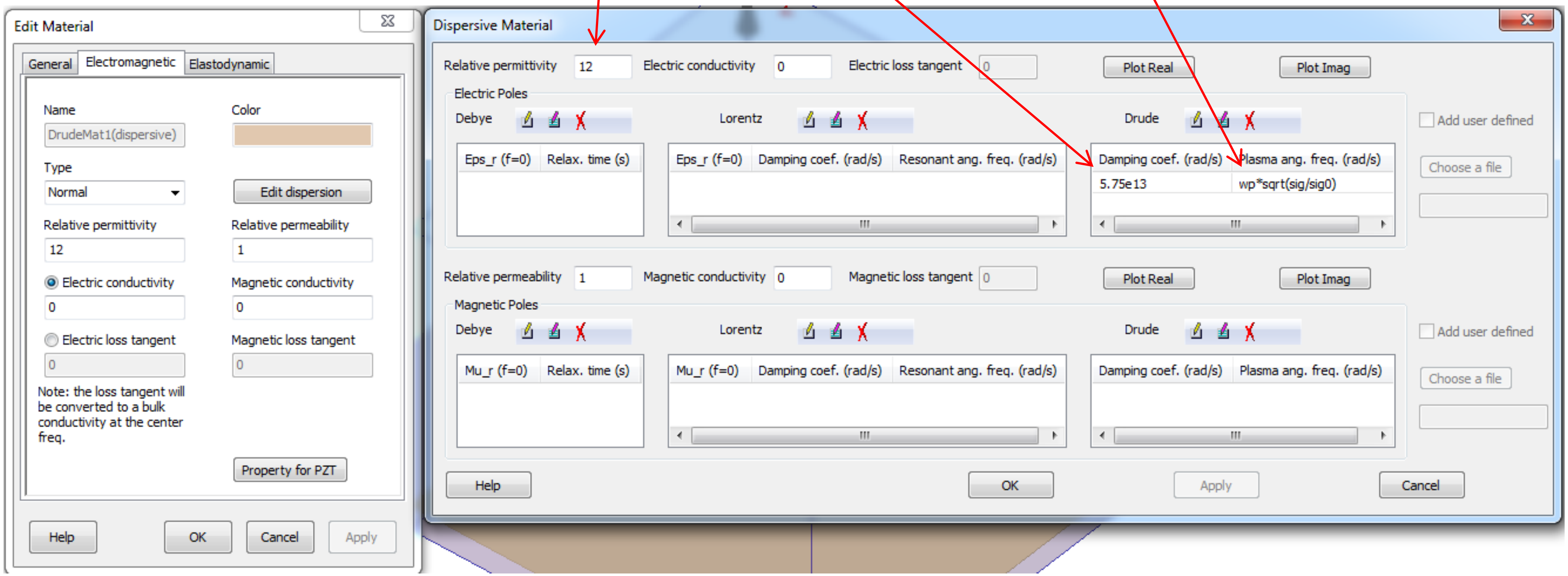
with $\sigma_0=3\times10^3\ \Omega^{-1}cm^{-1}$, $\omega_p(\sigma_0)=1.4\times10^{15}\ rad/s$, and $\gamma=5.75\times10^{13}\ rad/s$

$$\omega_p^2(\sigma)=\frac{\sigma}{\sigma_0}\omega_p^2(\sigma_0)$$, which is depend on σ

We define variables: sig0=σ_0; sig=σ, wp=ω_p as following



$$\varepsilon(\omega)=\varepsilon_{\infty}-\frac{\omega_p^2(\sigma)}{\omega^2+i\gamma\omega} \qquad \omega_p^2(\sigma)=\frac{\sigma}{\sigma_0}\omega_p^2(\sigma_0)$$

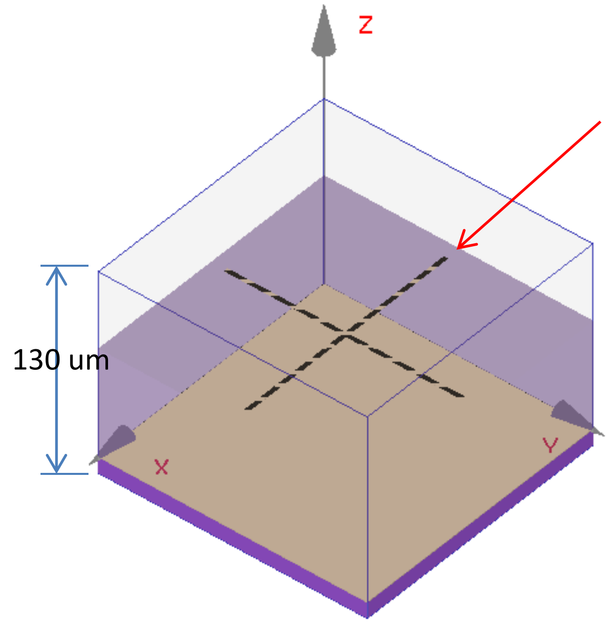


- Special automatic mesh

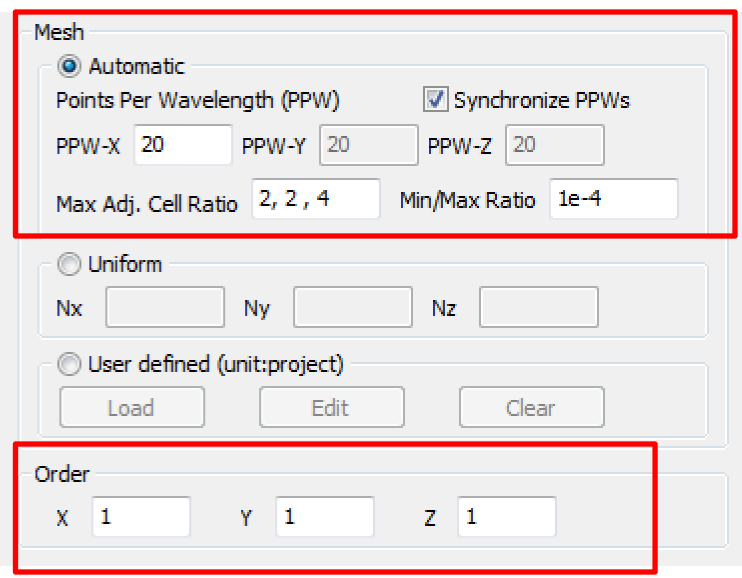
Due to the simulation freq. range is [0.3, 0.8] THz, under the f_{max} 0,8 THz, for the main structure: substrate S_iO_2, it is 0.5λ only. Therefore, this case will be oversample even with order=1. Because in X, Y and Z axis, there are at least 2 cells to capture the structures.

Here, we set the adjacent cell ratio in Z as 4, and the Min/Max cell ratio as 1e-4, to capture the Au layer in Z, with a minimum cell number in Z.

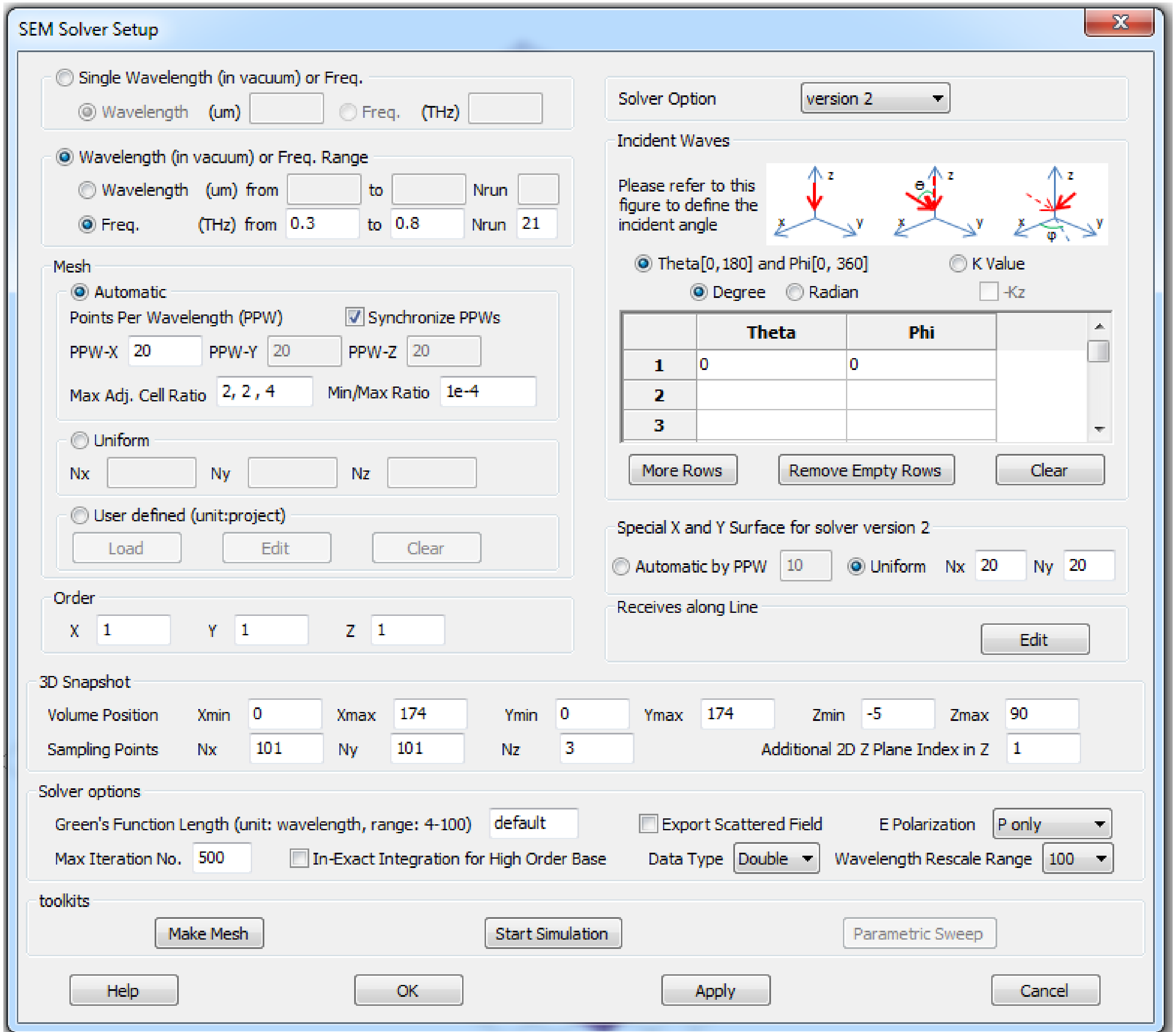
Because this case is oversampled, the order ***1*** in the solver should be good enough.



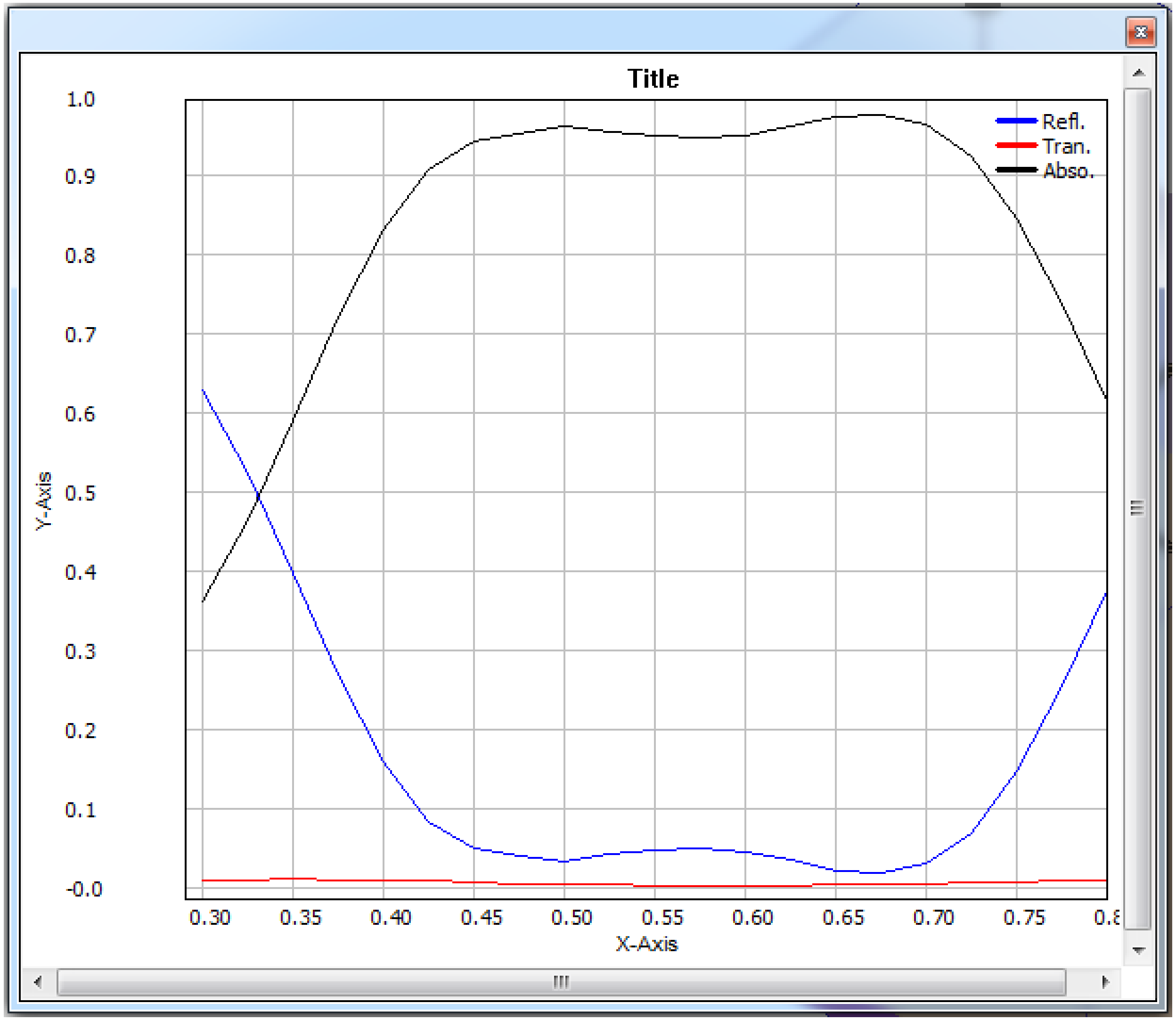
The cross shaped Au has a thickness of 0.02 um.



The final SEM simulation setup is



Following is the reflectance, transmittance and absorptance curve in from the freq. sweep. It matches with the data in the paper.



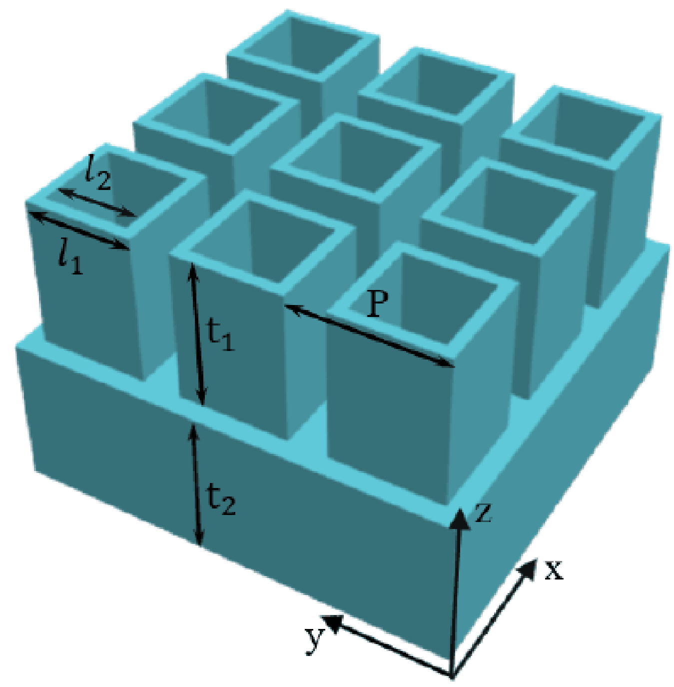
Benchmark Test X

Freq. sweep on a VO_2 filter

Application in THz

This case comes from the simulation model in the paper "Ultra-broadband wide-angle terahertz absorber realized by a doped silicon metamaterial", Mingwei Jiang, ZHENGYONG SONG, QING HUO LIU, *Vol. 471, 15 September 2020 | OPTICS Communications.*

Similar to the case IX, we will use a single filter to simulate the whole device.



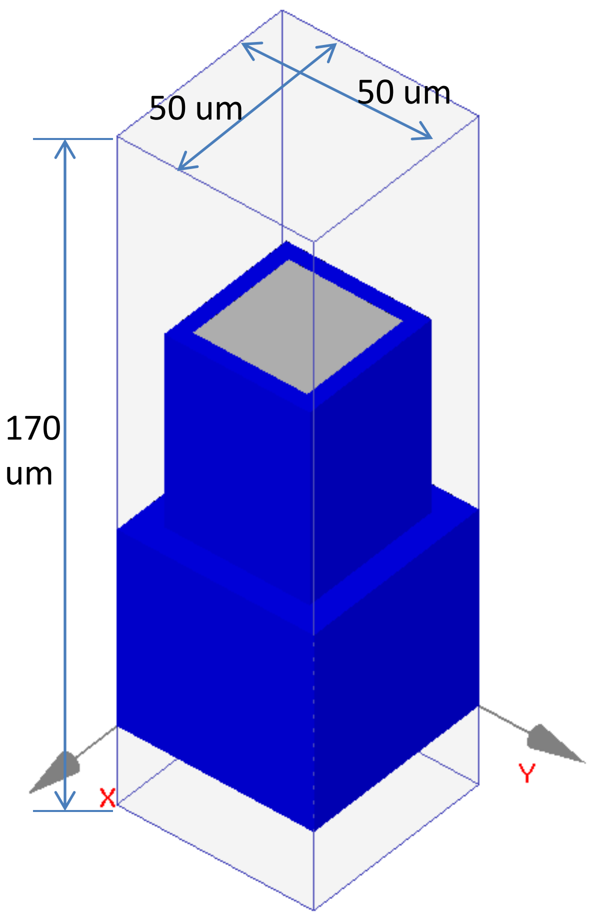
This case is built in the demo package:
sweep_freq_dispersive_material\filter_2\VO2 absorber_Si_5.wnt

In this case, we are going to sweep the freq. range [0.5, 6] THz.

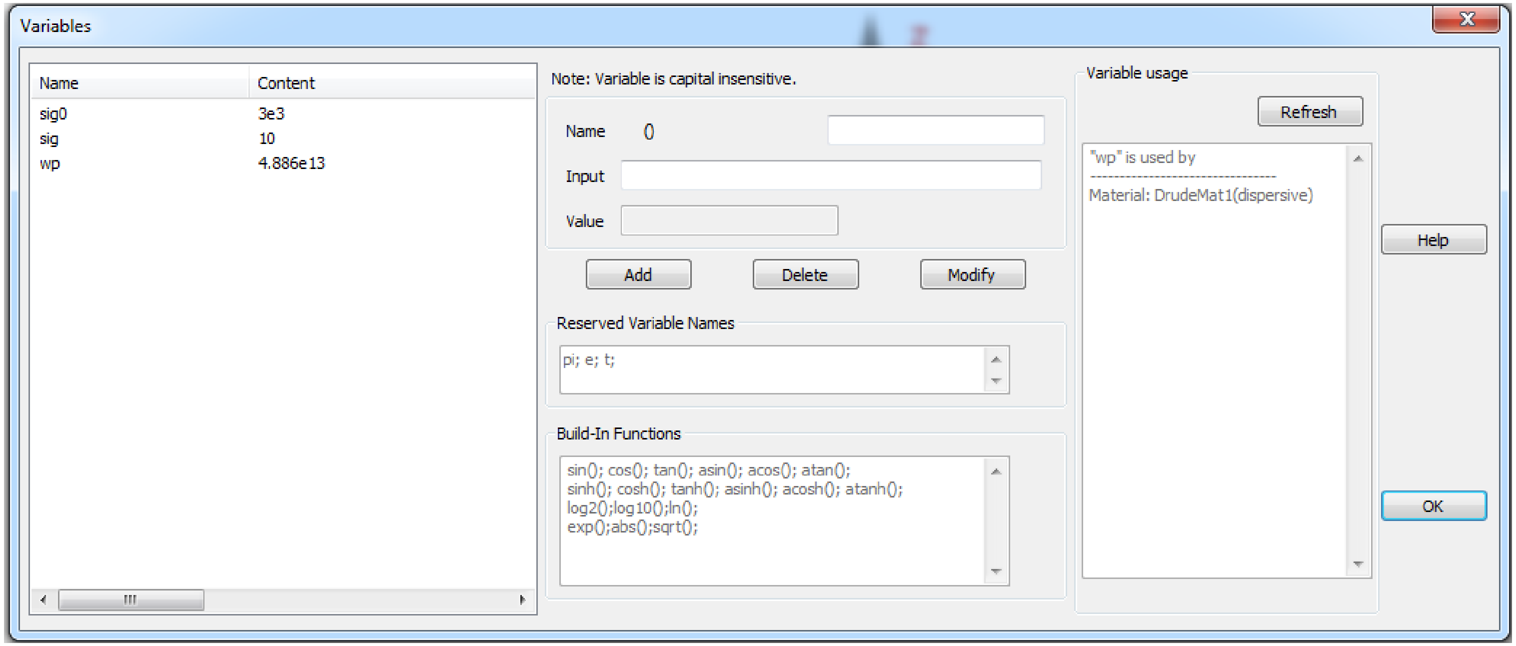
Due to the freq. range is different from that in the case IX, the dispersive material VO_2 has the following properties.

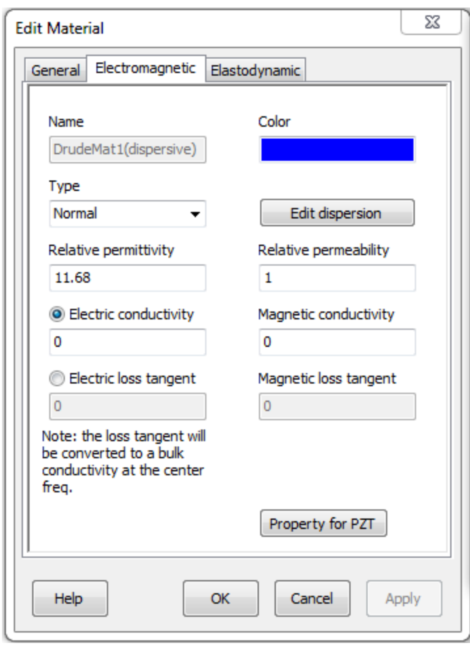
$$\text{Drude model} \quad \varepsilon = \varepsilon_c - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

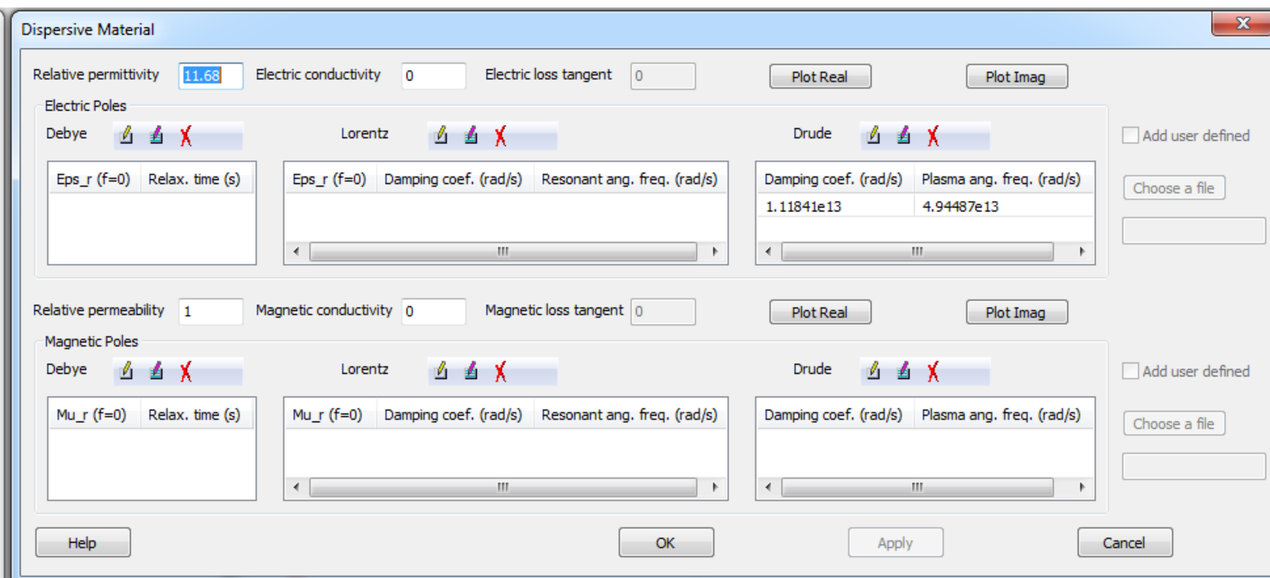
Where, $\varepsilon_c = 11.68$, $\omega_p = 2\pi \times 7.87$ THz, $\gamma = 2\pi \times 1.78$ THz



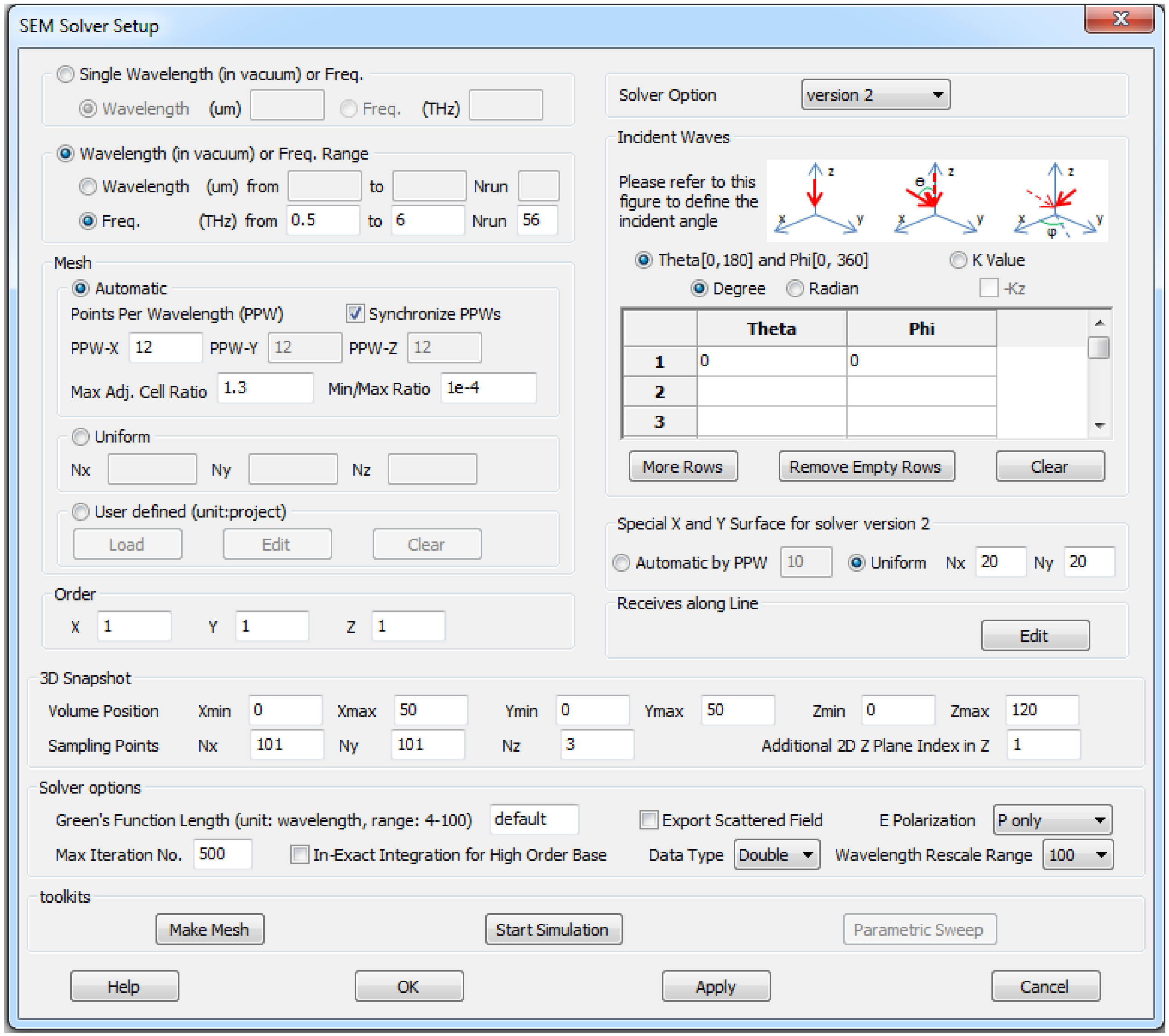
We define variables and the material property for VO_2 as following


Variables
Name
Content
sig0
3e3
sig
10
wp
4.886e13
Note: Variable is capital insensitive.
Name
()
Input
Value
Add
Delete
Modify
Reserved Variable Names
pi; e; t;
Build-In Functions
sin(); cos(); tan(); asin(); acos(); atan();
sinh(); cosh(); tanh(); asinh(); acosh(); atanh();
log2();log10();ln();
exp();abs();sqrt();
Variable usage
Refresh
"wp" is used by
Material: DrudeMat1(dispersive)
Help
OK

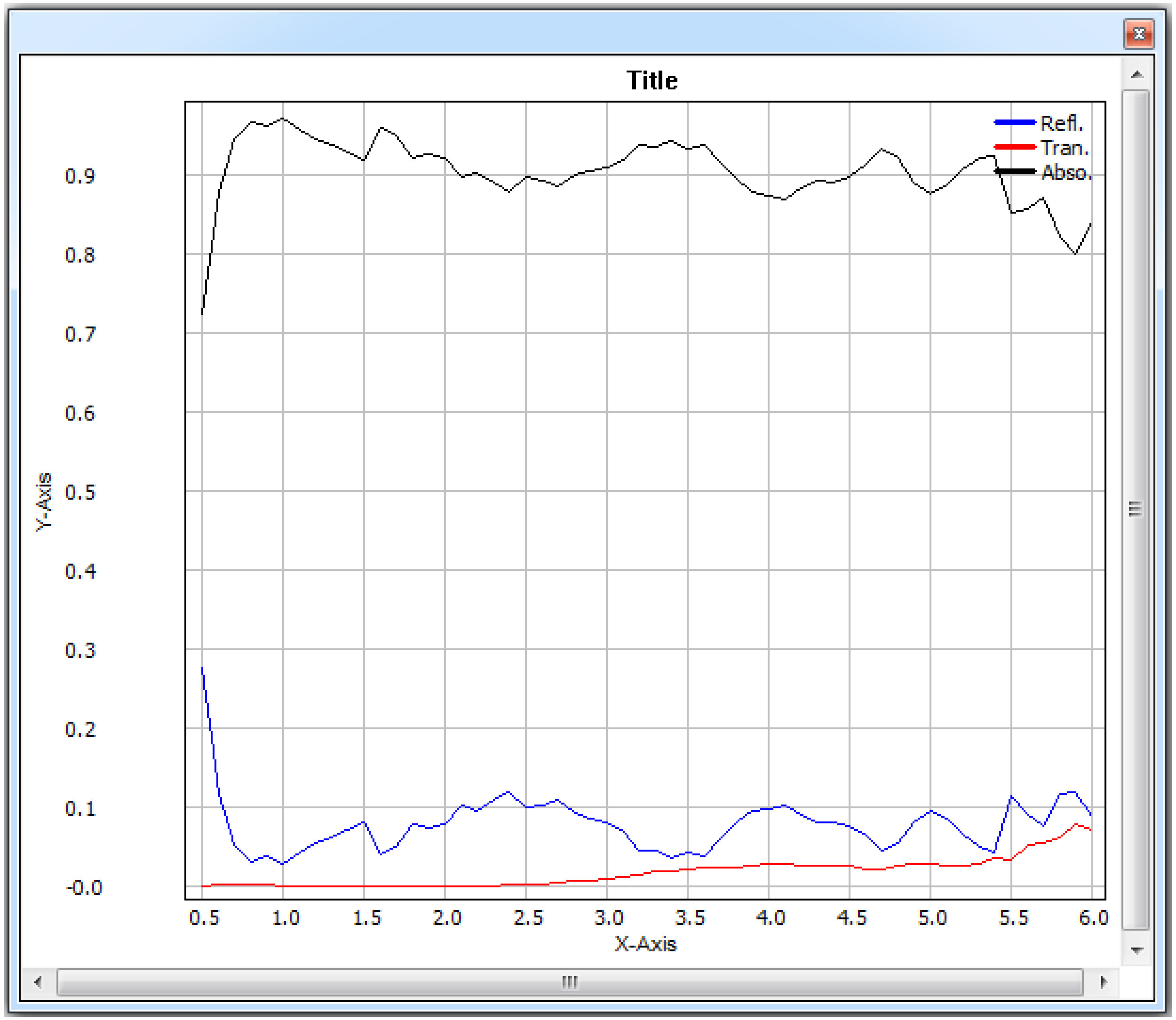

Edit Material
General
Electromagnetic
Elastodynamic
Name
Color
DrudeMat1(dispersive)
Type
Normal
Edit dispersion
Relative permittivity
Relative permeability
11.68
1
Electric conductivity
Magnetic conductivity
0
0
Electric loss tangent
Magnetic loss tangent
0
0
Note: the loss tangent will be converted to a bulk conductivity at the center freq.
Property for PZT
Help
OK
Cancel
Apply


Dispersive Material
Relative permittivity
11.68
Electric conductivity
0
Electric loss tangent
0
Plot Real
Plot Imag
Electric Poles
Debye
Lorentz
Drude
Add user defined
Eps_r (f=0)
Relax. time (s)
Eps_r (f=0)
Damping coef. (rad/s)
Resonant ang. freq. (rad/s)
Damping coef. (rad/s)
Plasma ang. freq. (rad/s)
1.11841e13
4.94487e13
Choose a file
Relative permeability
1
Magnetic conductivity
0
Magnetic loss tangent
0
Plot Real
Plot Imag
Magnetic Poles
Debye
Lorentz
Drude
Add user defined
Mu_r (f=0)
Relax. time (s)
Mu_r (f=0)
Damping coef. (rad/s)
Resonant ang. freq. (rad/s)
Damping coef. (rad/s)
Plasma ang. freq. (rad/s)
Choose a file
Help
OK
Apply
Cancel

The final SEM simulation setup is

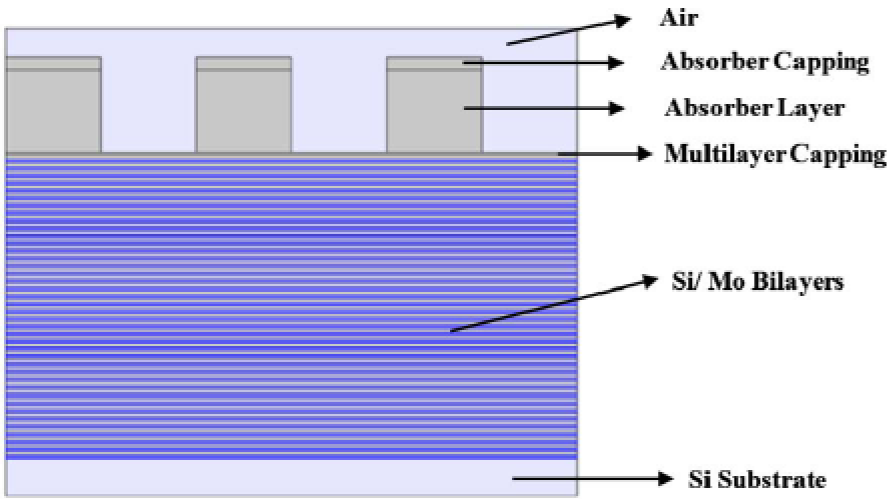


Following is the reflectance, transmittance and absorptance curve in from the freq. sweep.

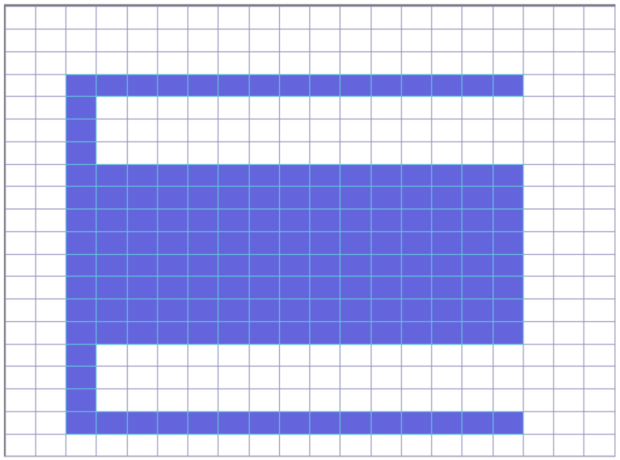


Appendix I
the Mask Editor for Lithographic Applications

For typical Lithographic applications, the base layers, including the Si/Mo bilayers and the Si substrate, are fixed. Only the absorber layer and the capping layer (mask layers) will be variant in different applications. Meanwhile, the structures in mask layers can be decomposed by fixed size boxes due to the fundamental element shape in the lithographic application is fixed. Based on these features, WCT GUI provides an editor to generate the mask pattern in a simple way.

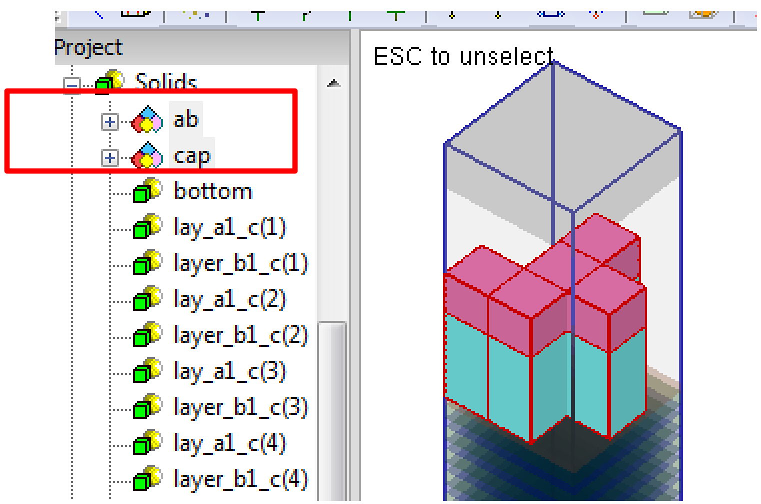


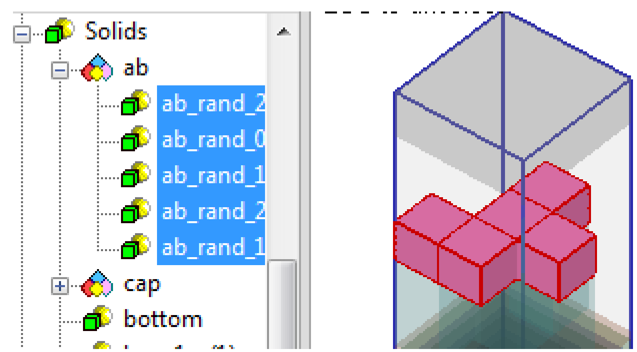
A mask pattern



- Requirements to use the mask editor
  - All 3D solids should be grouped into different layers (component) by the Z positions
    - in each layer, all solids should have the same Z size
  - All 3D solids in each layer should be a box aligned to X and Y axis

Following figures show 2 layers created by the mask editor





The mask editor can

- ➢ create patterns for multiple empty layers

- ➢ edit multiple layers with existing patterns

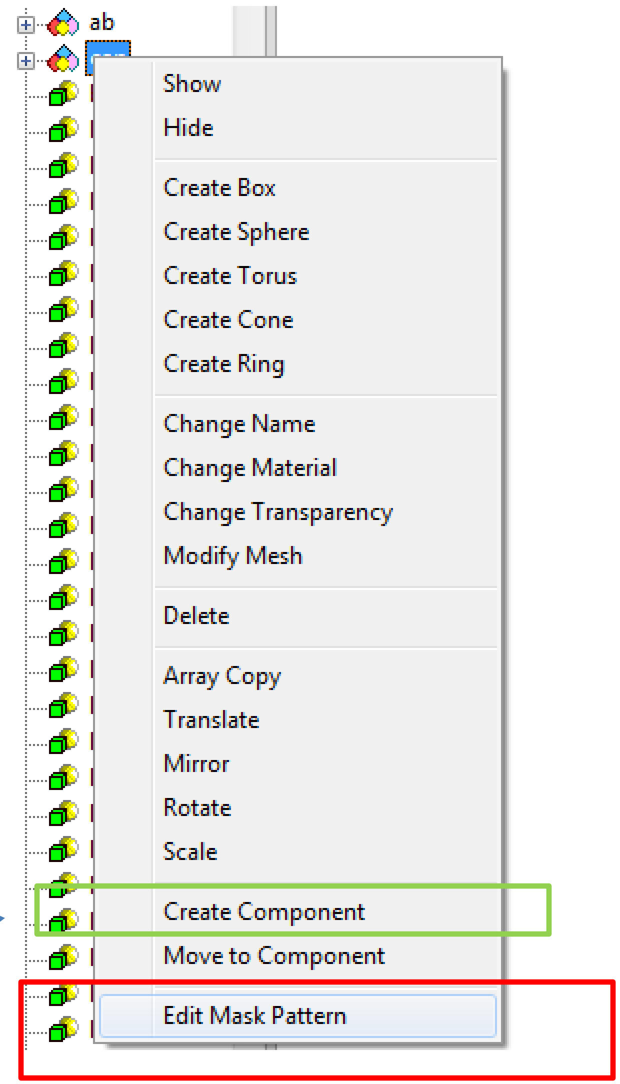
- ➢ generating multiple projects with random patterns and start the lithography solver to solve these projects automatically

- ➢ generating multiple projects with parametric sweeping patterns and start the lithography solver to solve these projects automatically

The Mask Editor

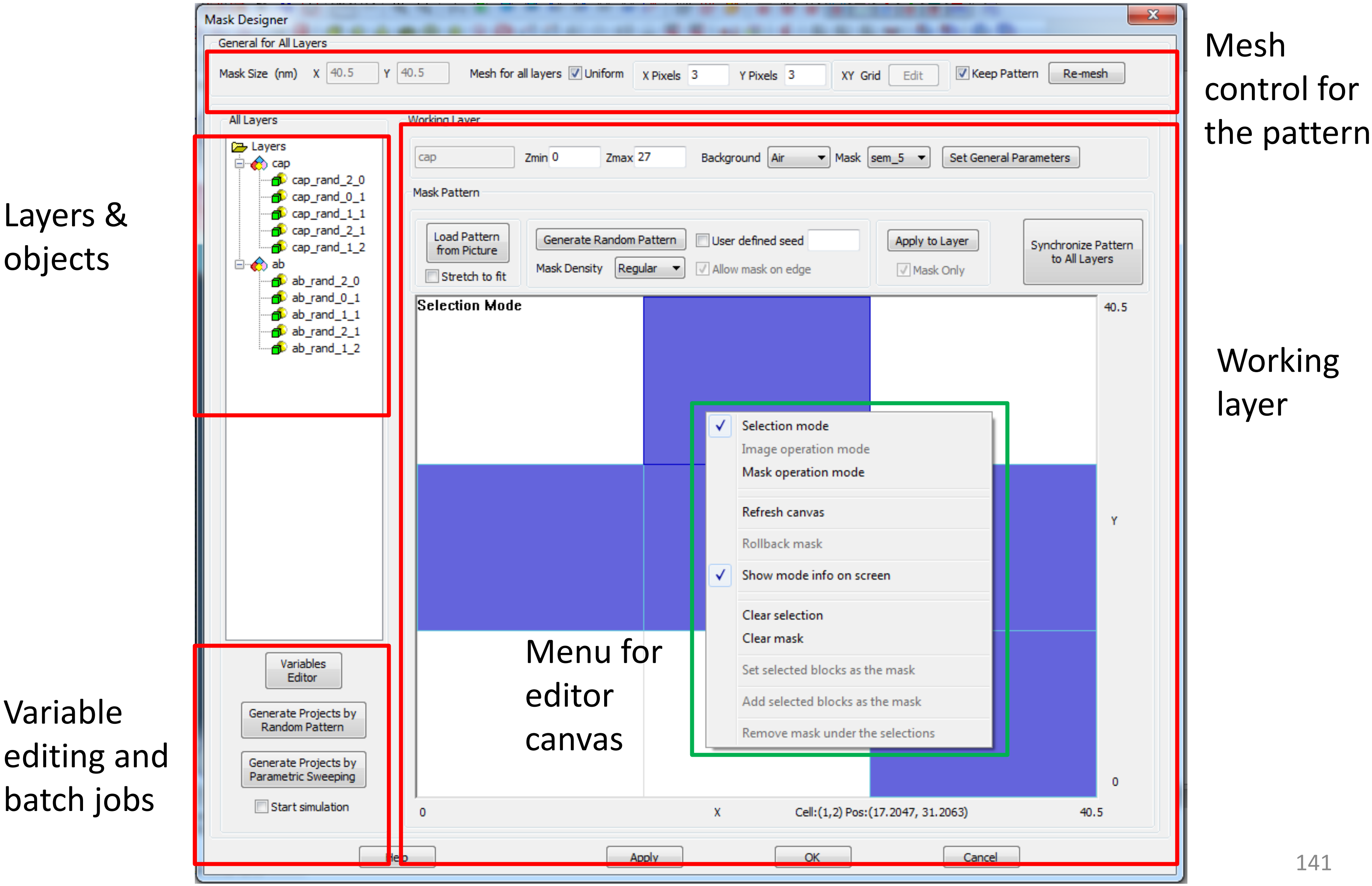
1) In order to start the mask editor, user need to select 1 or multiple components in the project tree to popup the menu as the figure.
   - Here, each component represents a layer
   - Each layer can have zero or multiple boxes

   Then use menu item "Edit Mask Pattern" to enter the mask editor



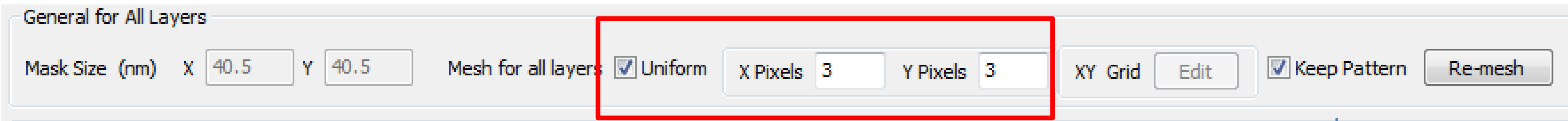
Note: If the solids are not organized by components, please create the components and drag the corresponding boxes into those components.

The Layout of the Mask Editor



a) Mesh control for the pattern

Note: this mesh is for geometry generation purpose. It is unnecessary the same as the real simulation mesh in the WCT solver. However, in order to make the pattern match the simulation mesh. It is suggested to load the SEM solver mesh as the pattern mesh.

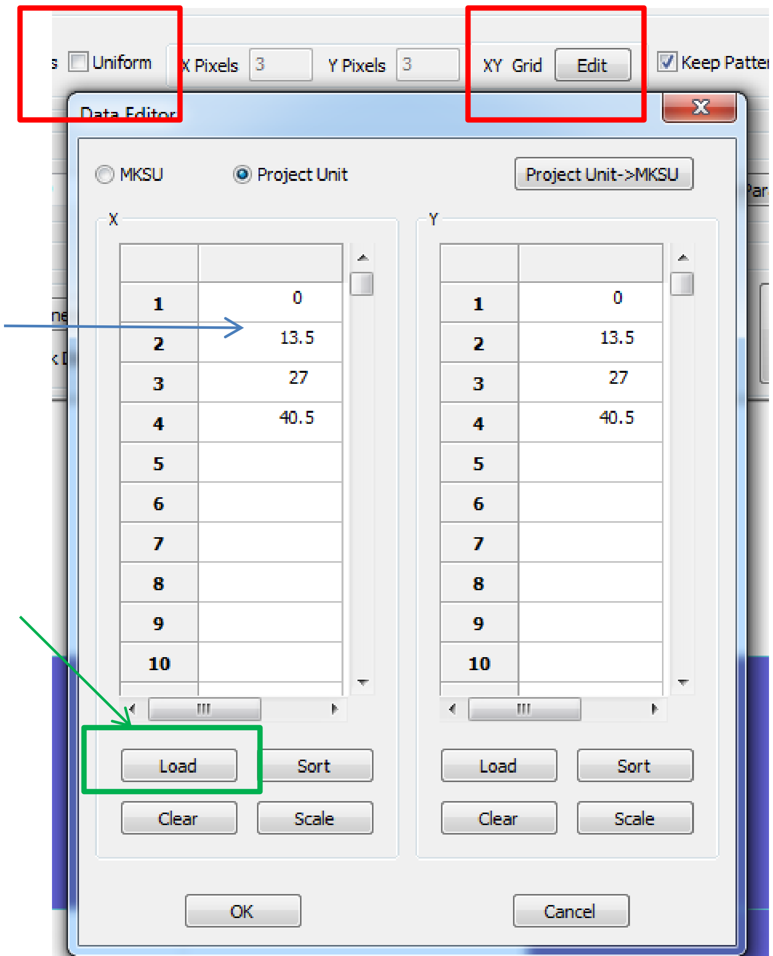


Project X & Y size

Uniform mesh

Un-check to switch to a non-uniform mesh

Edit the non-uniform mesh



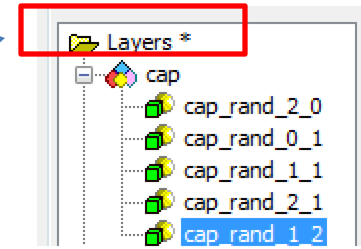
The mesh grid will be displayed in the editor canvas. The grid is **editable** in this dialog.

User can load the grid from a single column ASCII data file in project unit, as

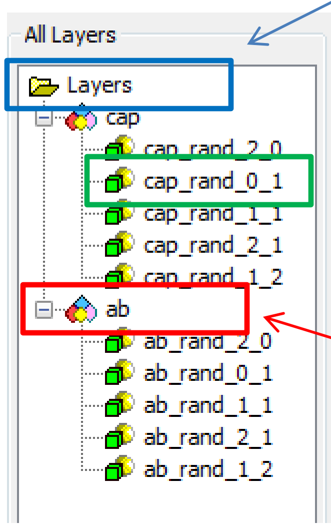
0
13.5
27
40.5

If "**keep Pattern**" is *un-checked*, after re-mesh, all existing solids in layers will be removed.

b) All editable layers in the editor

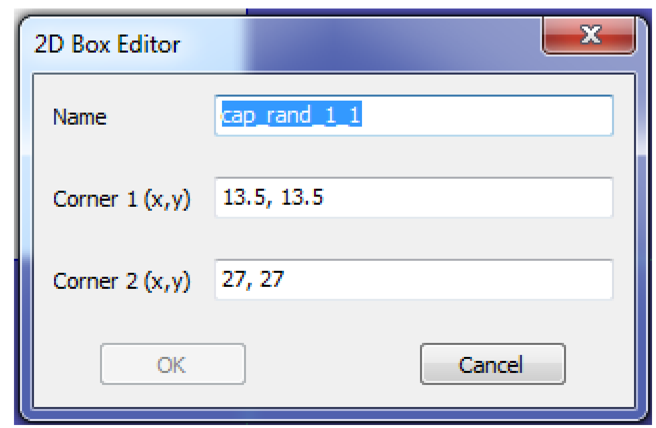


If any content in the layers has been modified, a “*” label will be added as



One box in this layer, ***double click*** on it will enter a 2D box editor for this object, as following

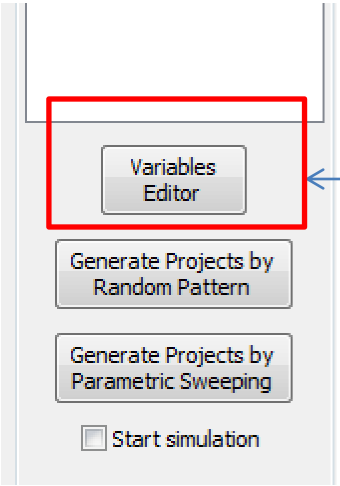
Layer node, ***double click*** on it will set this layer as the working layer in the left part of the editor



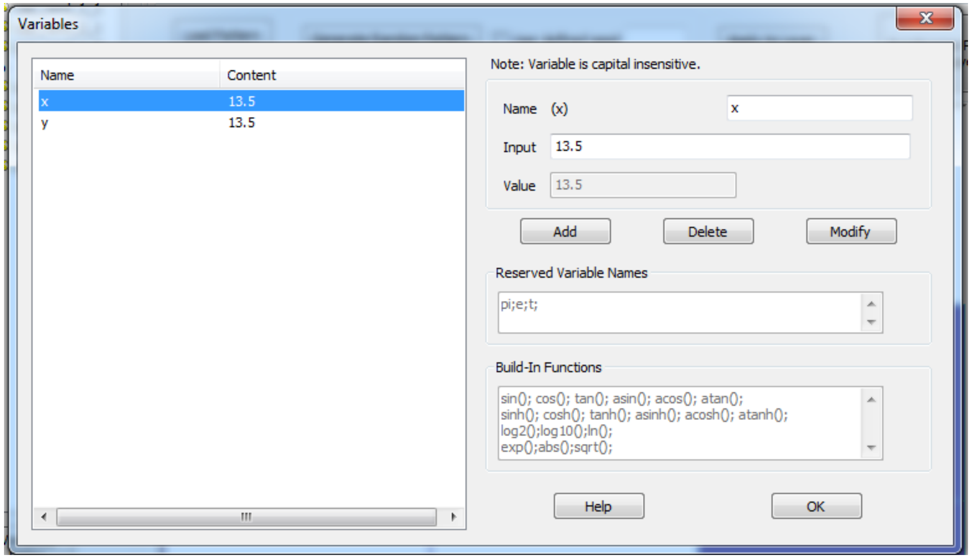
Note: the definition of box corner can use variable. For example, there is variable x=13.5 in the project. So, the definition of “Corner 1” as “x, 13.5” is the same as “13.5, 13.5”

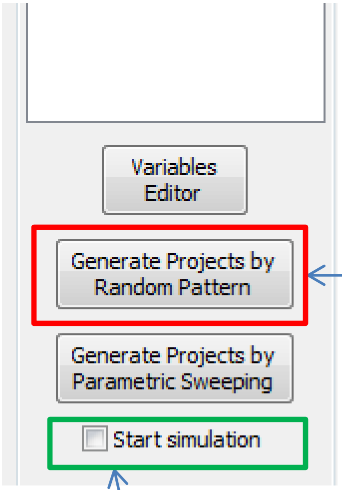
c) Global buttons

Variable Editor



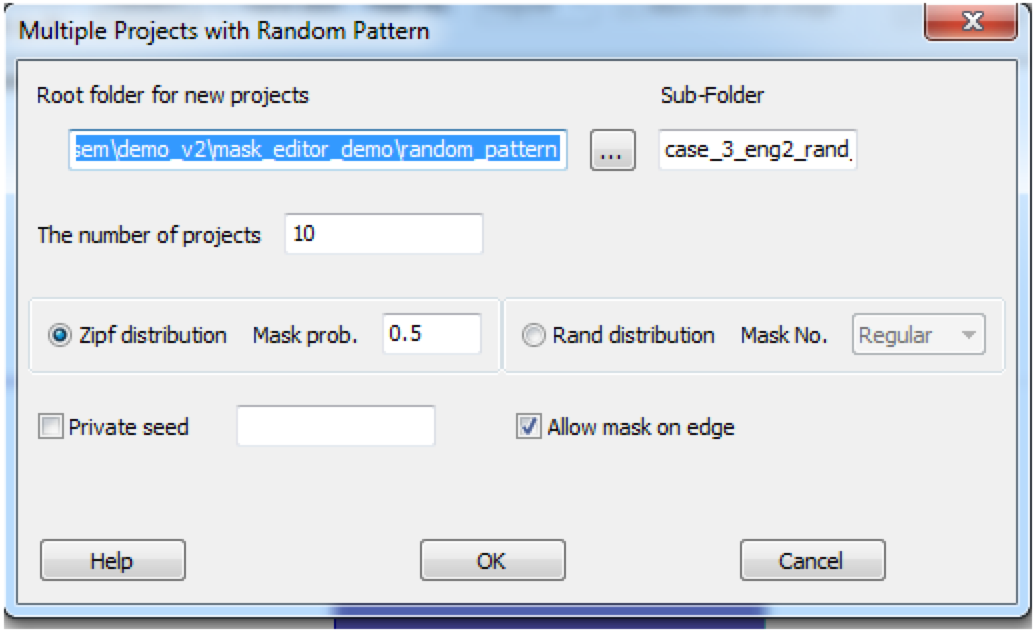
Popup the variable editor for this project.





Multiple Random Patterns

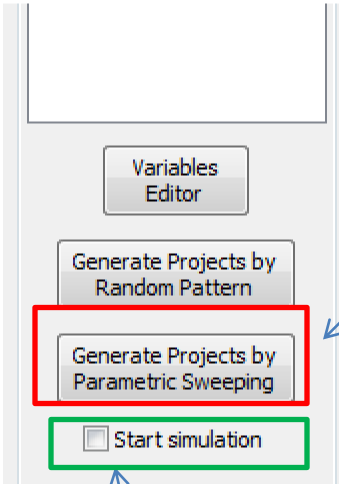
Generating multiple projects. Each project will have a random pattern. The setup control for these projects is shown as



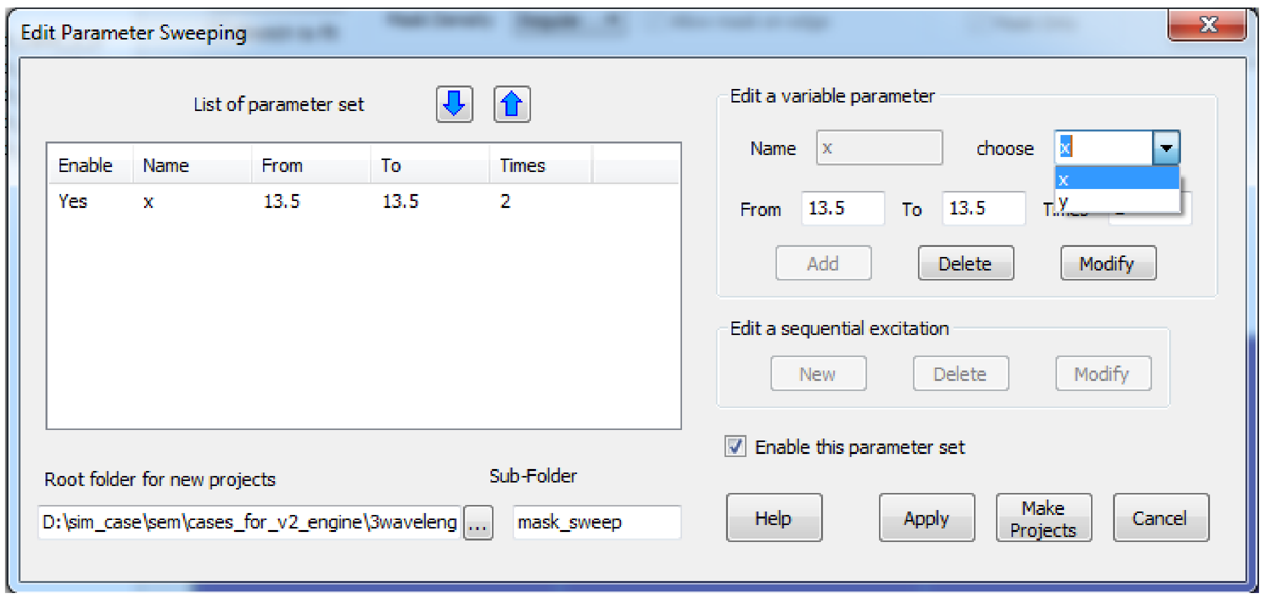
Whether need to start simulation automatically after these projects are generated

More details will be shown in the demo case.

Parametric Sweep



Generating multiple projects. Each project will implement a value of the variable in the sweeping range. The setup for these projects is as



Whether need to start simulation automatically after these projects are generated

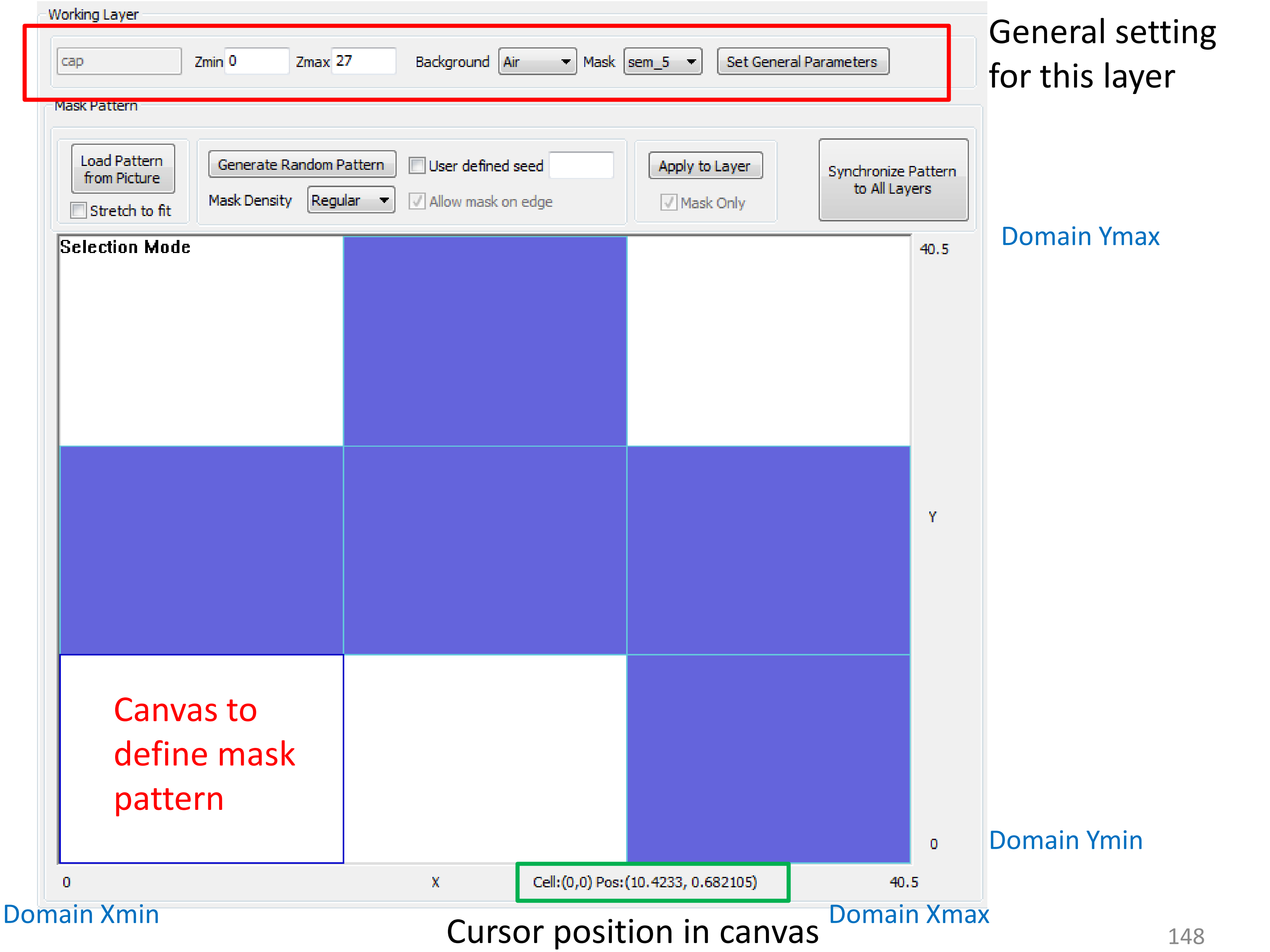
More details will be shown in the demo case.

Apply the modified content to the project, but still stay in the editor

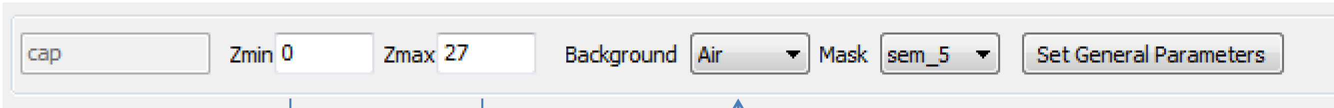
Skip the modification and quit the editor

Apply the modified content to the project, then quit the editor

d) Working layer



General setting for this layer



Layer's name

It will not be used in this version. Because the editor generate the box for mask only

Set left definitions to the working layer

The Z range of this layer. For an empty layer, it can be any values. For not empty layers, the Z ranges can't be intersect.

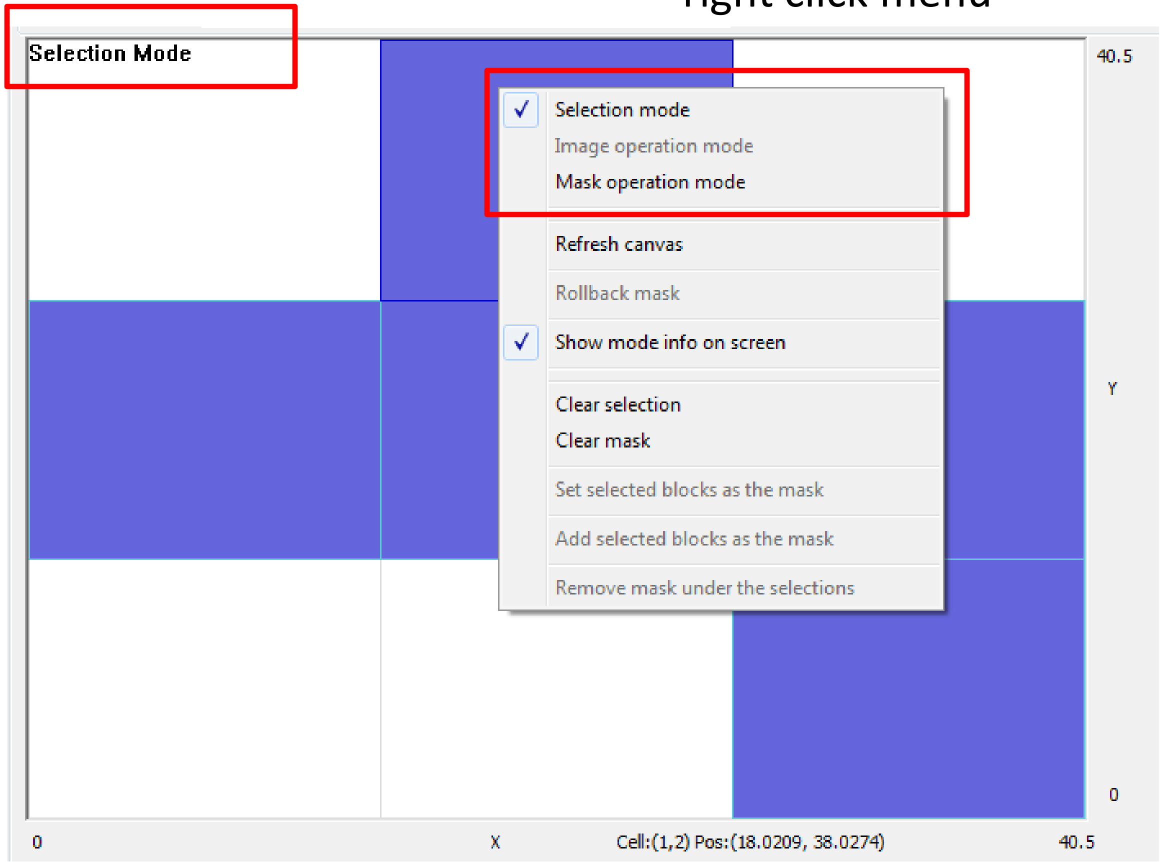
All the boxes in the mask pattern will use this material

Pattern Canvas

- there are 3 modes for this canvas
  - ❑ selection mode
  - ❑ image operation mode
  - ❑ mask operation mode

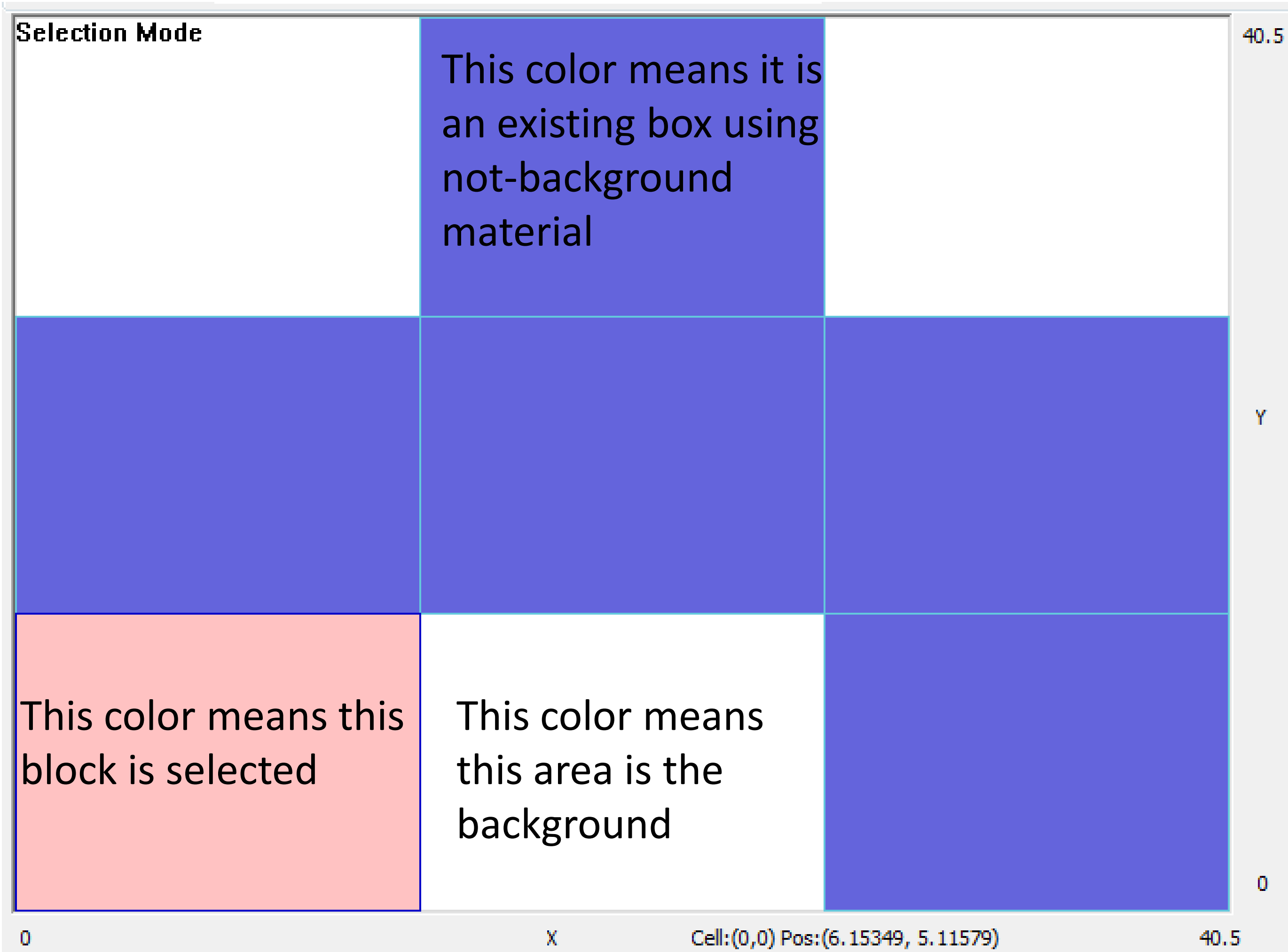
Switching modes by right click menu

Mode is shown here

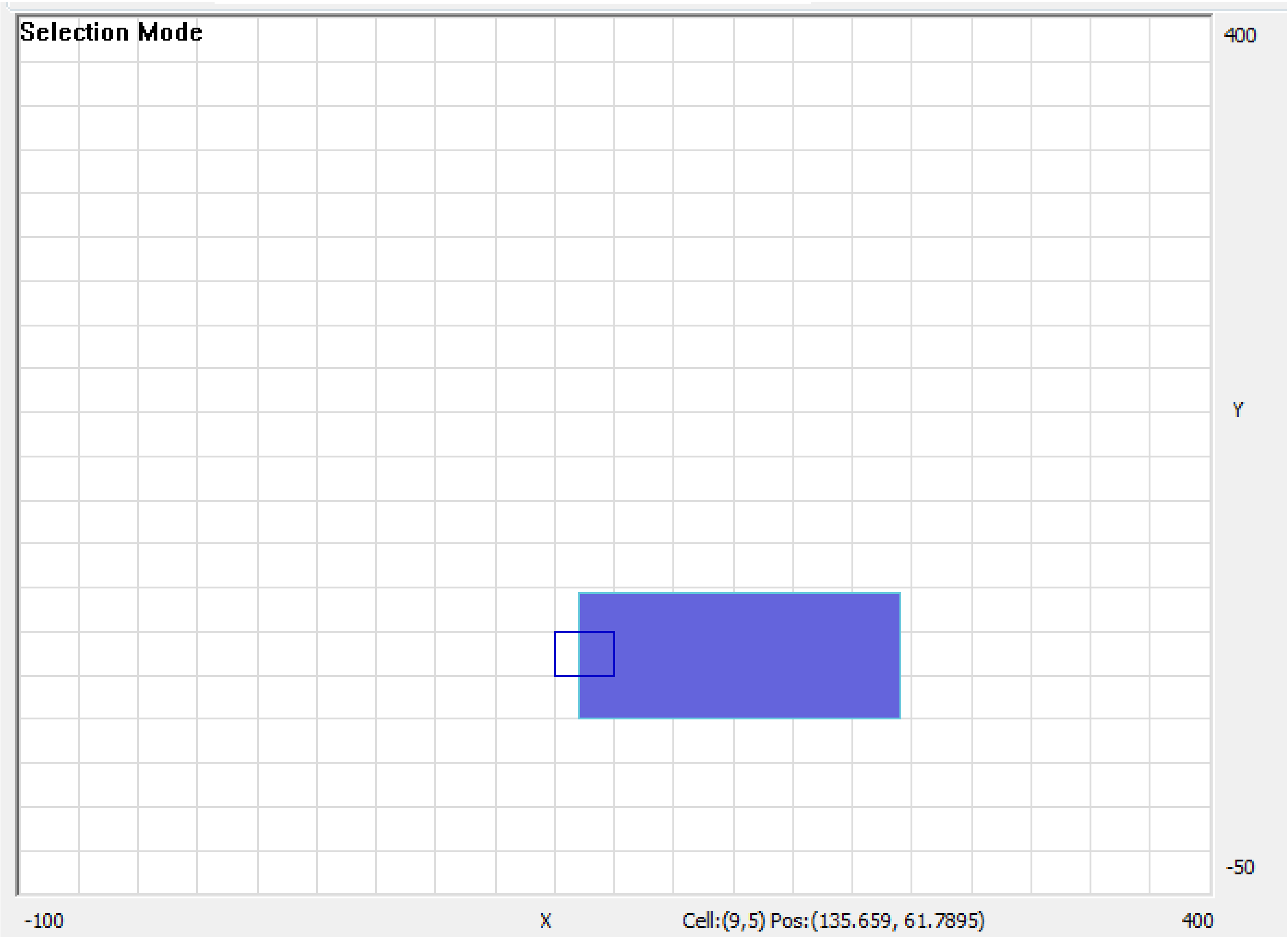


General information

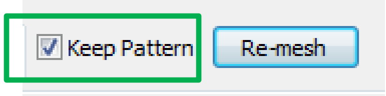
- the canvas is divided into block by the mesh defined on the top of the editor
- for each block:



Note: an existing box can be not exactly aligned to the mesh grid, as shown in the following figure

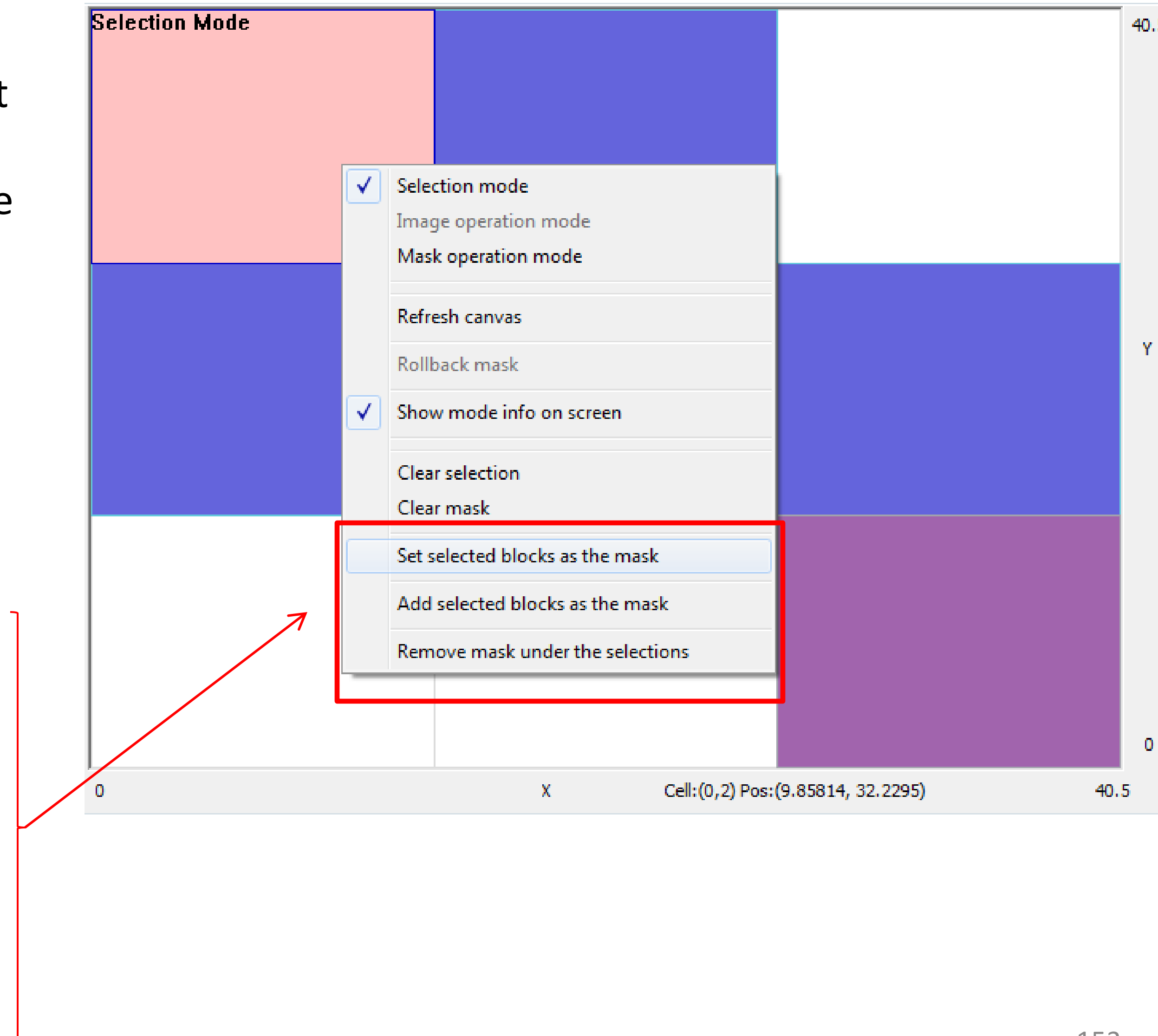


This is very common when the mesh is changed with the existing pattern kept as

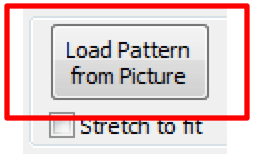


Pattern Canvas:: selection mode

- the bounding box a block under cursor will be shown
- left click mouse will select the block under cursor
  - additionally, with the "*Ctrl*" key is pressed, the block can be added/removed from existing selections
- with right click menu, the selected blocks can be
  - **set as the mask**, the old mask will be removed
  - **add the block to existing mask**
  - **remove them from mask**, it is equal to set these block as the background

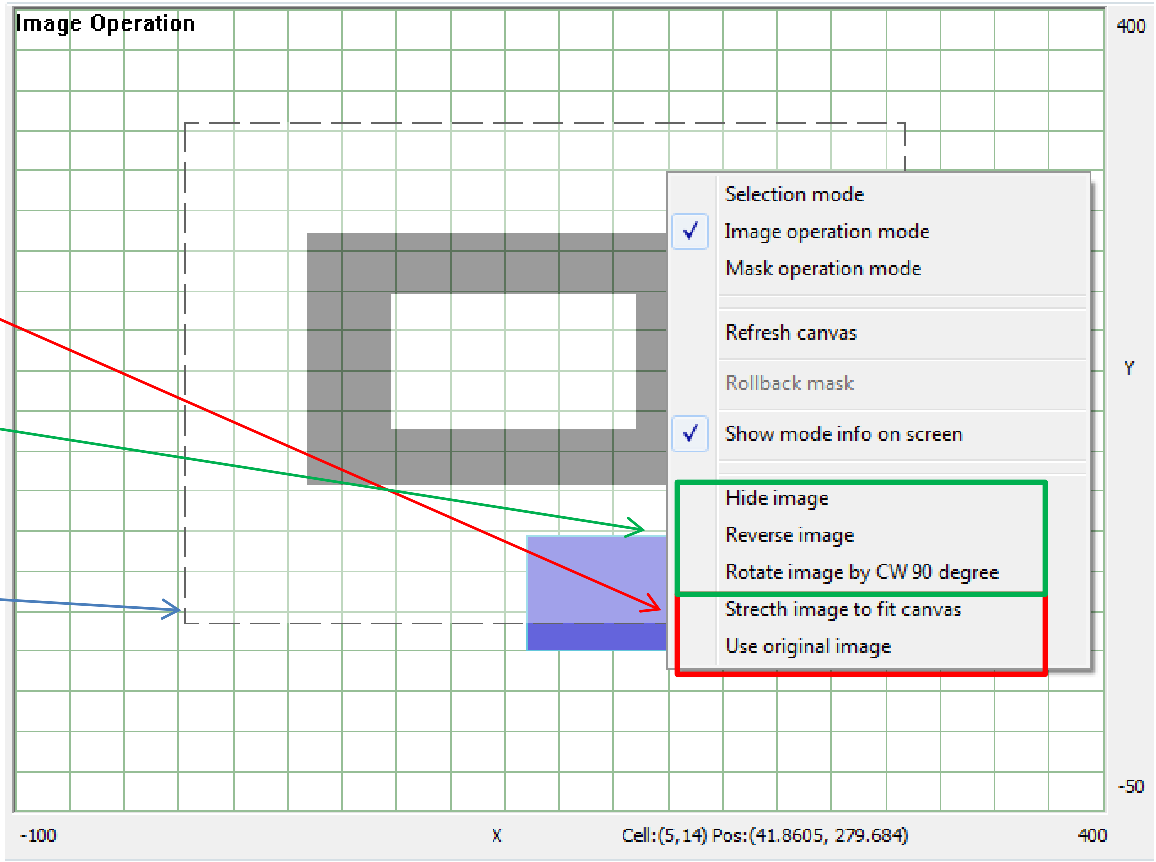


Pattern Canvas:: image operation mode

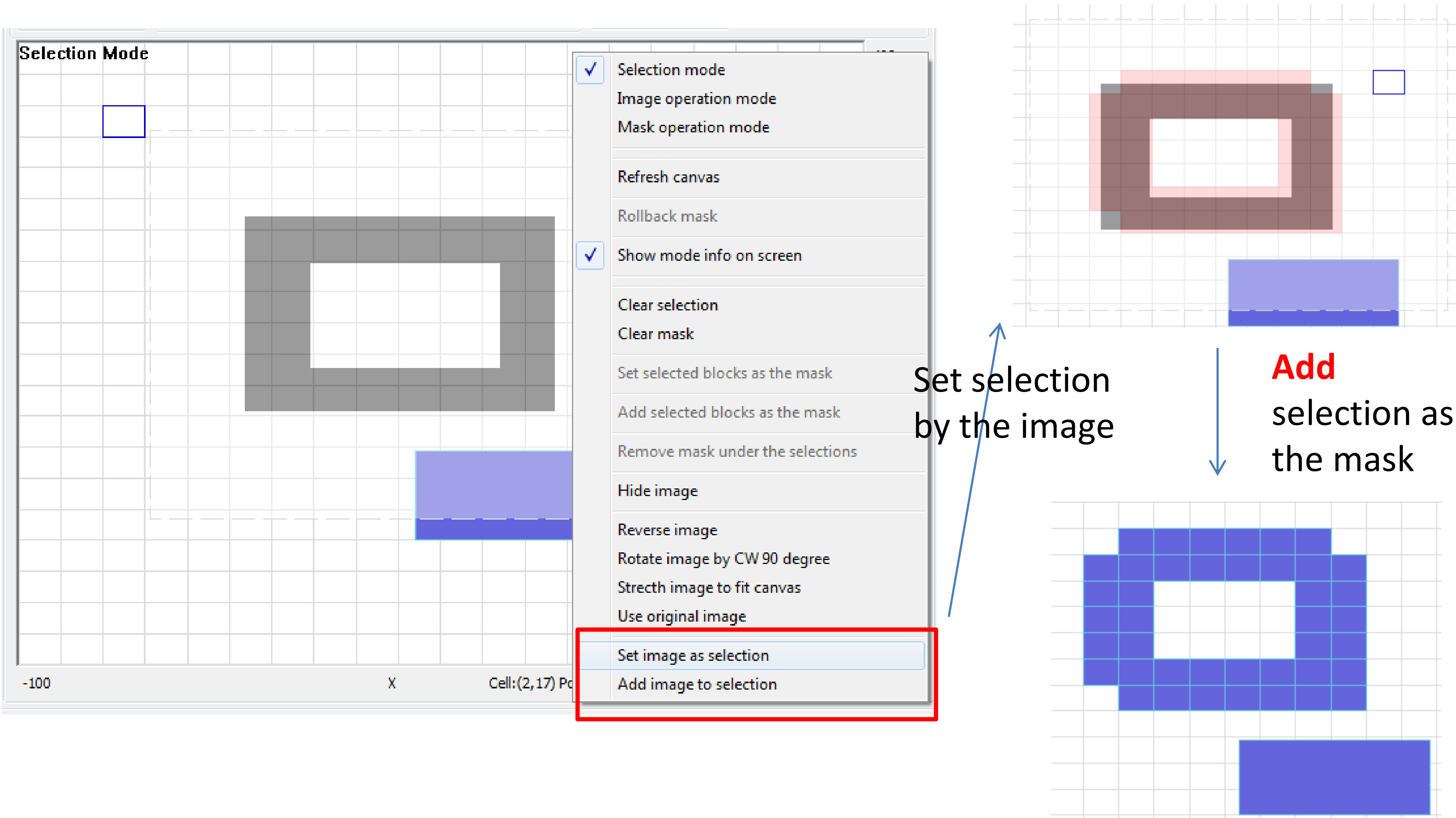


With this button, a image can be loaded in to the canvas in any mode

- the image will be converted to mono-color
- the image can be shrink to the original size, or extent to fit the size of canvas
- the image can be operated as
- user can drag the image to any position in the canvas



With an image is loaded, in the selection mode, user can define the selection area by the dark area of the image, then convert this selection to mask.

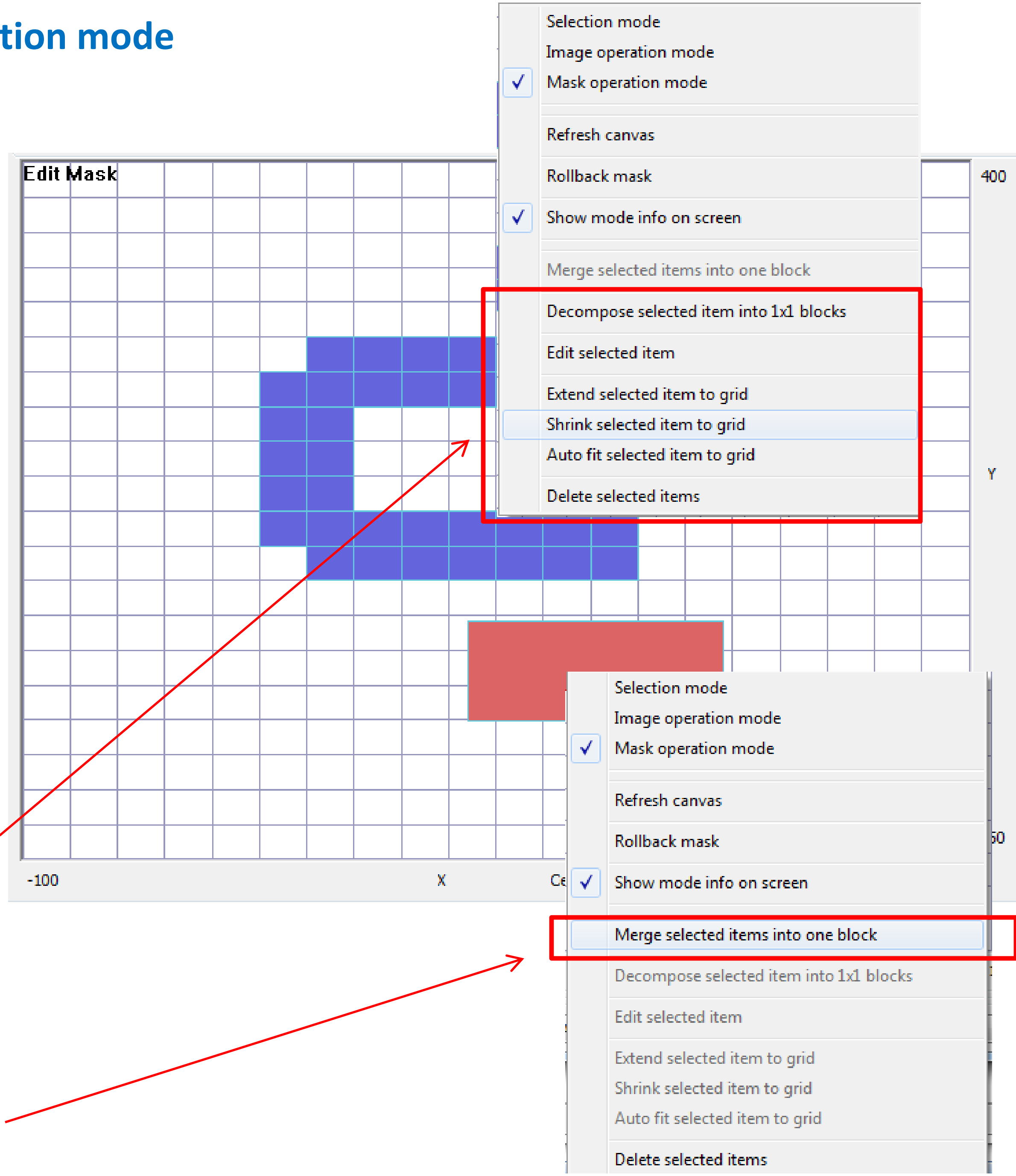


Pattern Canvas:: mask operation mode

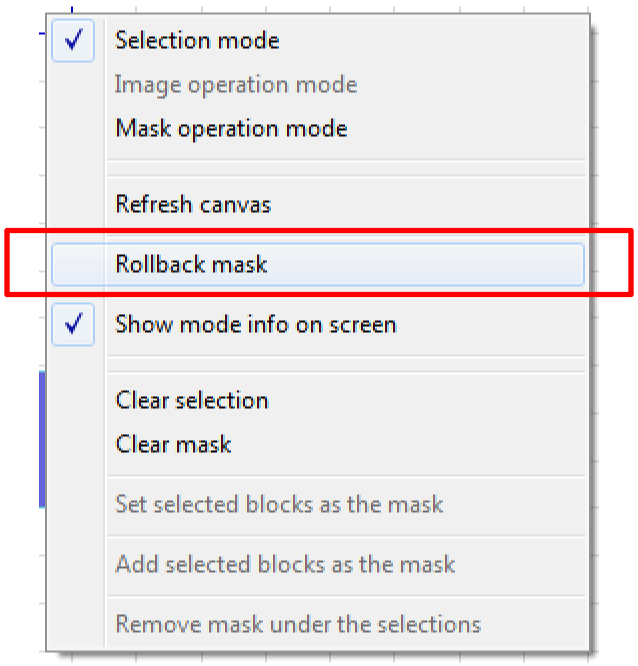
- the bounding box a box under cursor will be shown

- left click mouse will select the box under cursor
  - ❑ additionally, with the "***Ctrl***" key is pressed, the box can be added/removed from the existing selections

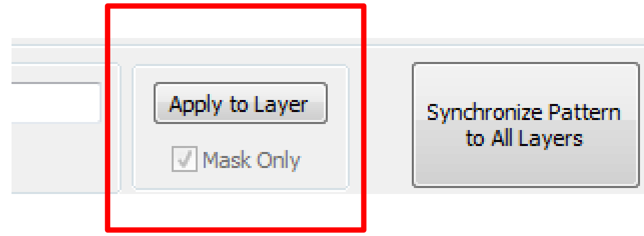
- with right click menu
  - for a single selected box
    - ❑ **shrink**, **extend**, **auto align** to grid
    - ❑ **edit** it's corners by user input
    - ❑ **decompose** a big box into multiple 1x1 blocks
    - ❑ **delete** the box
  - for multiple selections
    - **merge** them into a big box



If the mask in the canvas is changed, user can go back to the previous pattern by the menu item “**Rollback mask**”

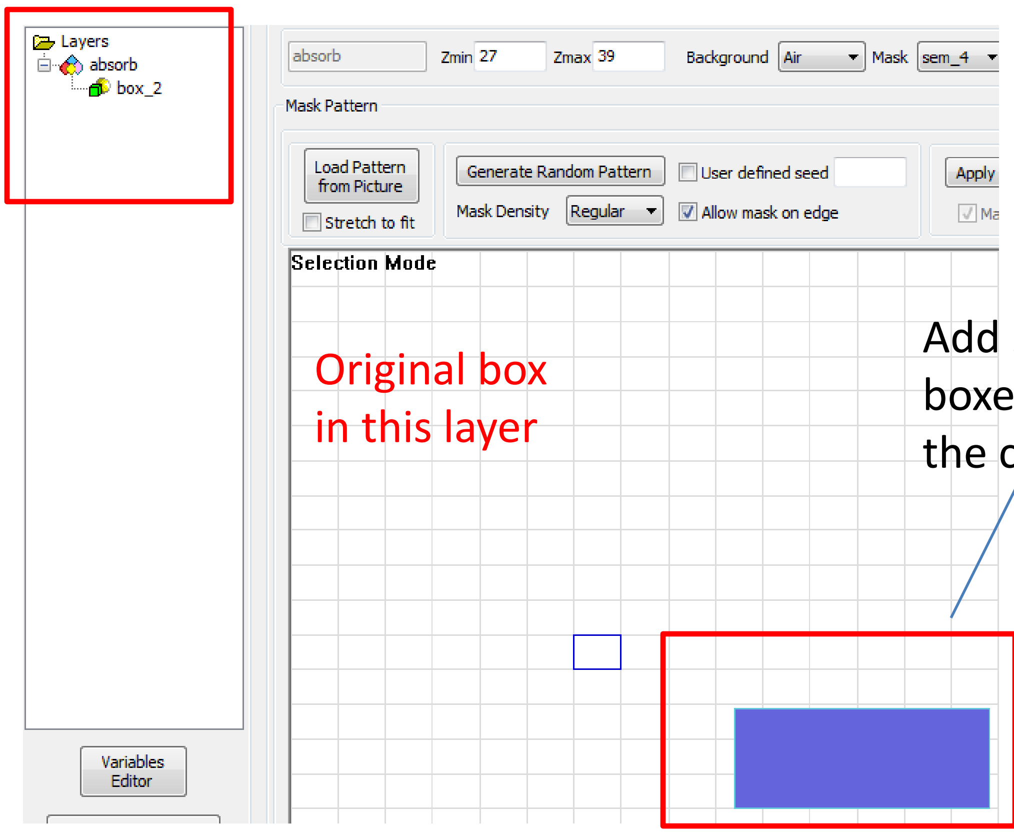


Apply the editing mask in the canvas to the layer



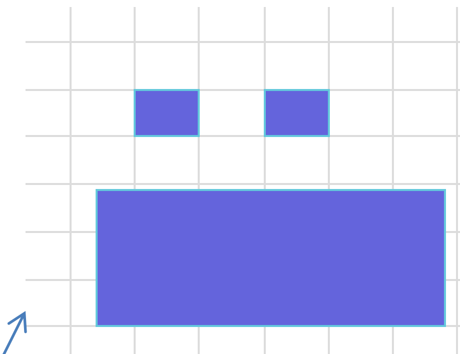
- ➢ all blue color boxes shown in the canvas will be converted to 3D boxes in the layer. These boxes use the mask material of this layer.

- ➢ If a box is not assigned a name in canvas, the new box will be automatic assigned a name by GUI

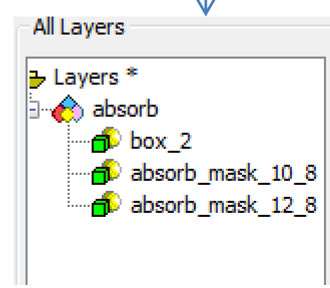


Original box in this layer

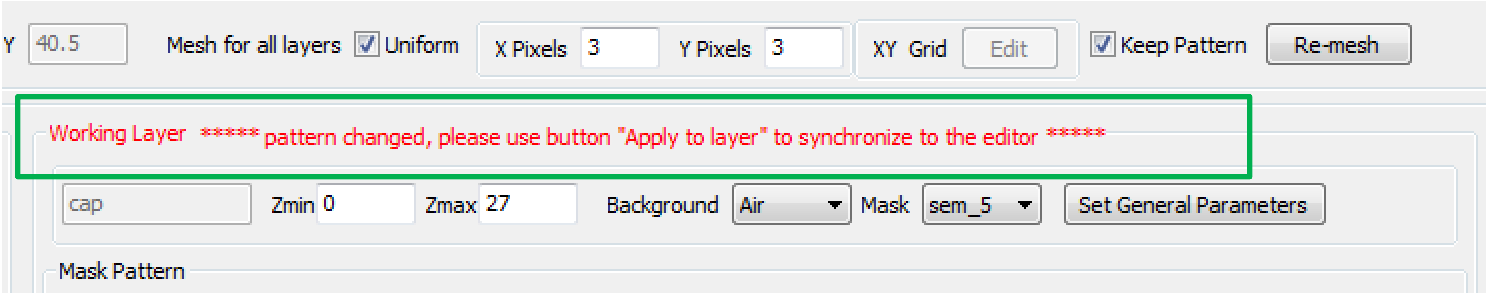
Add 2 boxes in the canvas



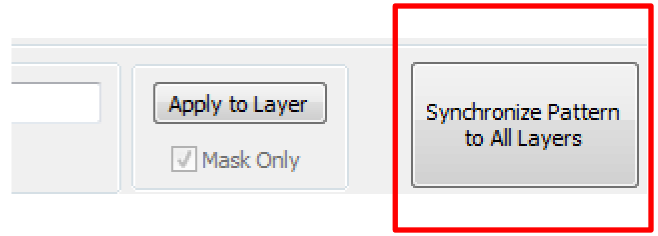
After “Apply to Layer”



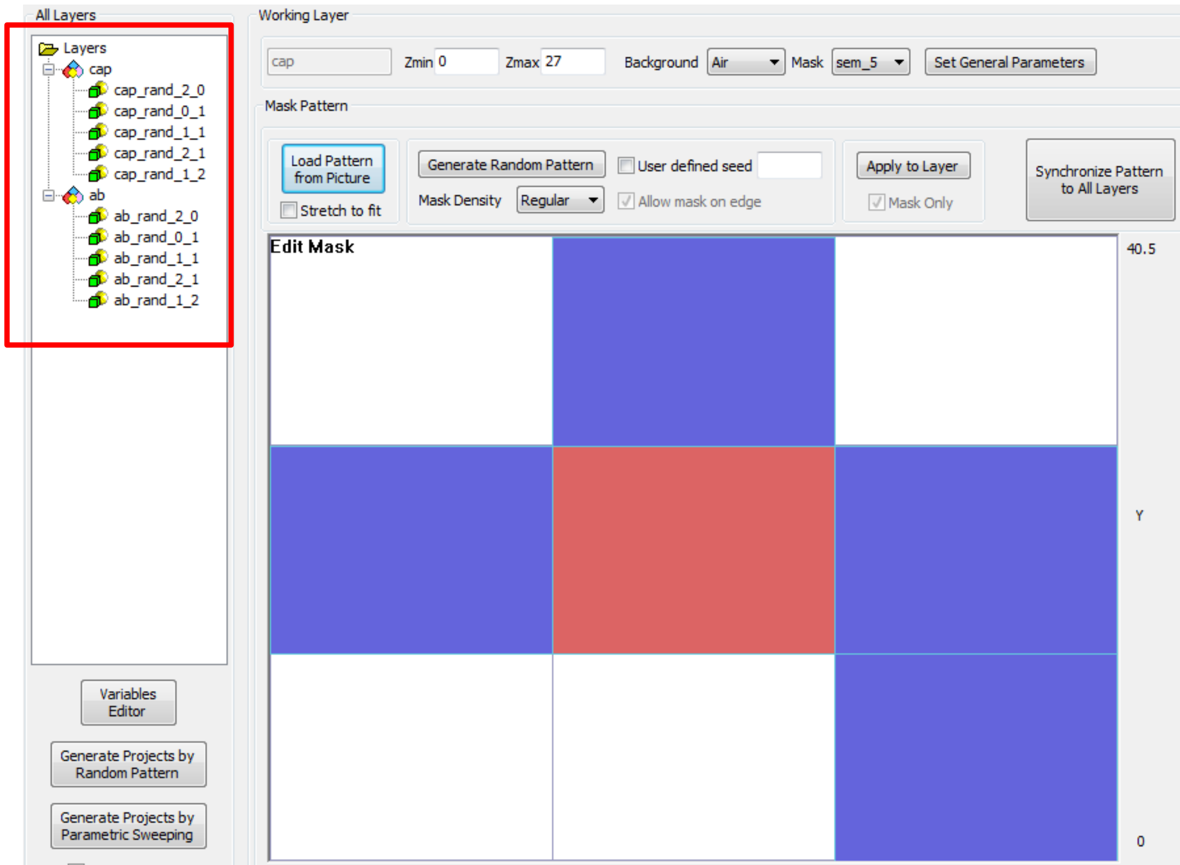
Note: if the mask in the canvas has been changed, there will be a warning message shown in the editor.



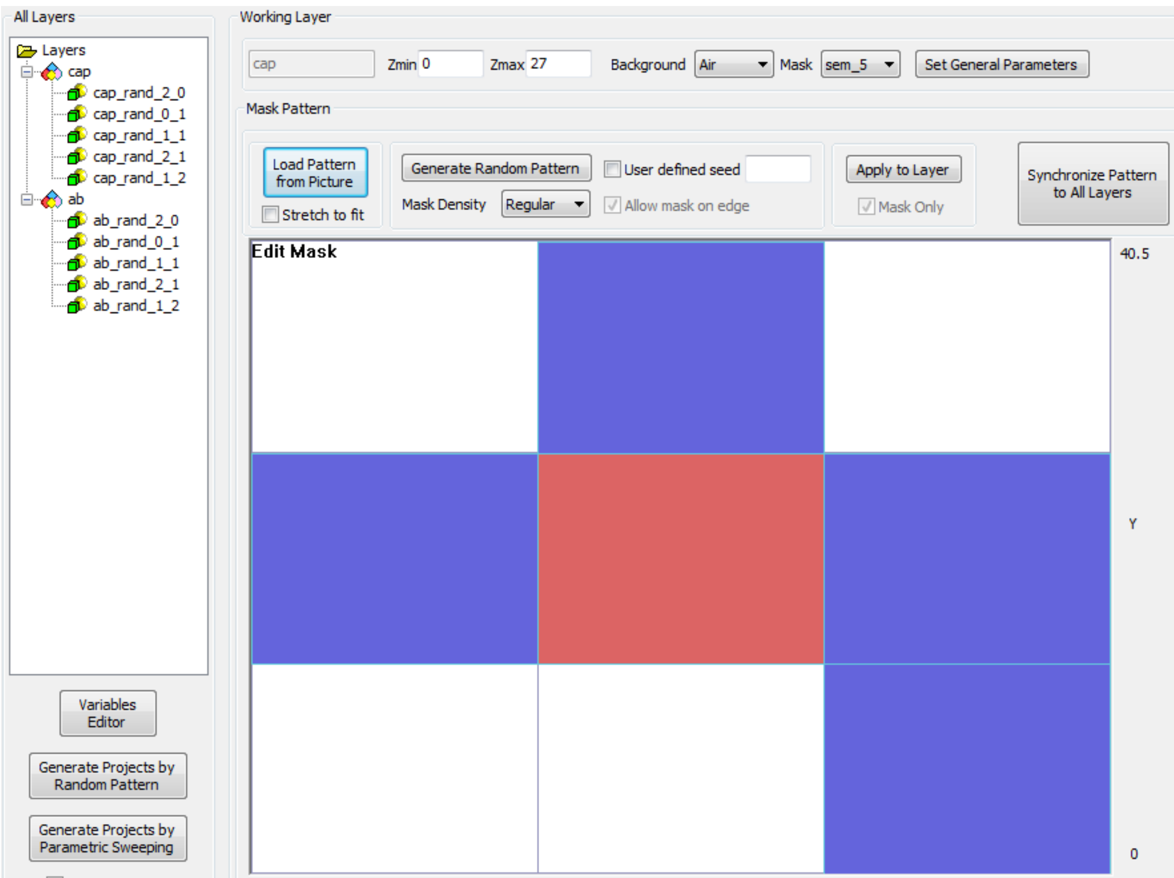
Set the pattern of all listed layers as the same as the working layer

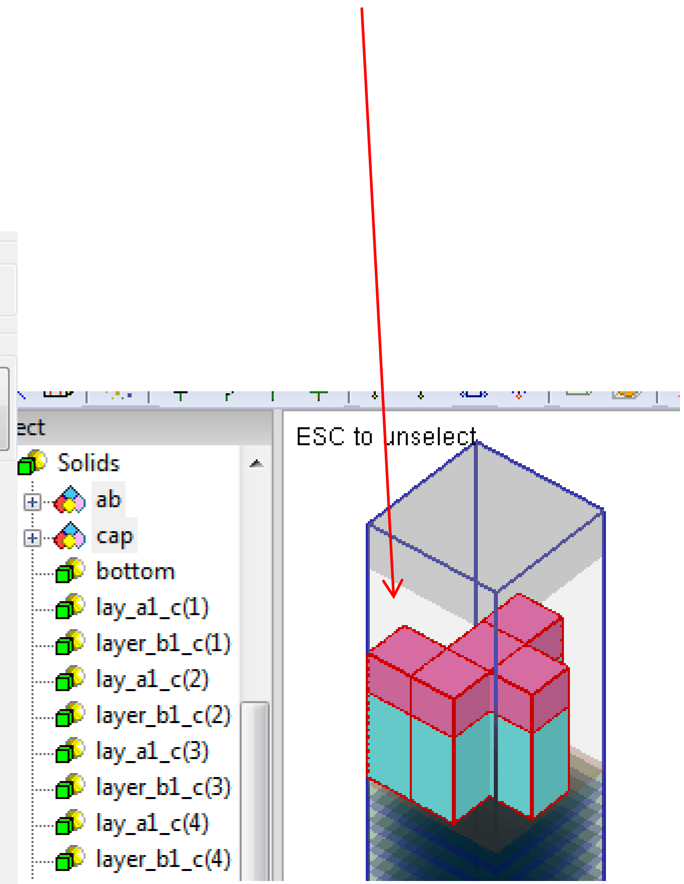


As shown in the following figure, both 2 layers will have the same mask pattern.
But in each layer, the box of mask will use the mask material of this layer, and also use the Z range of this layer only.

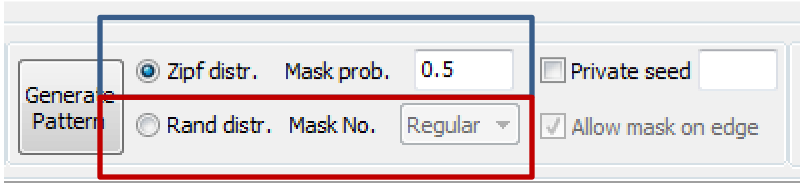


After the mask for all layers are finished, press “**Apply**” or “**OK**” button to implement these mask patterns in the project. The boxes will be shown as





Note: the random mask pattern generating



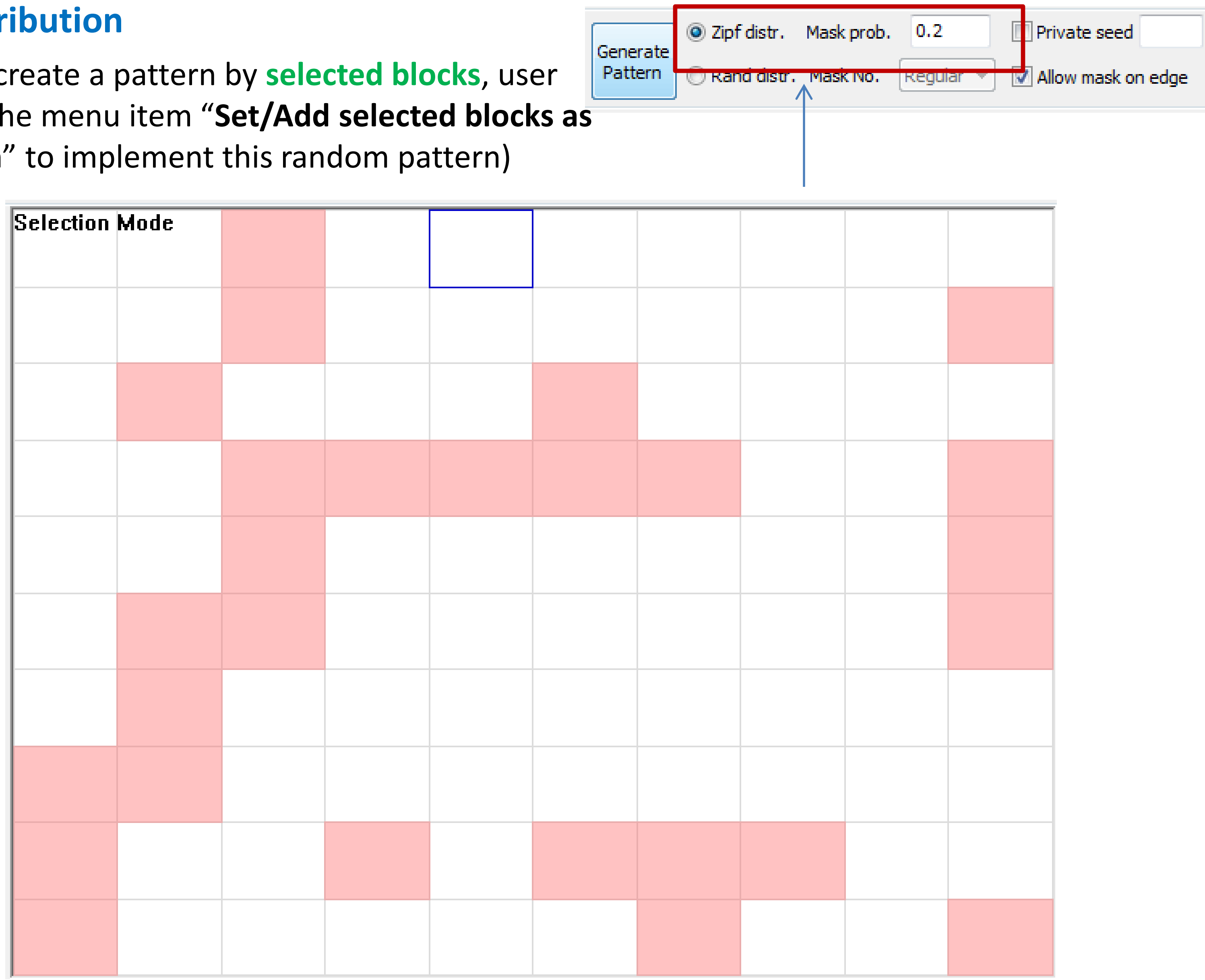
There are 2 random methods

1) Zipf distribution - user need to define the probability of mask cells appear in the pattern. For example, for a pattern with 100 cells, if user define the probability as 0.2, the number of mask cells appears in the pattern will be around 20.

2) Normal random distribution – the GUI will generate random number for each cell, if the number is higher than a threshold, the cell will be marked as mask cell.

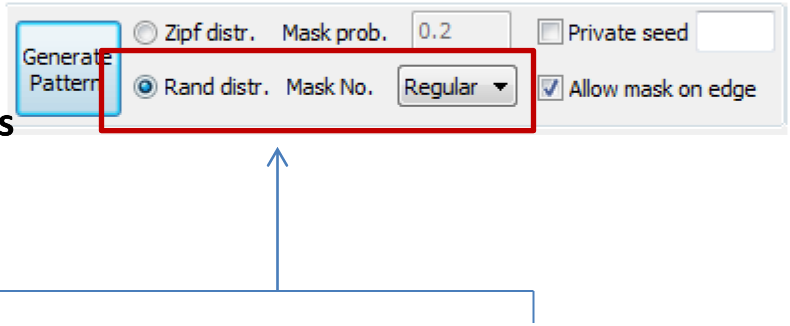
Generating a random mask pattern by Zipf distribution

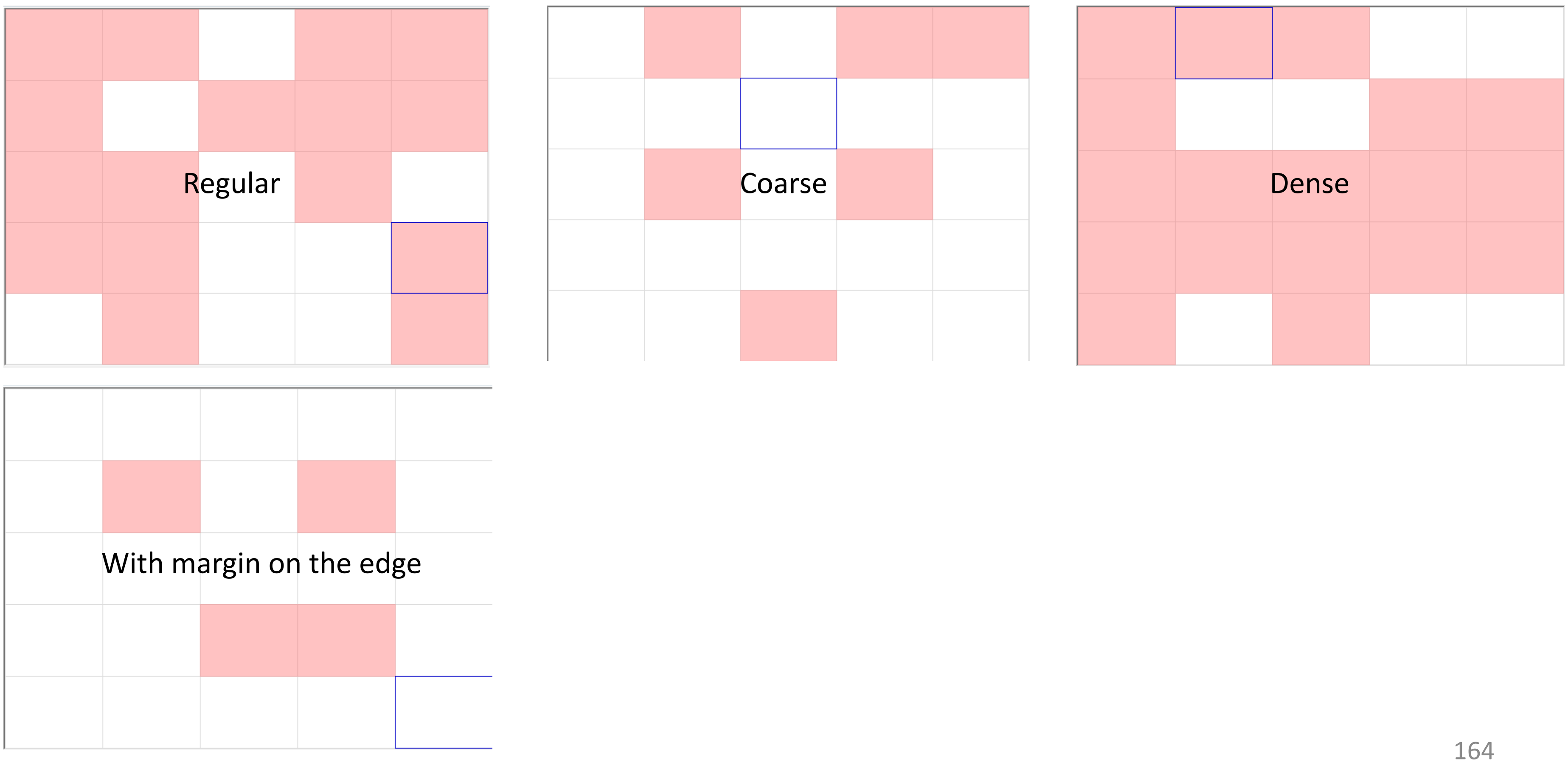
(Note: it will create a pattern by **selected blocks**, user need to use the menu item “**Set/Add selected blocks as mask pattern**” to implement this random pattern)



Generating a random mask pattern by normal random distribution

(Note: it will create a pattern by **selected blocks**, user need to use the menu item "**Set/Add selected blocks as mask pattern**" to implement this random pattern)

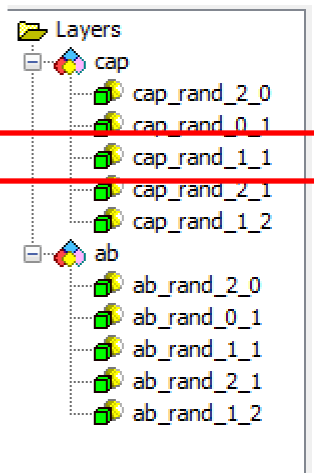


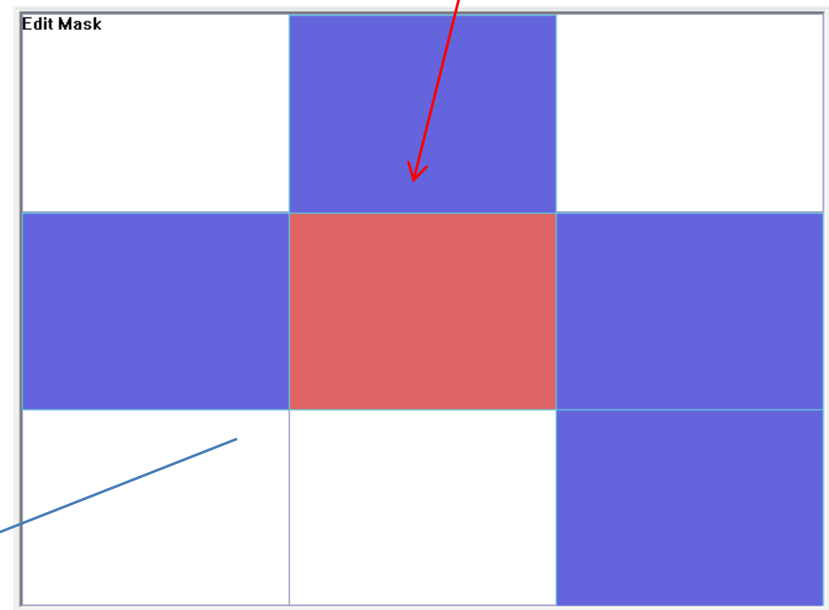


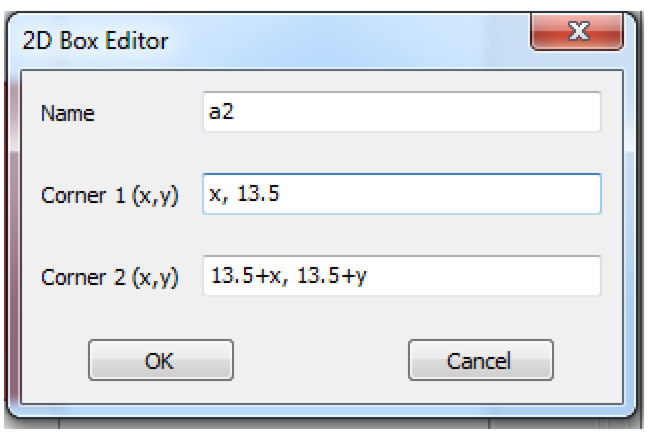
Manually editing a box, including the variable usage

Or, in the "**Edit Mask**" mode, double click the selected item.

Double click any box in the tree







User can modify

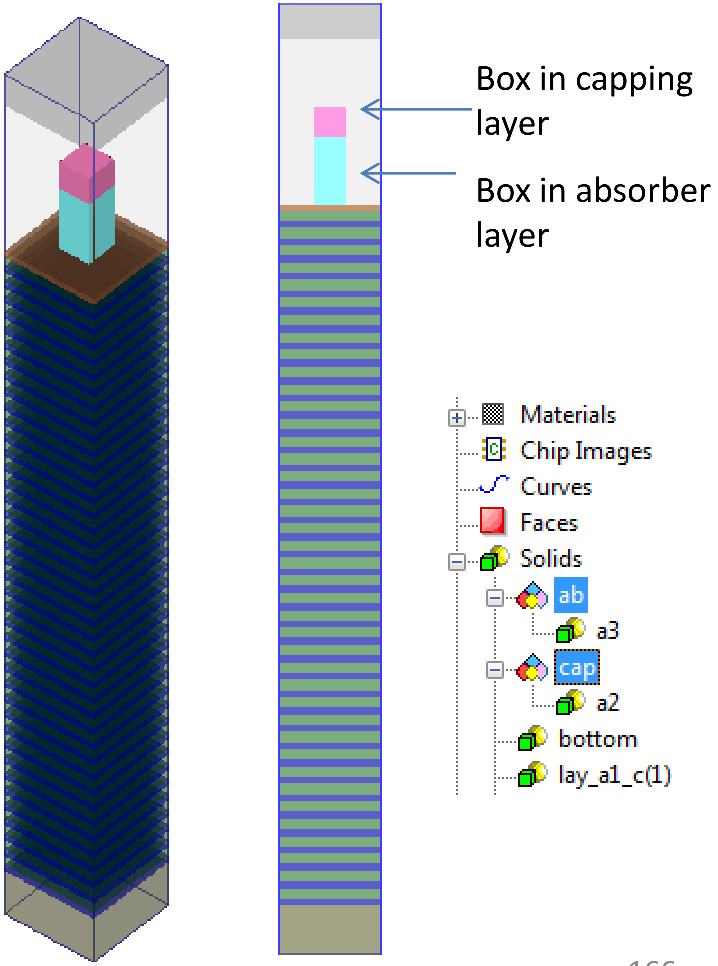
- Name: if the name part is empty, means that it will use the name assigned by GUI
- Corners: the coordinates can use variable

  Please check here to show variables in GUI

Demo I

Automatic batch simulation for multiple Lithographic projects with random mask patterns

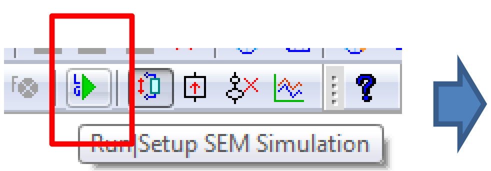
- We have an existing 40.5x40.5 nm^2 EUV case shown as the figure
- **All layers and SEM solver must be set up correctly before we do this batch job**
- For the capping layer and the absorber layer, there is only one box in these two layers (or there can be empty layer also)
- We want to simulate multiple projects with random mask patterns

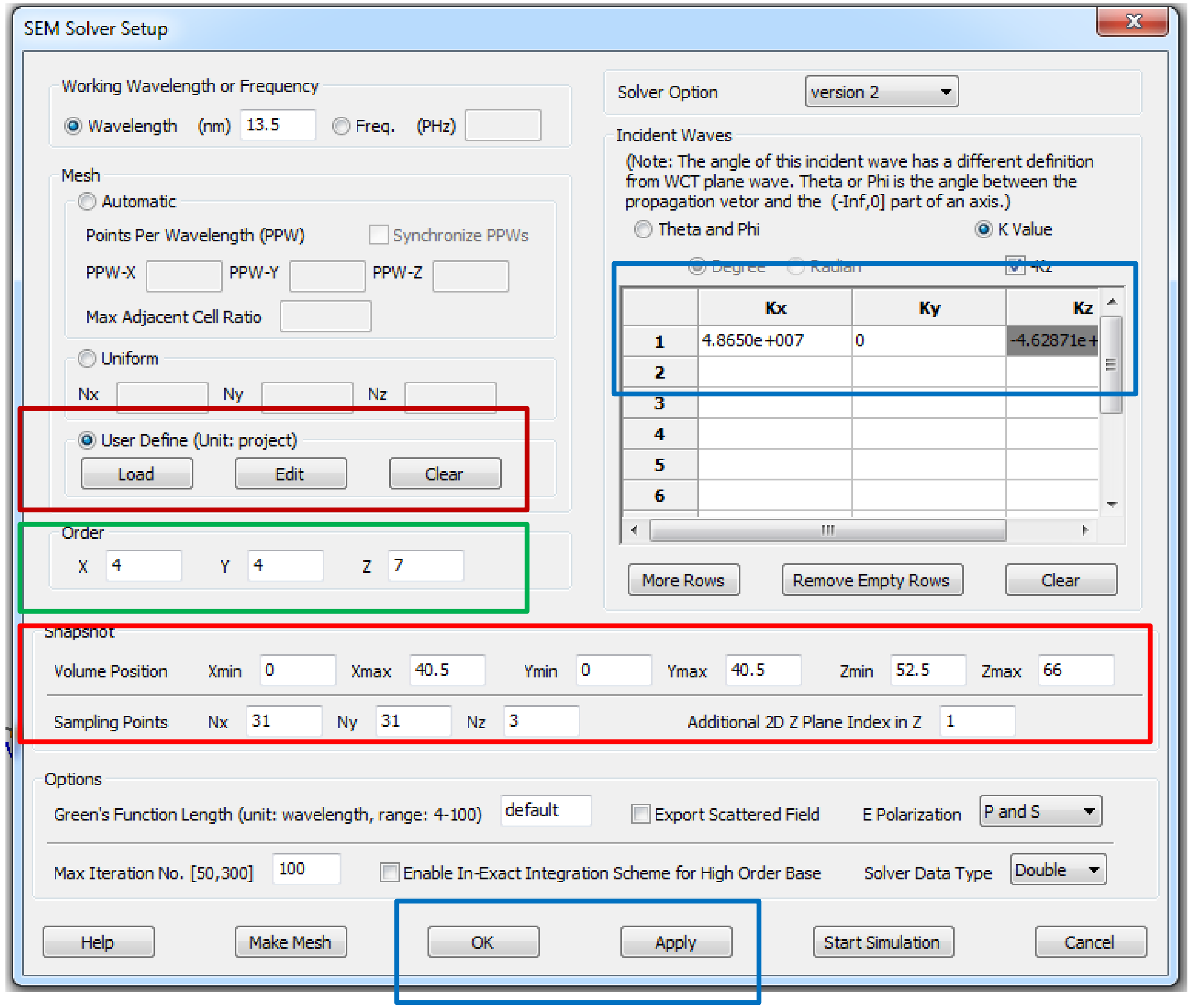


Assuming the existing project is the “**case_3_eng2_rand.wnt**” in the folder “**D:\sim_case\sem\cases_for_v2_engine\3wavelength_with_hole**”

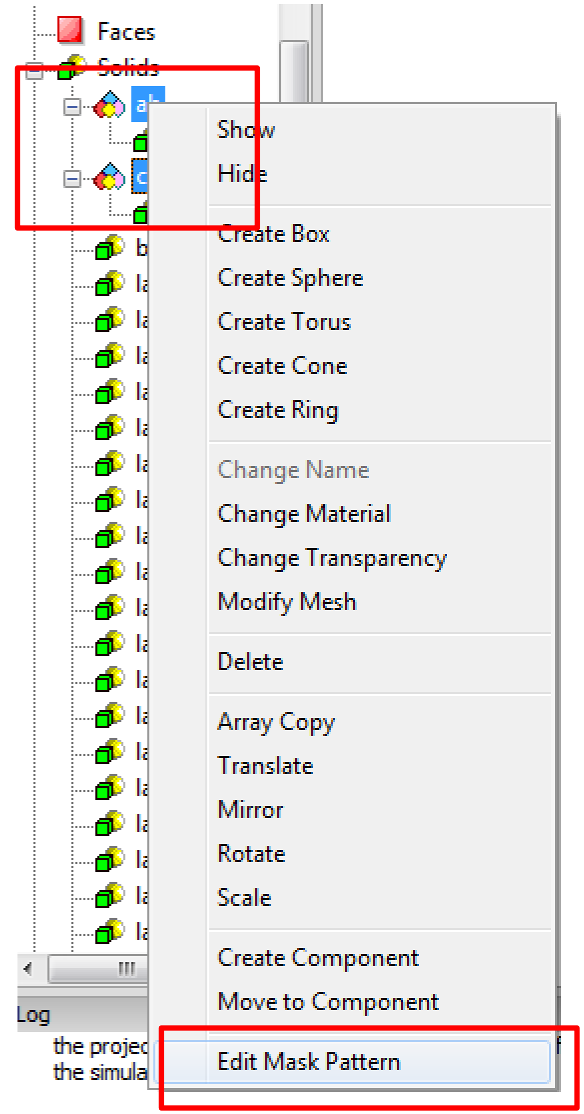
- Load Project into GUI

- Make sure the SEM solver setup and snapshot definition are correct. Because all projects created for auto simulation will use these setup





➢ Select layers “ab” & “cap”, enter the Mask Editor by popup menu item “**Edit Mask Pattern**”

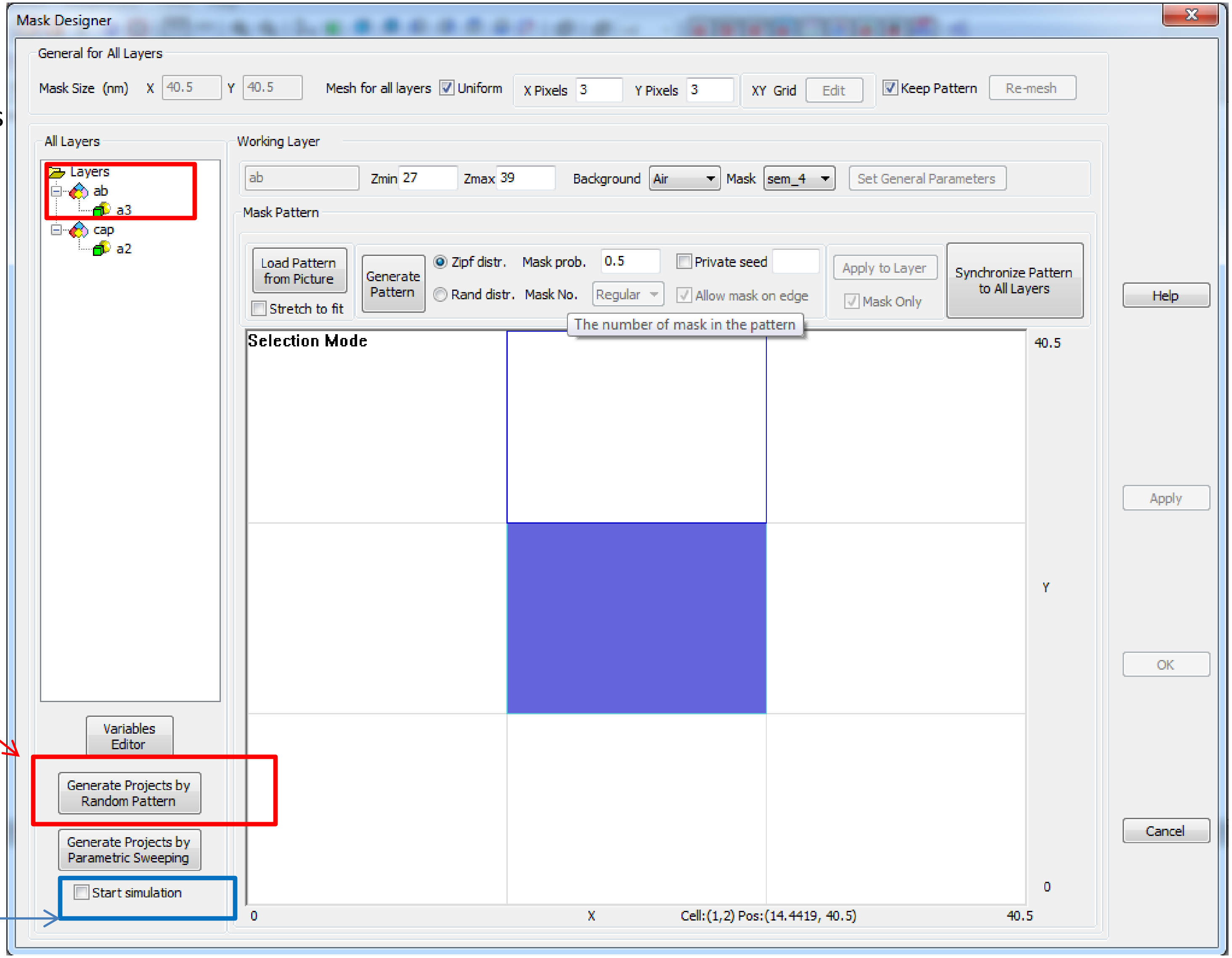


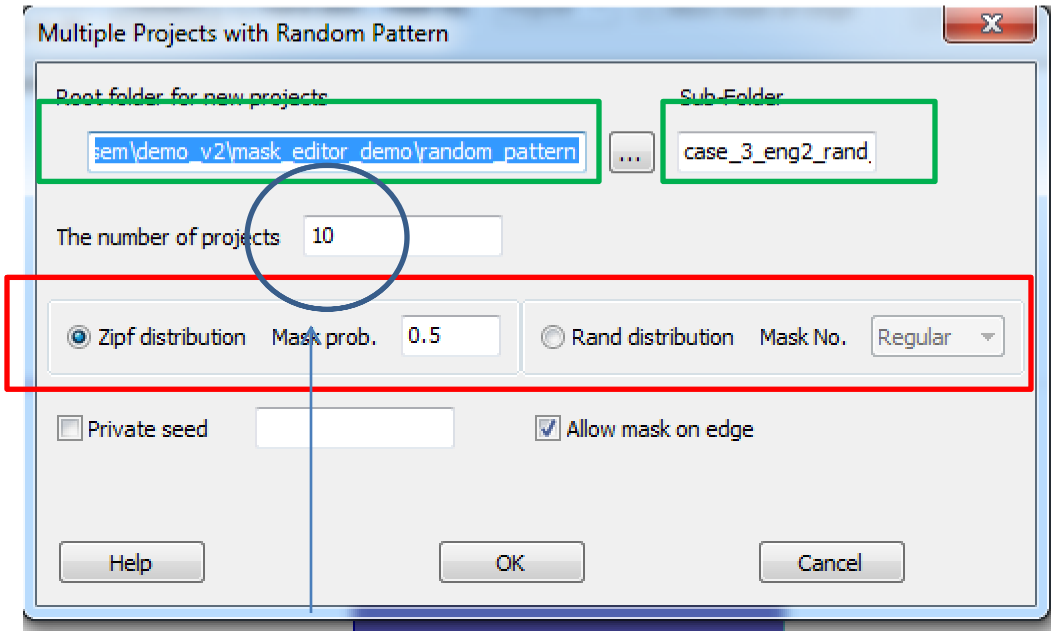
In the Mask Editor, **double click** each **layer-node** to check whether those items are correct or not.

- Z range of the layer
- the material for the mask

If all setting are correct, press this button to set up the batch control.

If user want to start simulation automatically after multiple project are generated, please check this option



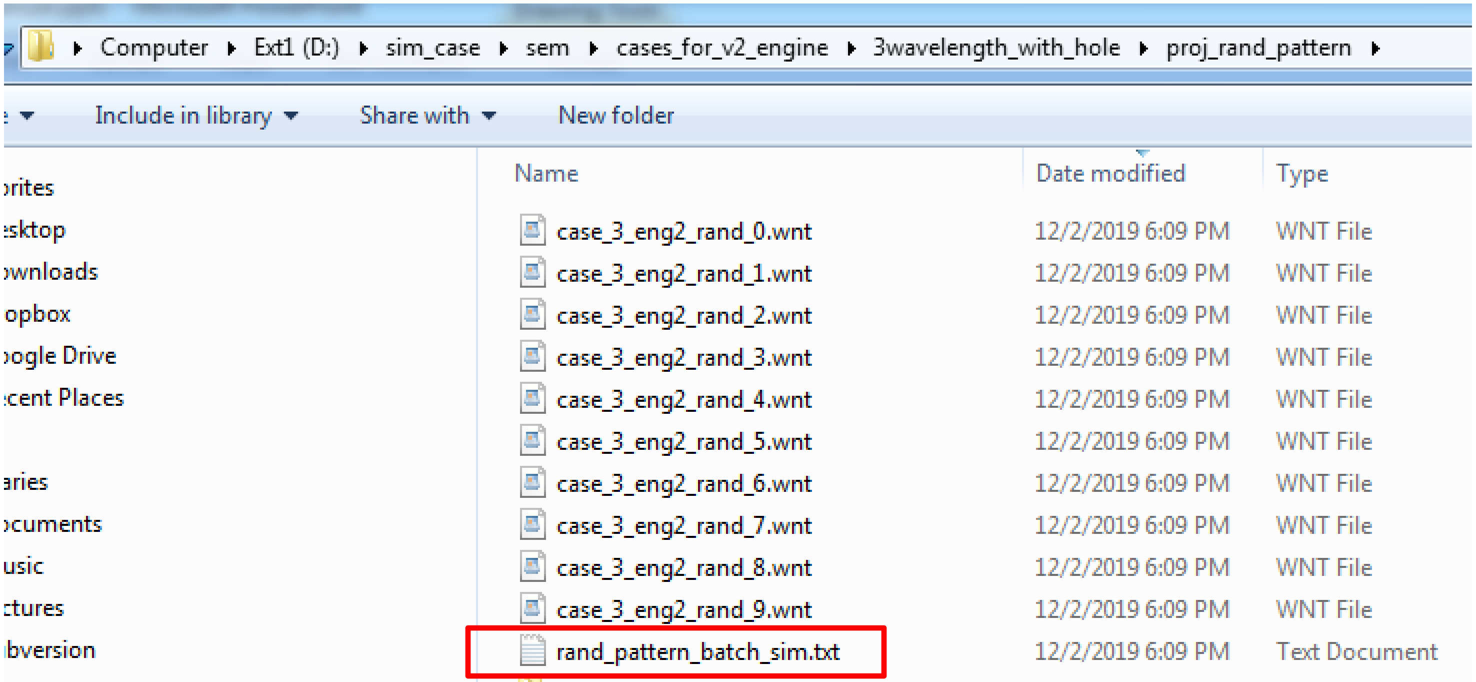


The target projects will be stored in this folder

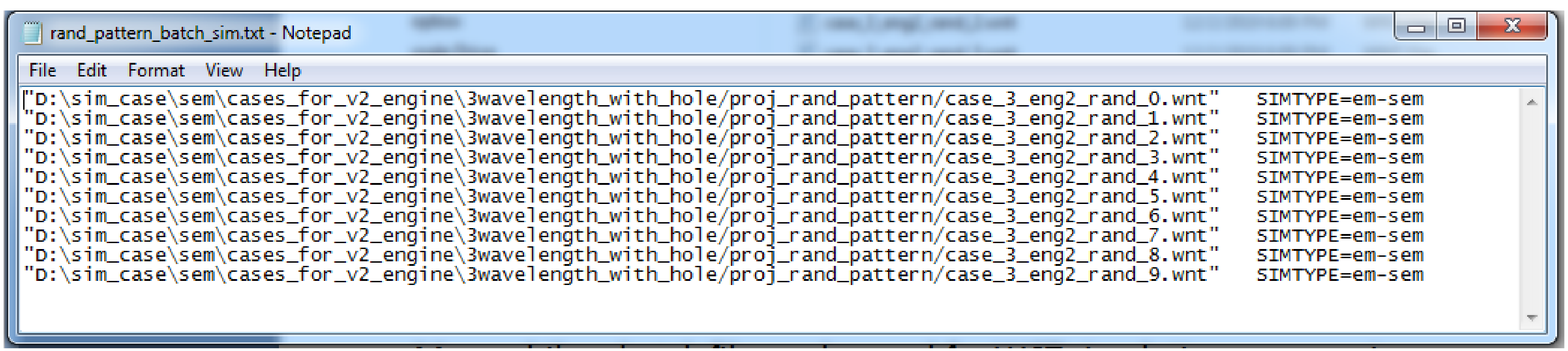
The meaning of these parts are the same as the definition in here.

How many projects we will generate. Each project has a mask pattern generated by random number.

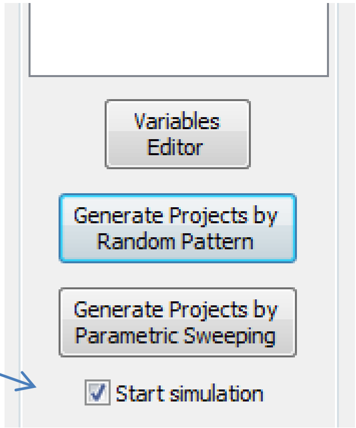
After “OK”, we can see 10 projects are created in the target folder.



Meanwhile, a batch file can be used for WCT simulation manager is created as

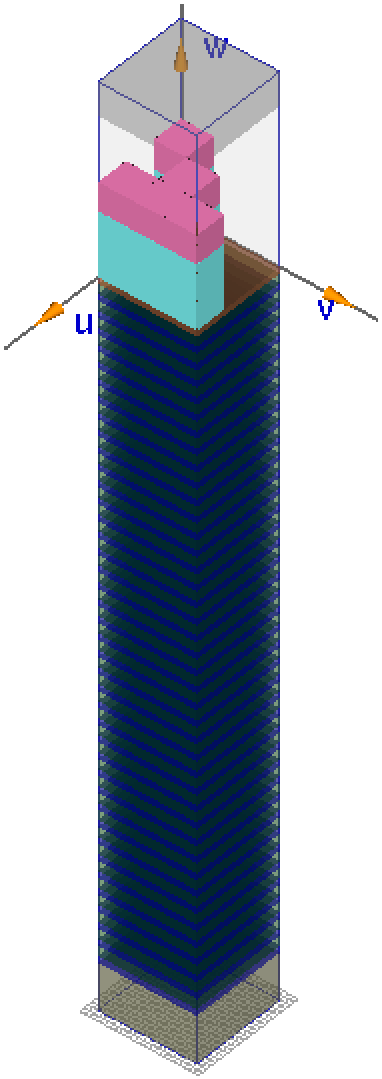


If the “**Start Simulation**” option is checked in generating these projects, the WCT simulation manager will be open to load that batch file and start simulation on these projects automatically.

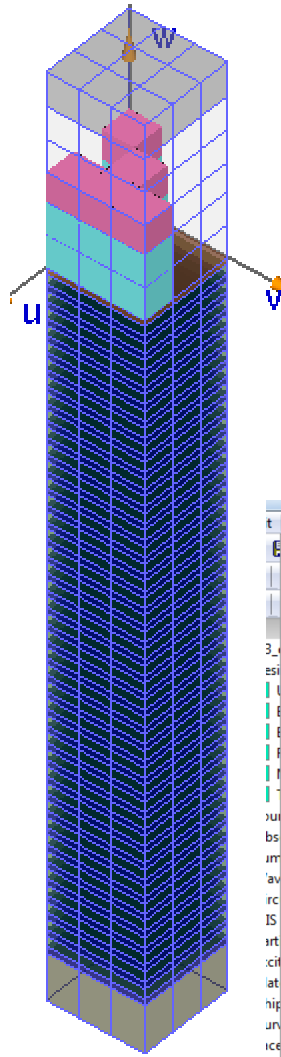


If user don’t want to simulate these case immediately, he still can use the WCT simulation manager to simulate these projects later.

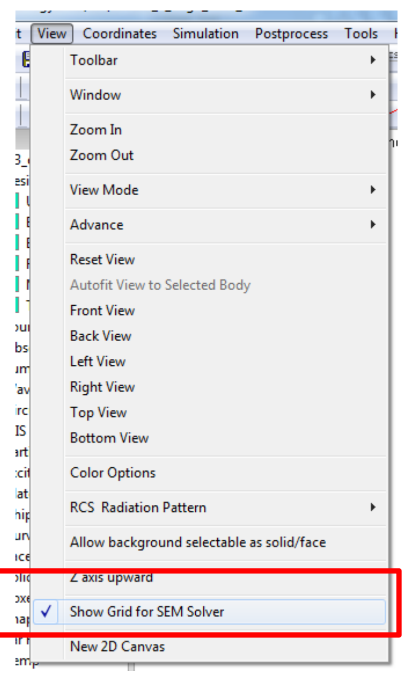
Here, we show the "case_3_eng2_rand_9.wnt" create from previous steps.



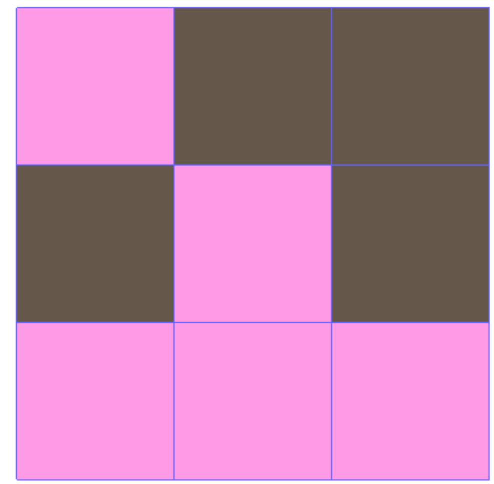
Angle view of project



Angle view of project with the SEM grid



X-Y view

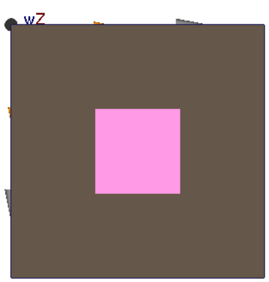


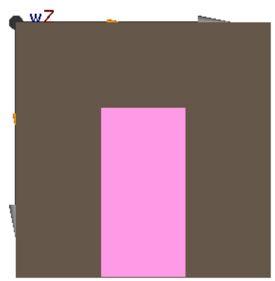
Demo II

Automatic parametric sweeping for Lithographic project

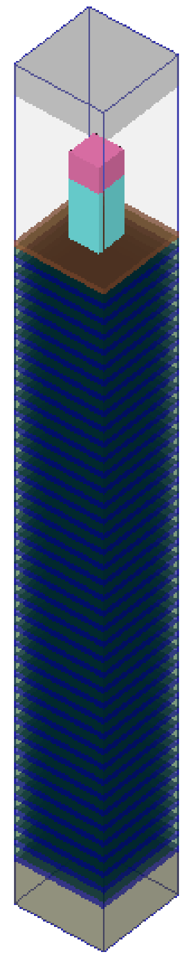
- We have an existing 40.5x40.5 nm^2 EUV case shown as the figure
- **All layers and SEM solver must be set up correctly before we do this batch job**
- For the capping layer and the absorber layer, there is only one box in these two layers (or there can be empty layer also)
- We want to simulate multiple projects by sweeping the mask from x=13.5 to 27 by a step of 13.5.

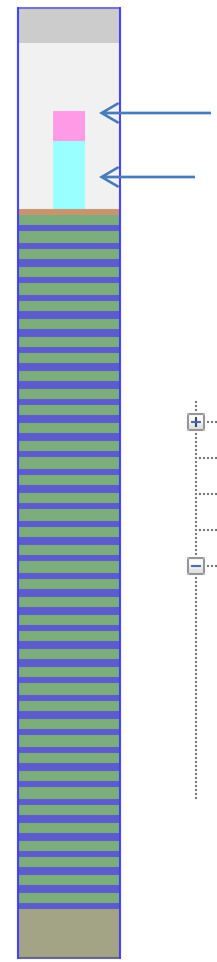
X=13.5

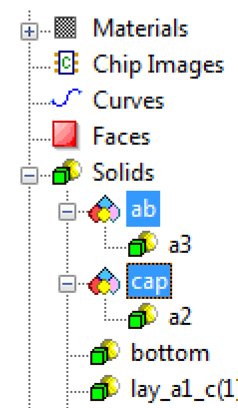




X=27



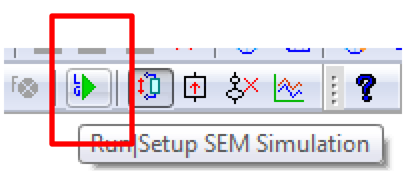


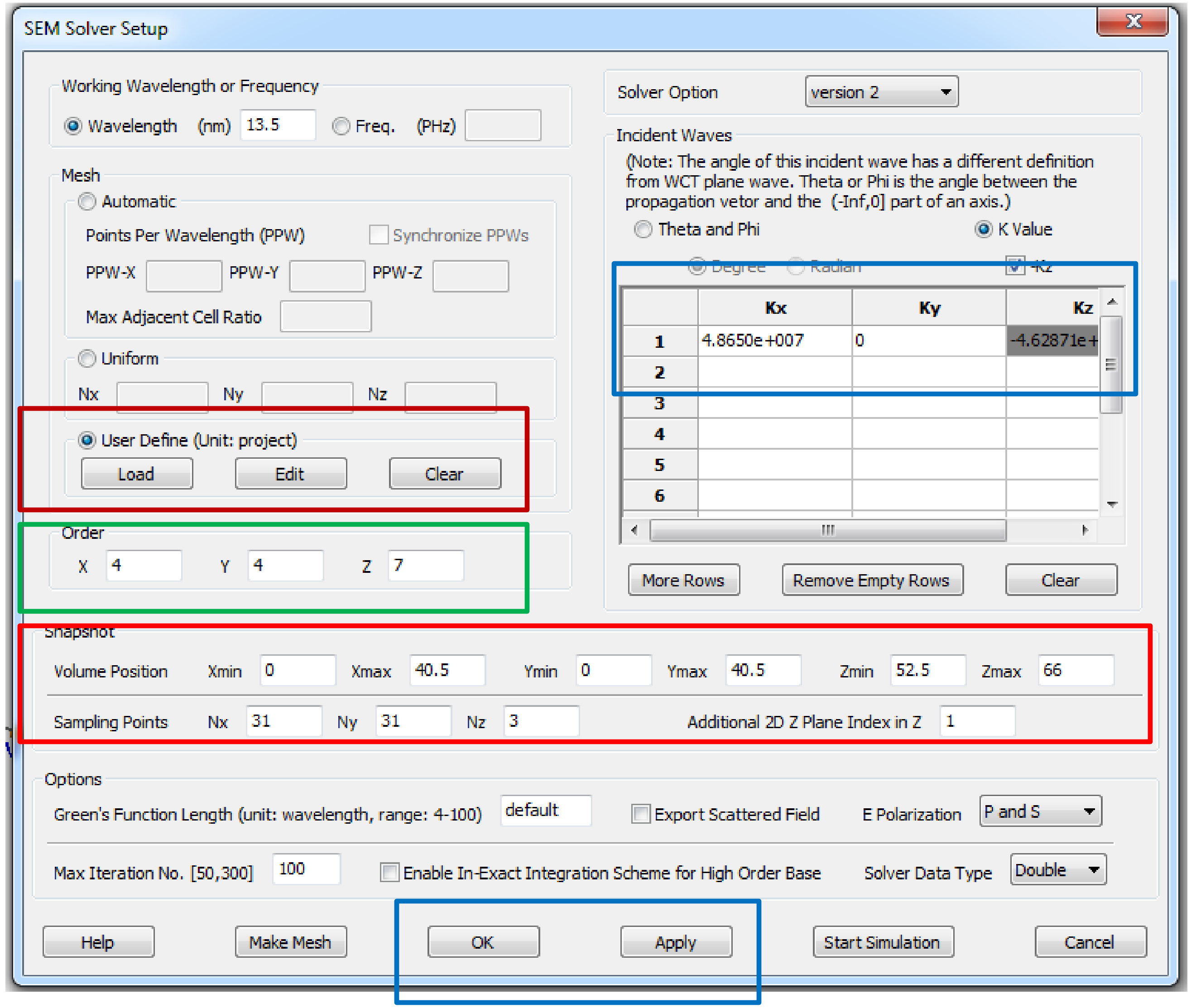


Assuming the existing project is the “**case_3_eng2_para.wnt**” in the folder “**D:\sim_case\sem\cases_for_v2_engine\3wavelength_with_hole**”

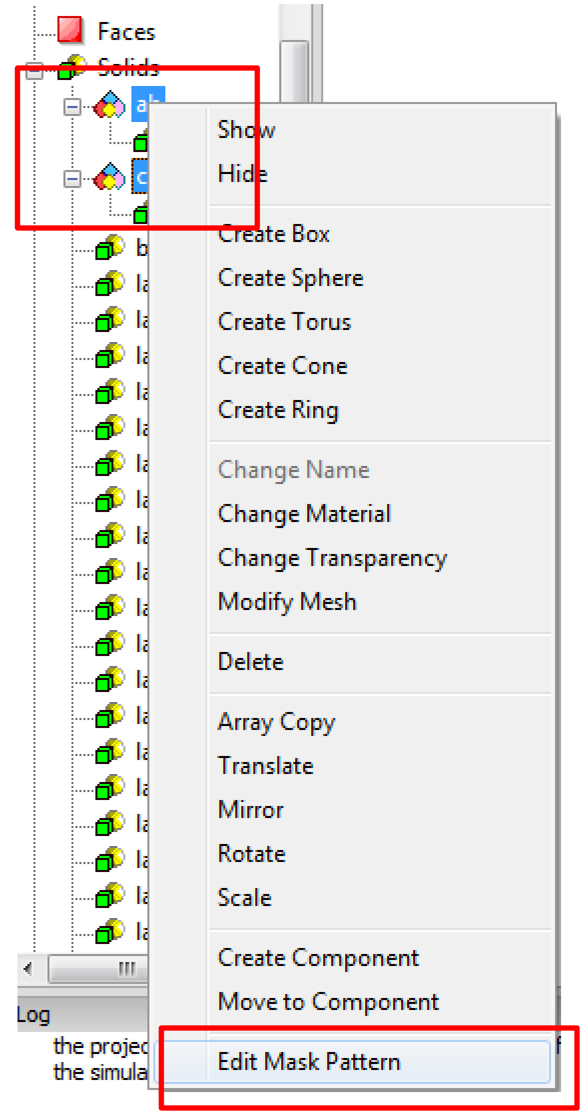
- Load Project into GUI

- Make sure the SEM solver setup and snapshot definition are correct. Because all projects created for auto simulation will use these setup



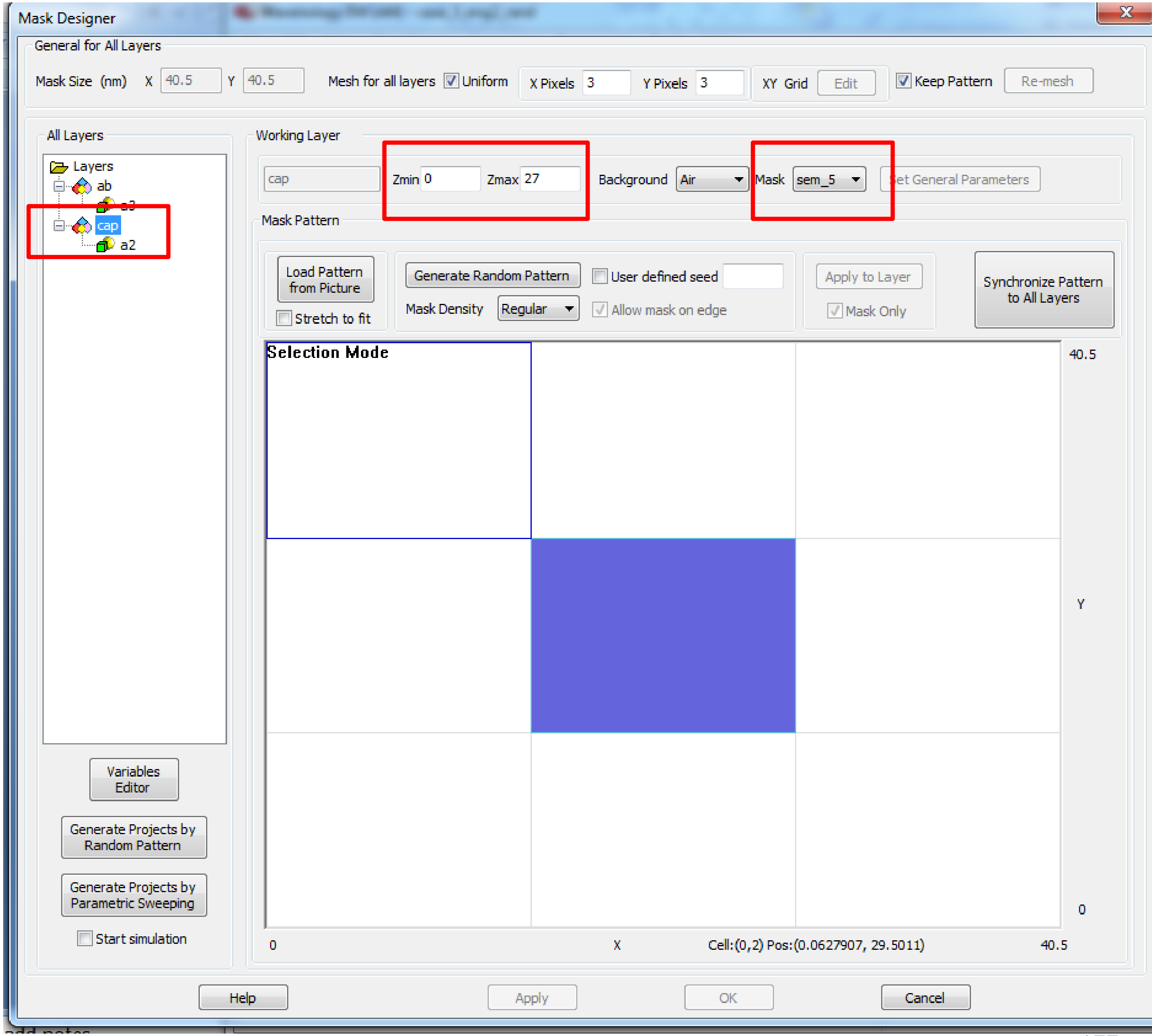


➢ Select layers “ab” & “cap”, enter the Mask Editor by popup menu item “**Edit Mask Pattern**”



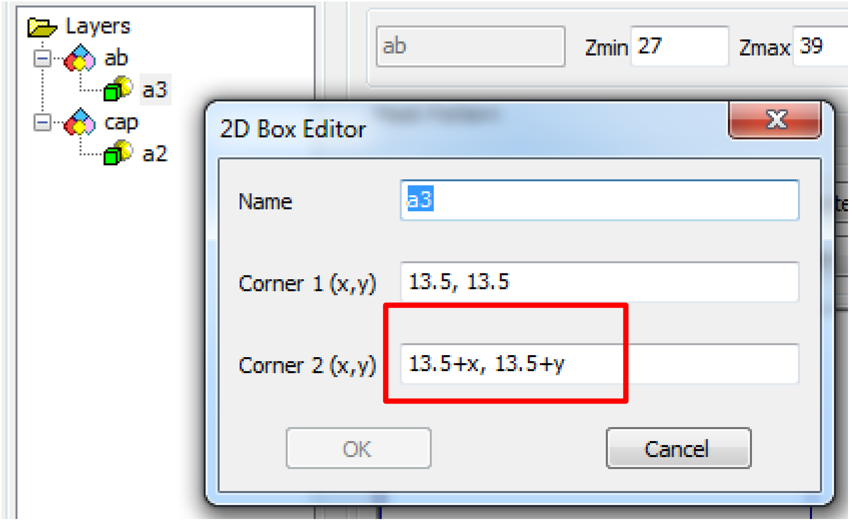
In the Mask Editor, **double click** each **layer-node** to check whether those items are correct or not.

- Z range of the layer
- the material for the mask

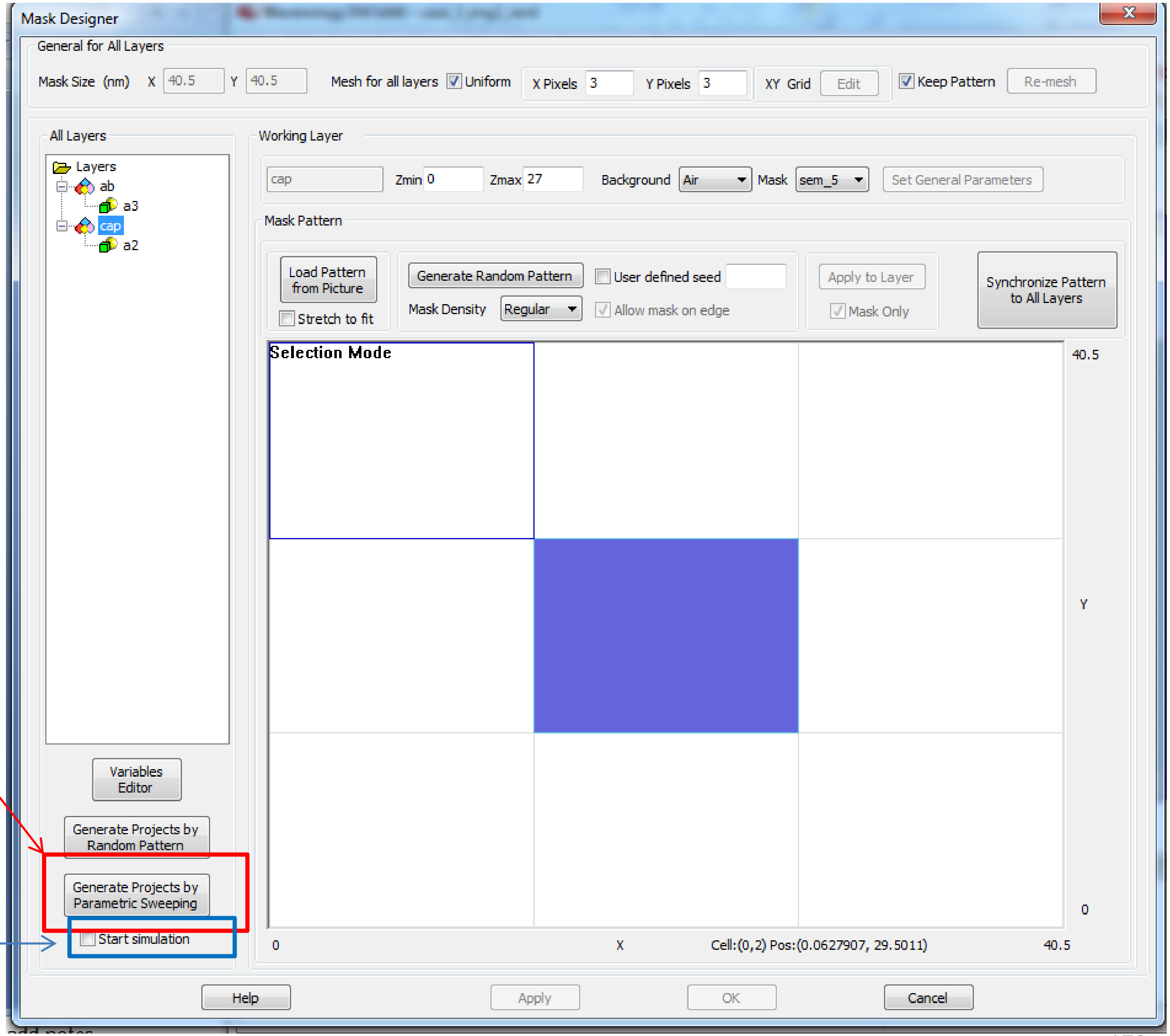


Make sure that:

- 2 layers have the same shape of pattern
- the corresponding box that will be swept has been defined by variable

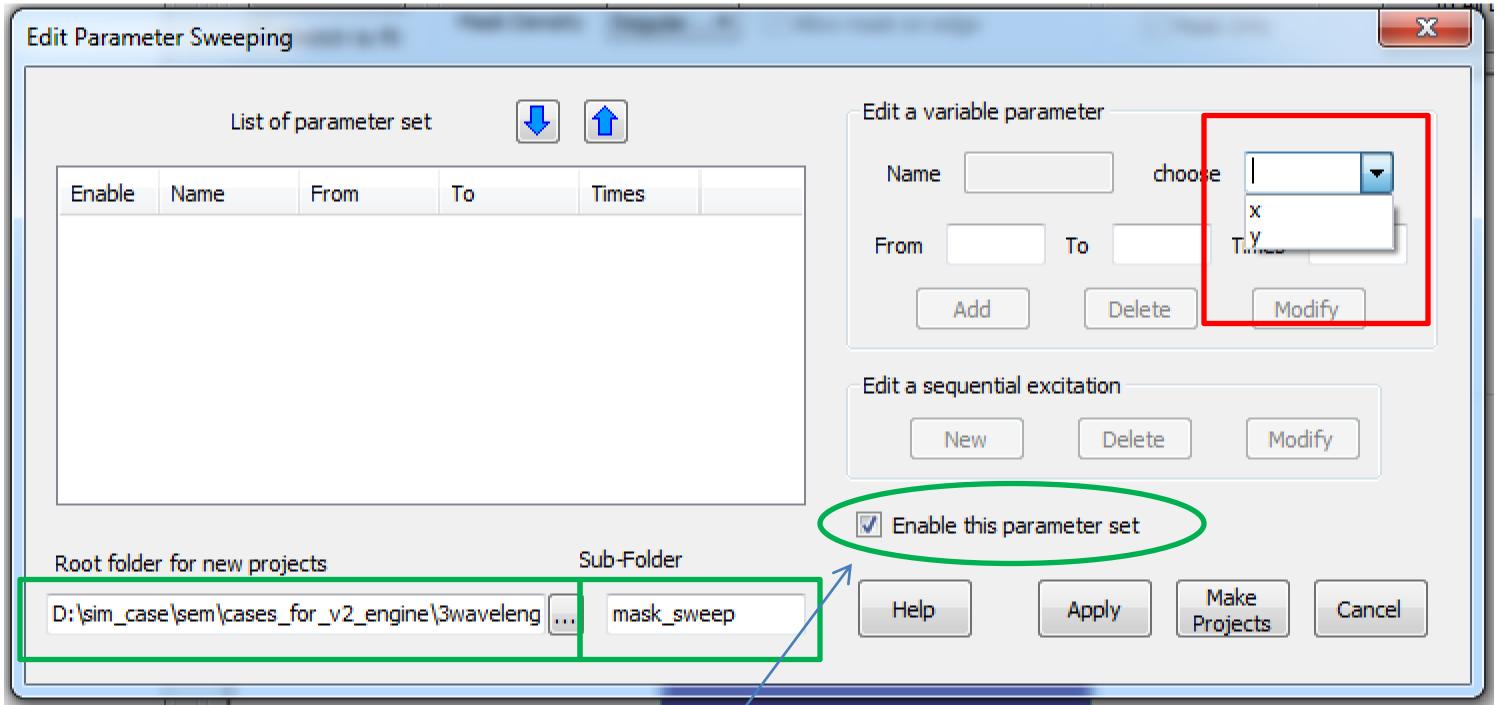


Here, user can define one layer correctly, then use "**Synchronize Pattern to All Layers**" to build other layers. It can simplify the procedure.



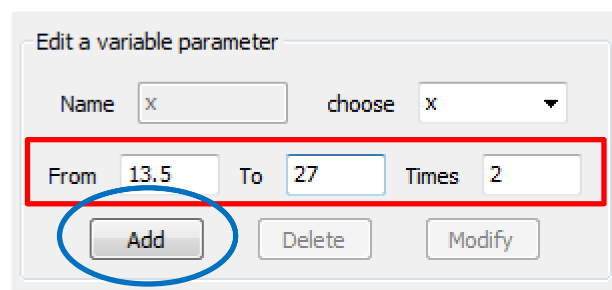
If all setting are correct, press this button to set up the batch control.

If user want to start simulation automatically after multiple project are generated, please check this option



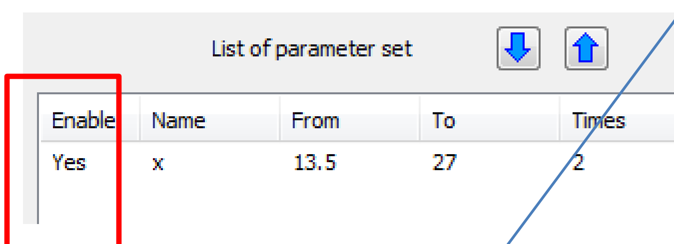
Select the variable **x**

The target projects will be stored in this folder



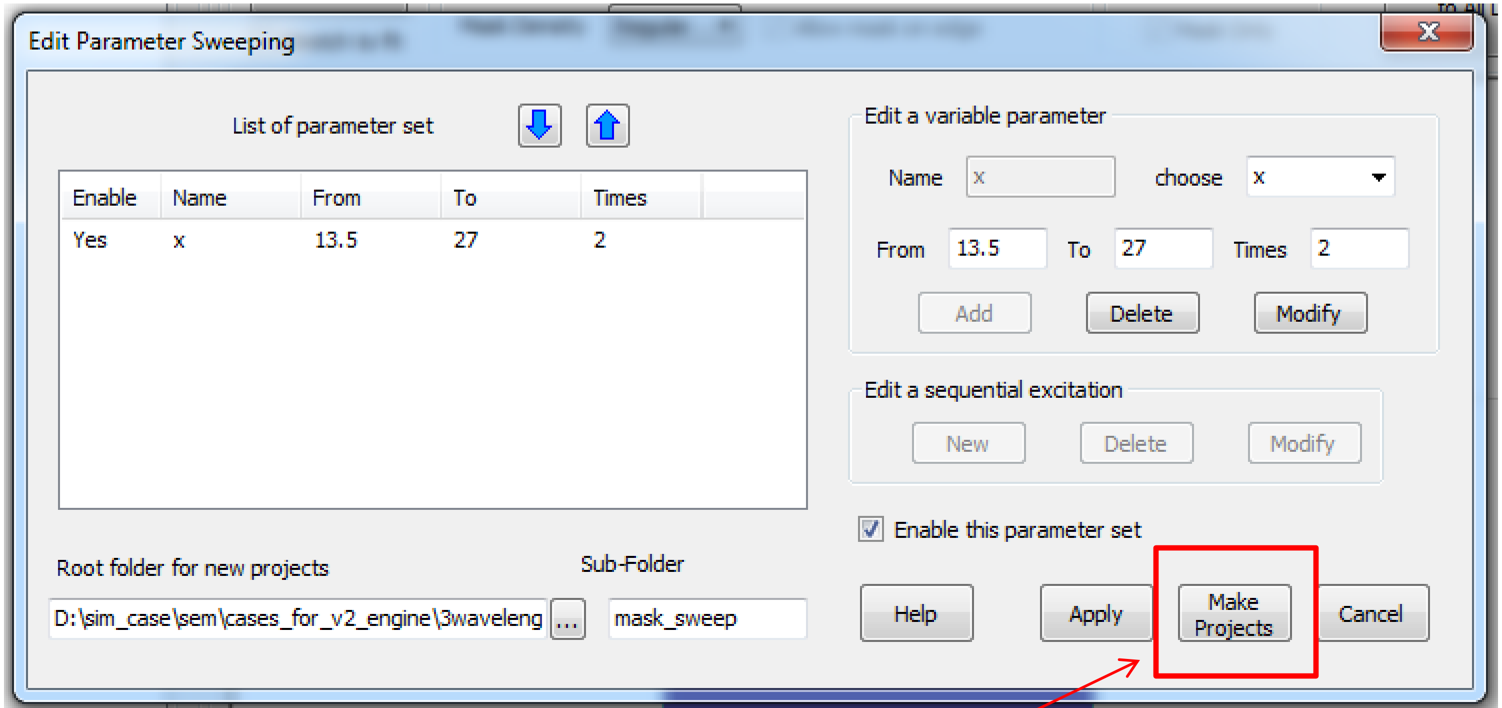
Define the seeping range and steps for x

Then add it to the parameter set



Make sure this set is Enabled

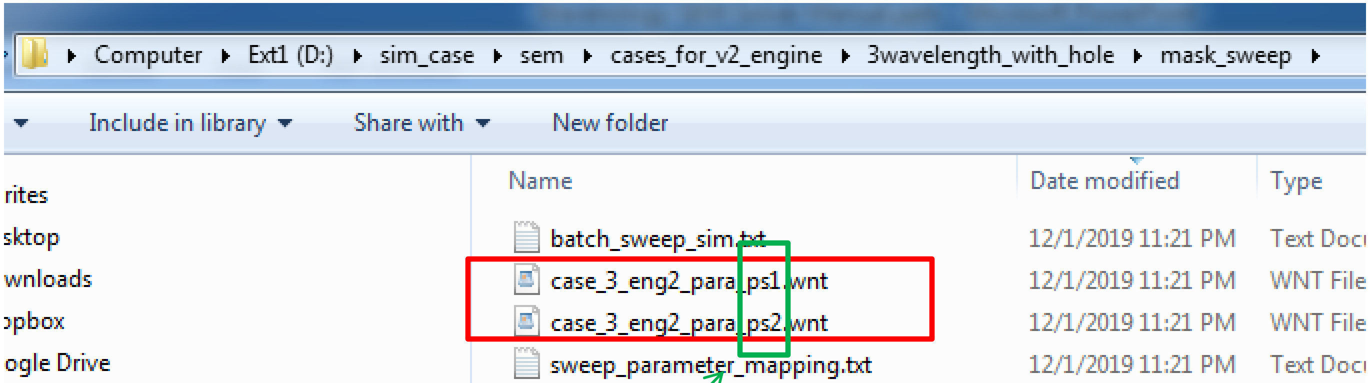
If there are multiple variables for the box, more sweeping can be added by the same way.



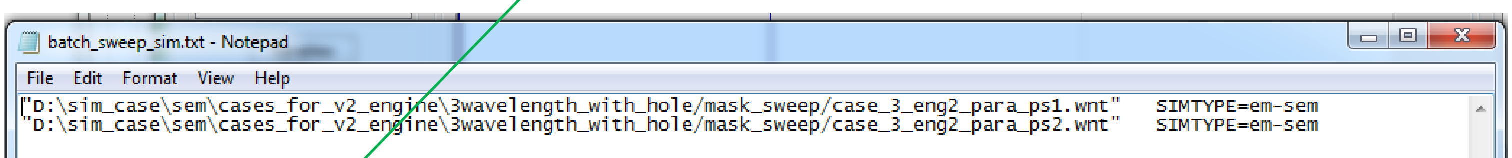
After the sweeping definition is done, user can generate the multiple projects by "<u>Make Projects</u>" button.

If the "**<u>Start Simulation</u>**" option is checked in generating these projects, the WCT simulation manager will be open to load that batch file and start simulation on these projects automatically.

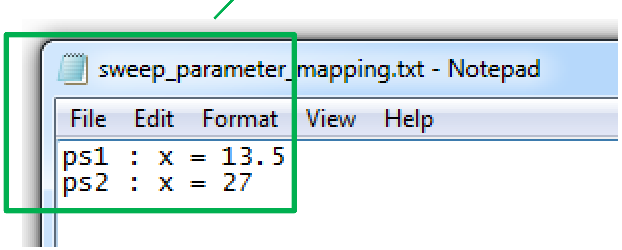
We can see 2 projects are created in the target folder.



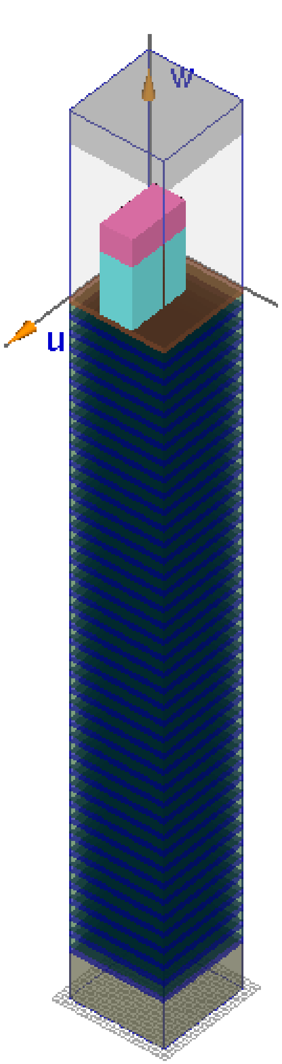
Meanwhile, a batch file “**batch_sweep_sim.txt**” for WCT simulation manger is created also.



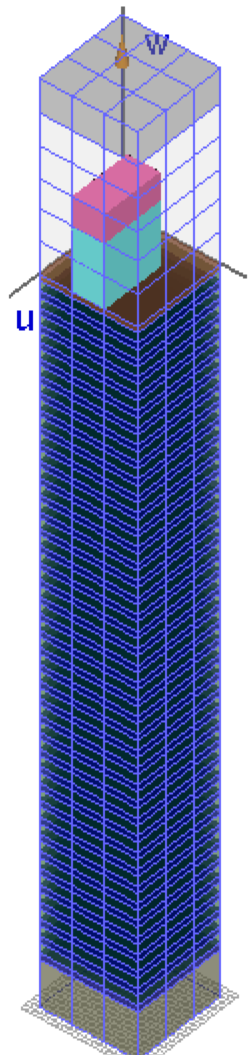
A mapping file “**sweep_parameter_mapping.txt**” to show the mapping of name to the real value of the variable is created also.



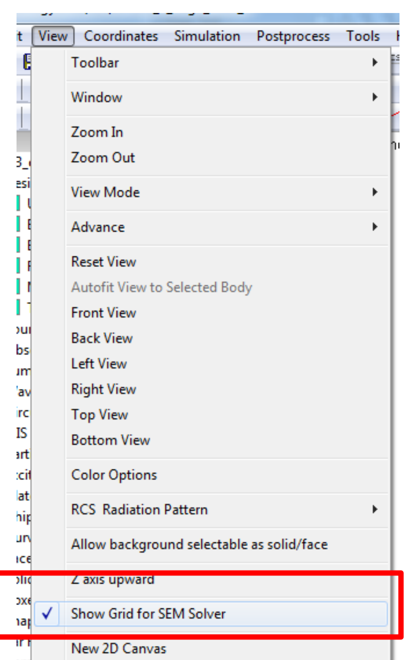
Here, we show the "case_3_eng2_para_ps2.wnt" for x=27 as shown in "**sweep_parameter_mapping.txt**"



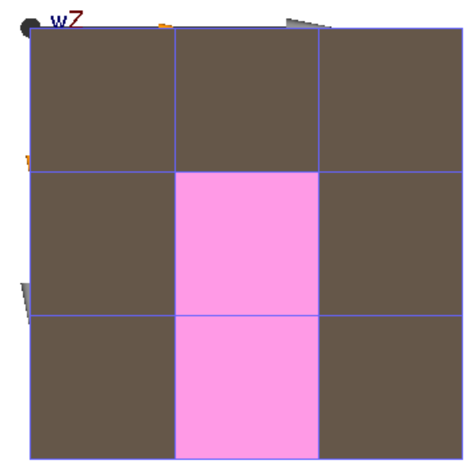
Angle view of project



Angle view of project with the SEM grid



X-Y view



Note:

- above 2 demo cases all are based on the "**layer defined by boxes**" example, this example comes from the EUV template: **layer_by_box** in the WCT SEM demo package.

- User can also use another example "**define layered media as background**" in the EUV template: **pure_layer**. The usage of the mask editor is the same.

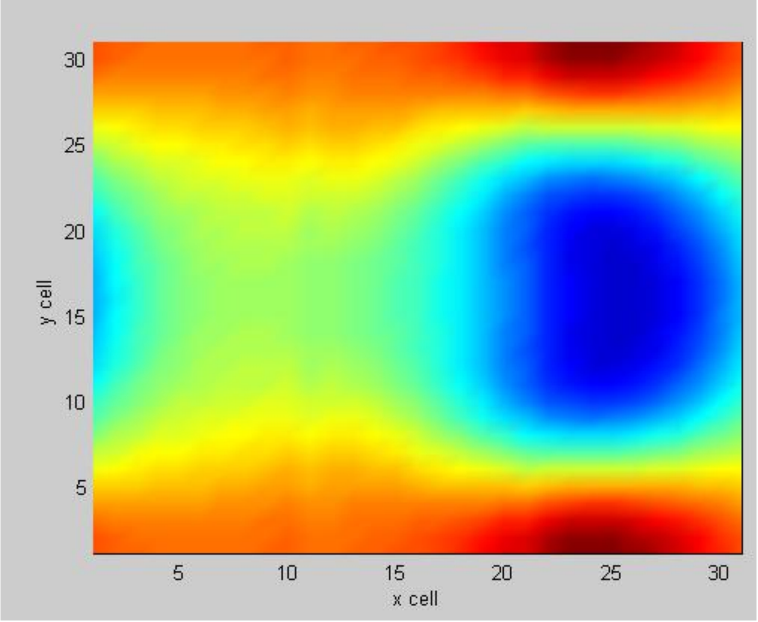
- The comment on the 2 EUV templates can be refer to
  - **layer_by_box** template
  - **pure_layer** template

Appendix II : Process Simulation Result Data by Matlab

Here, we show how to use Matlab code to read the simulation result file

- the folder storing the data file and the format of file are shown at here
- the demo case for the code is the 2nd parameter in the sweeping case
    - the case name is: **case_3_eng2_para_ps2.wnt**

Following is the figure in Matlab for the |Ex| at the 3rd Z planes in the snapshot. The source code is shown in the next page, the coresponding m file is "./ mask_editor_demo/parametric_sweep /check_sem_result.m" in the demo package.

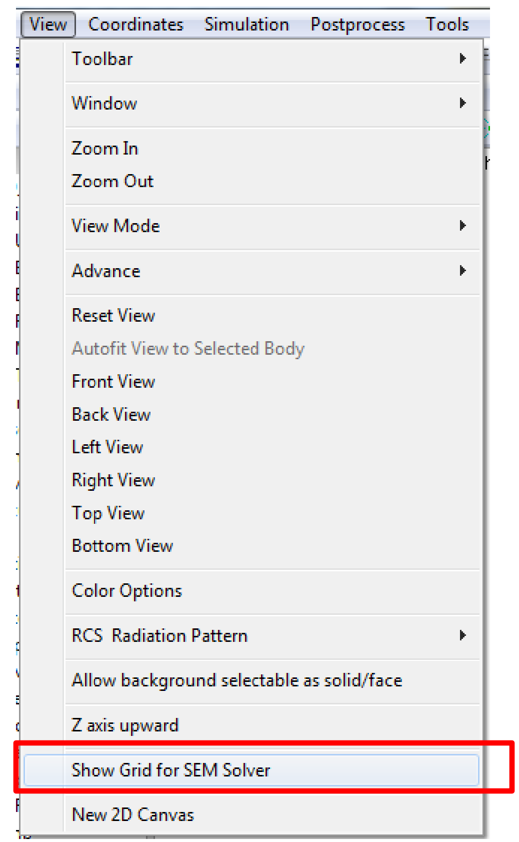


```
close all;
clear all;

%%%% the sub-folder to store the project files %%%%%
sub_folder = 'mask_sweep';

%%%% project name %%%%%
proj_name = 'case_3_eng2_para_ps2';

%%%% the full path for the E field data in P polarization, for whole snapshot
%%%%%
proj_full_path = sprintf( './%s/%s_res/sem/%s_snapshotEUV_k1_p_file2.txt',
sub_folder, proj_name, proj_name );

%%%% load the data file %%%%%%%
data = load( proj_full_path );

pos = data(:,1:3);
ex = complex( data(:,4), data(:,5) );
ey = complex( data(:,6), data(:,7) );
ez = complex( data(:,8), data(:,9) );

%%%% define nX, nY, nZ in each axis, these values can be obtained from WCT
%%%% SEM solver setup dialog
nX = 31;
nY = 31;
nZ = 3;

if( length(ex) ~= (nX*nY*nZ) )
   disp( 'the number of data does not fit, quit!' );
   return;
end;

%%%%%%%%%%% reshape data to 3D %%%%%%%%%%%%
ex = reshape( ex, nZ, nY, nX );
ey = reshape( ey, nZ, nY, nX );
ez = reshape( ez, nZ, nY, nX );

%%%%%%%%%%% extract one Z plane from 3D data array
zid = 3;
ex_a = squeeze( ex(zid, :, :) );
ey_a = squeeze( ey(zid, :, :) );
ez_a = squeeze( ez(zid, :, :) );

%%%%%%%%%% show abs of each component %%%%%%%%%%%%
tmp = abs( ex_a );
color_max = max( max( max( abs(ex) ) ) );
color_min = min( min( min( abs(ex) ) ) );

figure;
pcolor( tmp );
caxis( [color_min  color_max] );
shading interp;

xlabel( 'x cell' );
ylabel( 'y cell' );
```

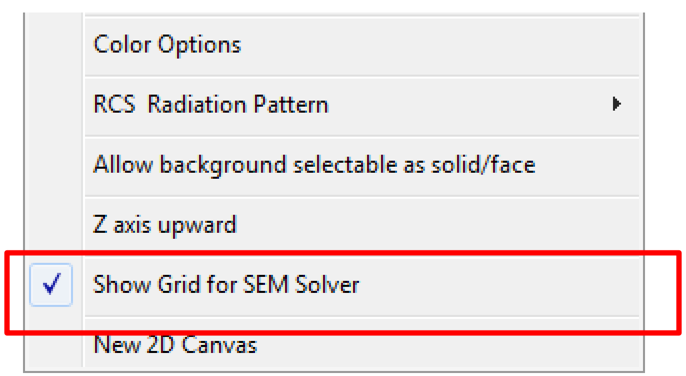
Appendix III : Displaying the mesh grid for the SEM solver

In some situations, user want to know whether the mesh grid for the SEM solver is setup correctly or not. Especially for the user defined SEM mesh grid. However, the default shown grid on the main canvas is the FDTD grid.

So, user need to switch the displaying mesh type to SEM grid by

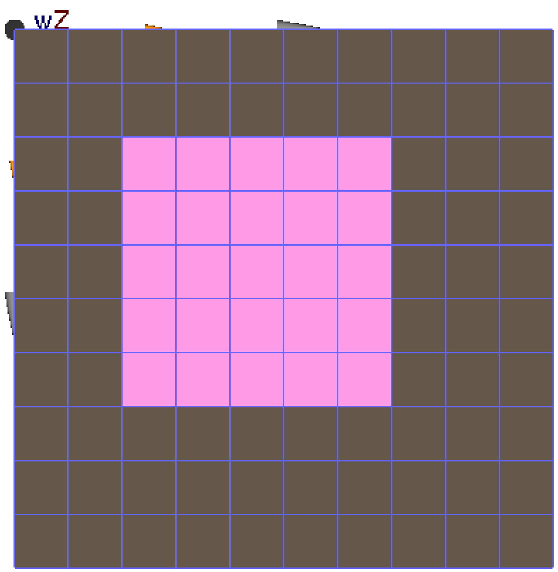


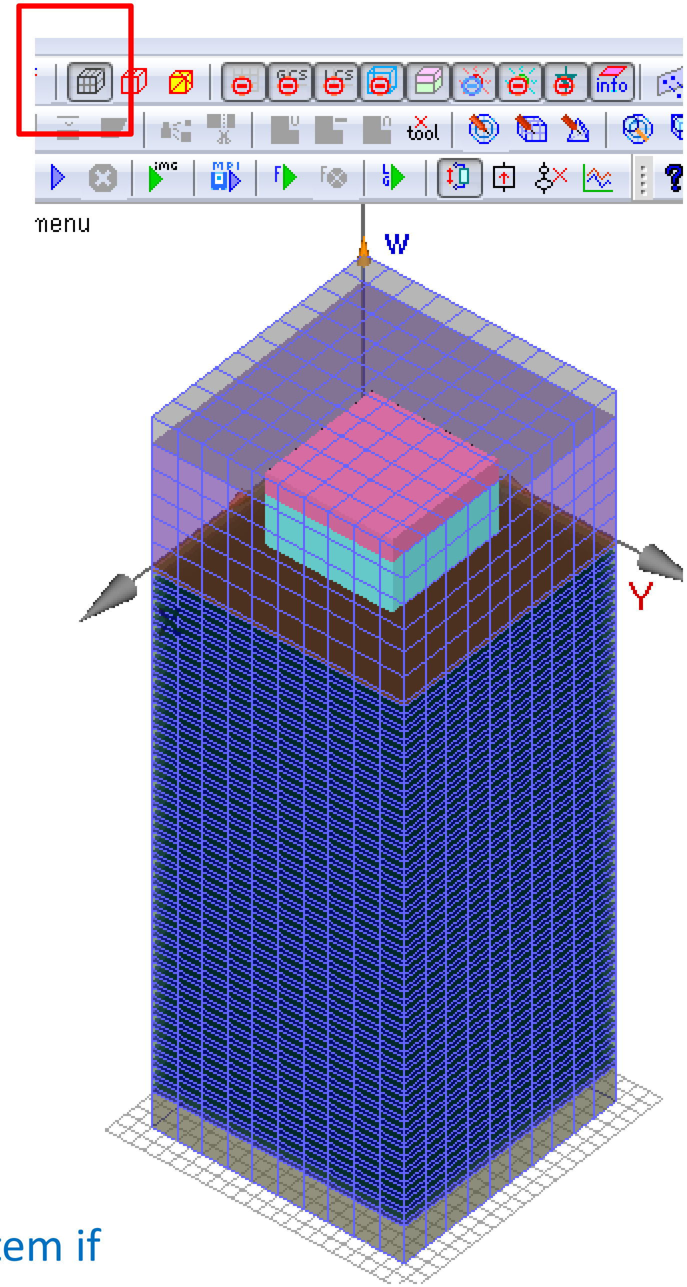
With this menu item is checked,



When click to show the mesh grid, the SEM mesh grid will be shown in the blue color.

Then, user can check the grid by different view angles.





(Note: user need to un-check this menu item if need to return to the FDTD solver)

END