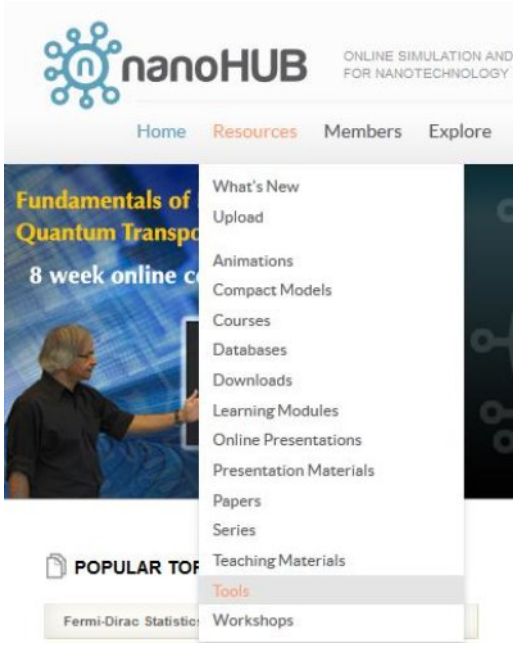
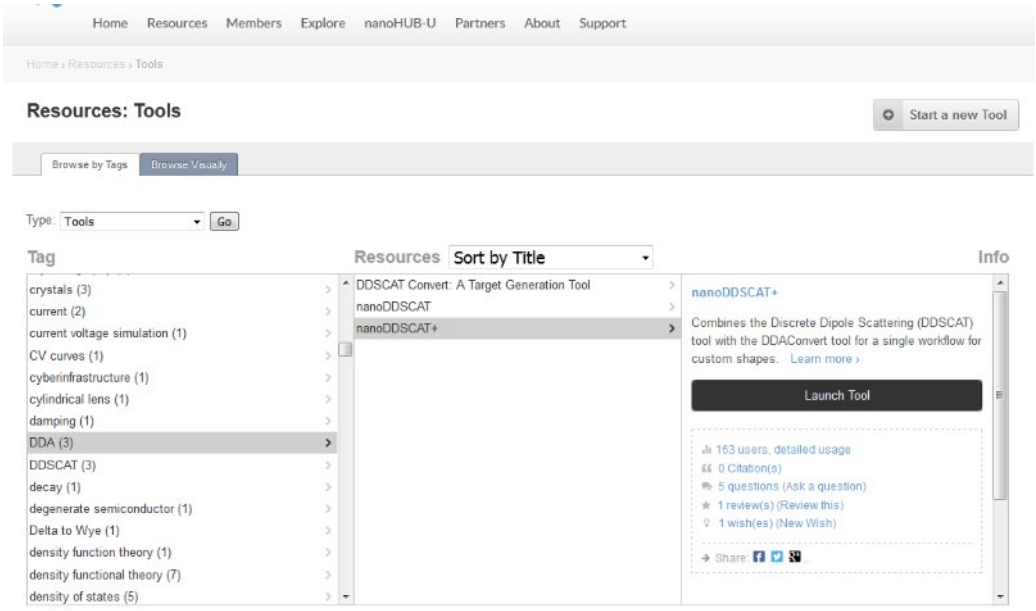
Credit: Prashant K. Jain, Jeremy G. Smith, AbderRahman N. Sobh

Getting Started

1) Log onto nanohub.org. You can either create a login to save your jobs for future reference, or login as a guest. Go to the resources tab and click on Tools.



2) From the list on the left, scroll down to DDA or DDSCAT.
From the central list, select nanoDDSCAT+. On the right hand list click launch tool.



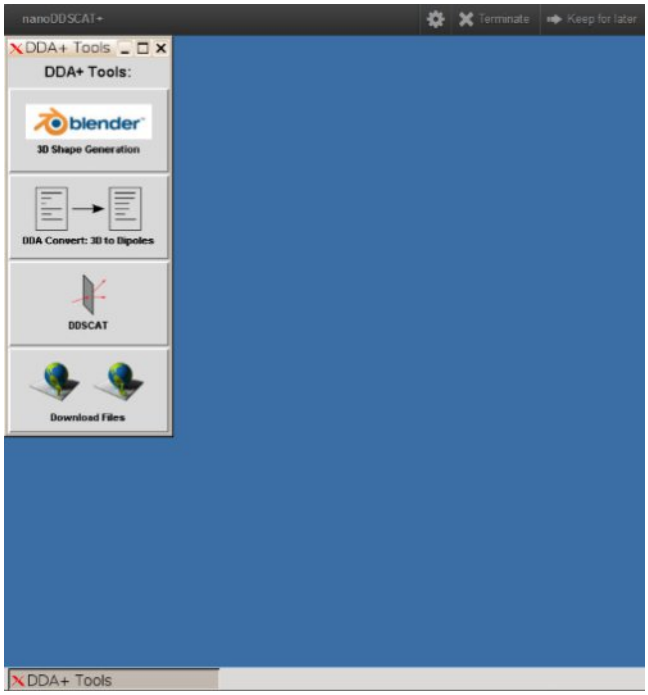
Now you have opened the DDA workflow tool on Nanohub which will perform the calculation for you. We must go through a number steps to correctly setup the calculation.

nanoDDSCAT+ (part 1/3, Blender):

The DDSCAT tool has a collection of fixed geometries such as ellipsoids and cylinders that can be used to generate shape files. While this can be instructive for learning purposes, most experimentalists prefer to use DDA calculations to simulate materials that they can synthesize in their labs. For this purpose nanoHUB has created the nanoDDSCAT+ tool.

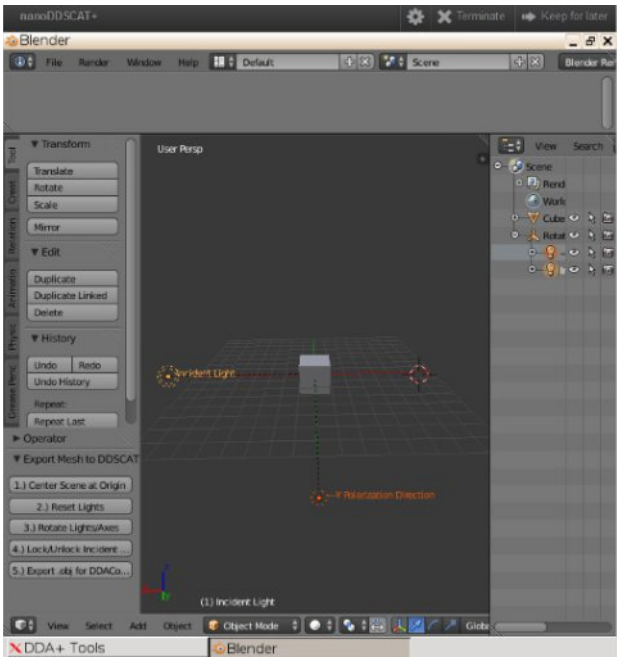
This tool allows a user to generate their own arbitrary objects and simulate the electric fields and scattering and absorption spectra of these materials.

1) Launch the nanoDDSCAT+ tool:

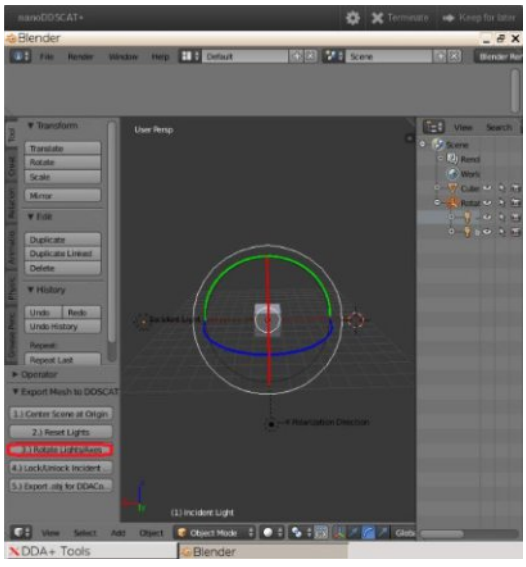


This is the nanoDDSCAT+ interface. It is logging you in to a remote desktop on a nanoHUB server that allows you access to three programs. You will need to navigate through them, in order, to generate and simulate the plasmonic properties of light interacting with an arbitrary structure. The first of these is the top tab, the one for Blender. The second button runs the converter which transforms Blender files and makes them ready to run in DDSCAT. The third button from the top is the actual DDSCAT program. Finally, the last item in this menu allows a user to Download and Upload Files that they have created at any stage including files made in Blender. Automatically, the tool will shuttle the necessary files along as we progress through the workflow and the user is also able to supply the files from disk at any stage as well.

2) Clicking this top button will launch the Blender application. Blender is primarily a 3D rendering and animation software, with a lot of powerful functionality, most of which will not be used by the typical user looking to run DDSCAT simulations. Some important basics will be needed however and are briefly discussed below before we continue with the simulation.

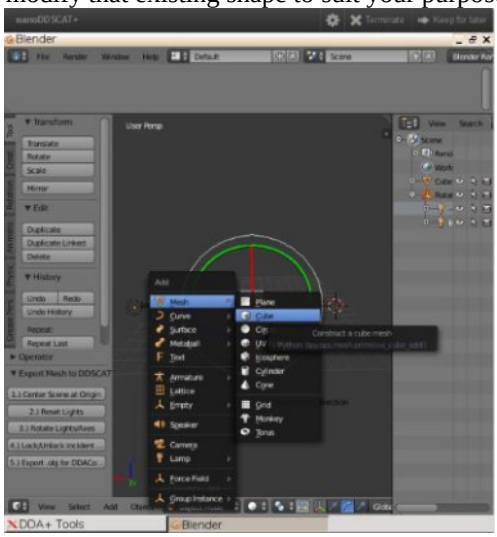


A) First, note the two parallel lines marked in the figure. The first of these is the light propagation direction, and the second is the light electric field polarization. This will define what direction the light is being shone on the object. Typically plasmon resonance will be excited based on the oscillating electric field (the magnetic field typically interacts with the electrons more weakly), and thus the electric field will define a plane along which excitations of the electrons occur strongly. Based upon the contours of the object in this plane, the scattering, absorption and electric field will change. When you create objects, keep in mind that rotating the electric field polarization may dramatically affect how the light interacts with the object. This can be changed easily by clicking the “Rotate Lights/Axes” button in the left menu titled “Export Mesh to DDSCAT”



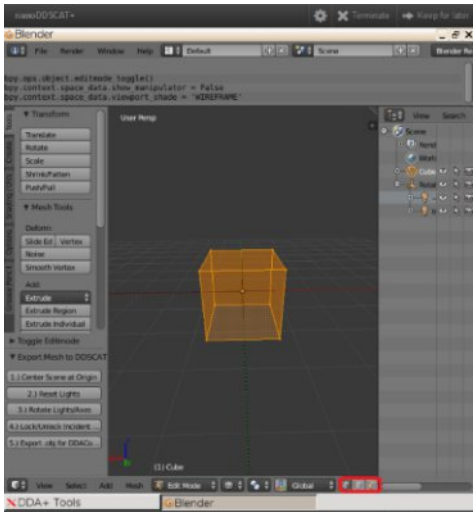
B) Some basic keyboard shortcuts will help you navigate in Blender:

- Holding down the center button (or the wheel) of typical mouse will allow you to rotate the scene to get a good look at your object.
- Objects can be selected by right clicking on them.
- Once selected objects can be deleted using the delete key.
- A new object can be added by pressing Shift+a. This will bring up a dialogue prompting you to add a new mesh, there are several useful built in shapes. Typically, it is easiest to start with a shape somewhat similar to the one you desire, and then modify that existing shape to suit your purpose.



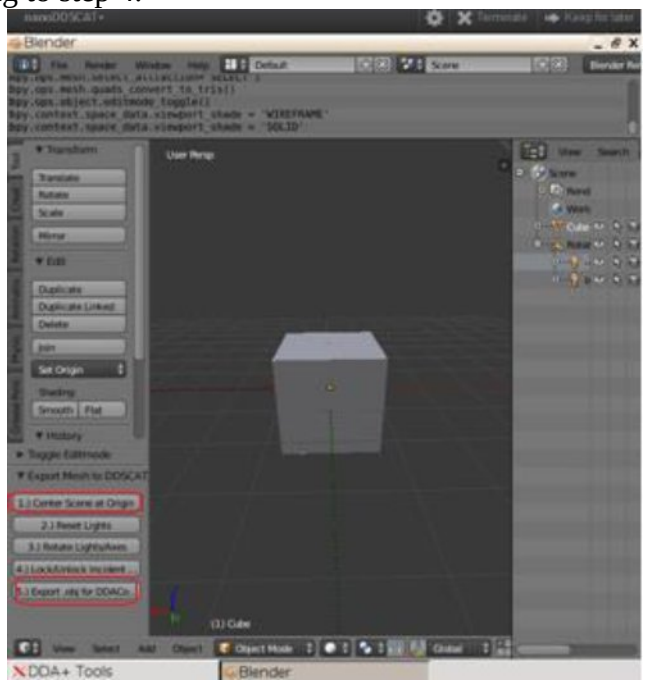
C) For object editing, it is usually easier to switch the view to wireframe. The mode everything starts in is called object mode, which is usually reserved for organizing multiple objects in a frame, not for modifying existing objects. To switch to object editing mode, press Tab.

- Three types of editing can be done, editing of faces, edges and vertices. These are changed in the bottom menu as shown below. Clicking on a particular vertex, edge or face and pressing “g” will allow you to move it freely. Left clicking on one of the red, blue or green arrows will allow you move these along a specific cardinal direction.



D) A very useful option is the subdivide option located in the mesh tools options on the left. This will allow you to create more vertices, or edges to make new faces and make your object more complicated. You can then drag these new vertices to define a shape. It is important to note that after subdividing objects you need to redefine the faces of your object. Do this by selecting all of the vertices which define a specific face and pressing "f". Failure to do so will result in your object not being simulated correctly.

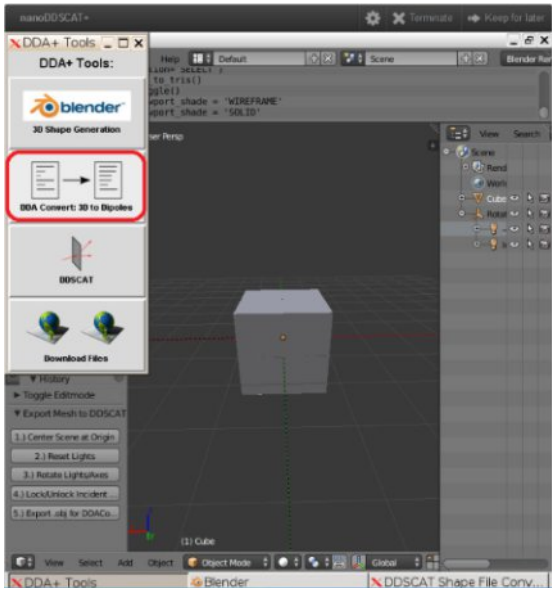
3) It is important to note at this point that the calculation will be done assuming the default center your object is at the origin. This is why the center object at origin button is provided, so you can get an accurate idea of where the electric field plane of the light will bisect your objects. Simply click the button labeled "1) Center Scene at Origin" at any time and it will translate the objects appropriately. You should always make sure this is set before continuing to step 4.

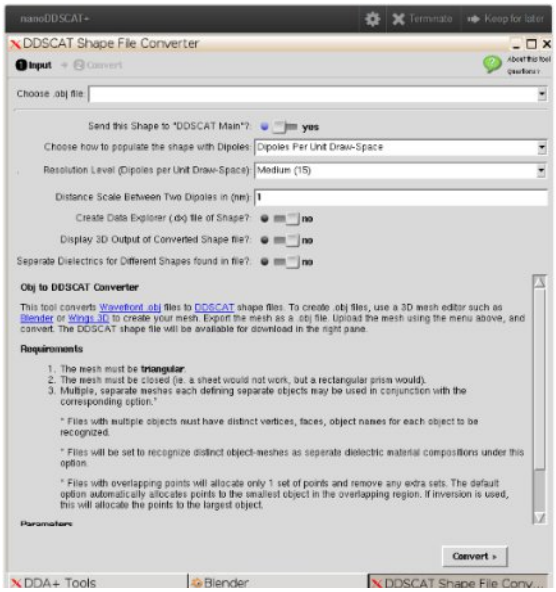


4) Once you have created a shape you are happy with and centered it, press the "Export .obj for DDSCAT" button. This will save your object in the correct format to run the DDA calculation using the tool. You are also free to download/upload any files that you create.

nanoDDSCAT+ (part 2/3, DDSCAT Shape File Converter):

The next step will be to open the second program in the work flow, which is the DDSCAT Shape File Converter tool.





1) In the top dropdown menu, you need to select “Blender file”. This will load the most recent Blender file that was saved in this nanoDDSCAT+ session. There is also an option to upload your own .obj file. You can choose this option if you prefer to run Blender locally on your own computer and then export a file to use with the file converter and DDSCAT. This is not advisable, as there are several specific details about formatting and saving the file which the specialized version of Blender on the website takes care of for you. These specifics are found under the header “Requirements” at the bottom of this tool.

2) Once you have selected your file, be sure to check yes in the second box to send the generated shape to “DDSCAT Main”. This will set up to run the DDA calculation in the following simulation.

3) Now you must choose the way to define the population of your shape with dipoles. Keep in mind that the real scale of the shape has not been defined yet as that will be done in the following step where we specify the distance in (nm) between two adjacent dipoles. What is being defined right now is simply the quantity of points (a.k.a. dipoles) that will be used to define your 3D system for the various calculations. As a result, asking for too few dipoles will leave you with incomplete drawings. Asking for too many dipoles will unnecessarily slow down processing. Typically, you want the resolution to be such that the sharpest point along your object is described by at least 2 dipoles. The time it takes to run the calculation will scale superlinearly with the number of dipoles, however, so you want to limit this value as much as possible. Finally, note that the dipoles will be forced to occupy a grid structure along the standard X,Y,Z axes.

There are 3 options are available under the “Choose how to populate the shape with Dipoles” dropdown menu. Each option will open up a different parameter entry that will be found right below this dropdown menu. They are defined as follows:

- Option 1, Dipoles Per Unit Draw-Space:
  Selecting this option allows for the user to specify the number of dipoles by relating them to the units used during 3D editing (i.e. Blender). Typically these units are not given real scale so we refer to them simply as units of “Draw-Space”.

  The entry that will open up is dropdown titled Resolution Level, the options allowed are estimated values that can populate the shape at 5 dipoles per unit of draw-space, 10 dipoles, and 25 dipoles. Additionally, the final option is to allow specification of a custom value here (note: this will create another entry just below Resolution Level where this value can be entered).

- Option 2, Dipoles along Max Cartesian Dimension:
  Selecting this option allows for the user to specify the number of dipoles by relating them to the longest dimension, in one of the cardinal directions, in the 3D system being considered. In other words, the longest of X, Y, or Z is considered and the user determines how many dipoles will be along that length. As a result, the system as a whole is defined by this ratio of dipoles-to- length.

  The entry that will open up is dropdown titled Dipole Length of the Longest Cartesian Axis, where an integer value can be entered in.

- Option 3, Total Dipole Volume:
  Selecting this option allows for the user to specify the number of dipoles by defining the maximum number of dipoles used to define the 3D system.

  The entry that will open up is dropdown titled Total Dipole Count, where an integer value can be entered in.

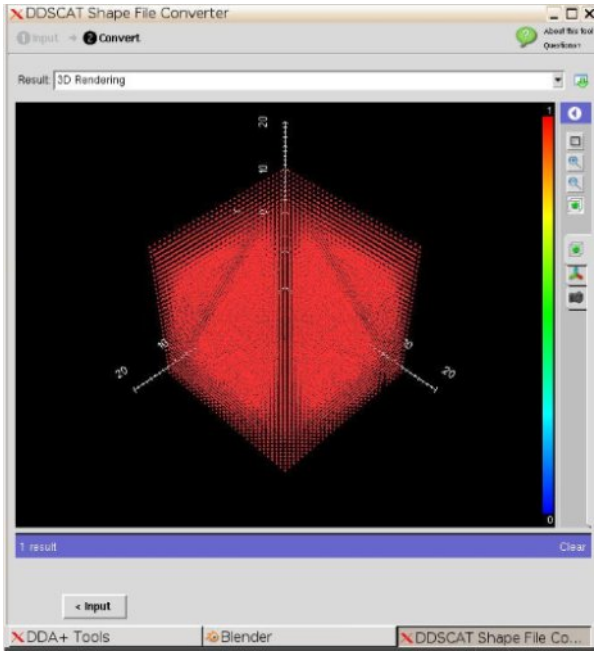
4) At this point you need to figure out the size you want your object to be (typically in nm for plasmonic materials). This is done by specifying the “Distance Scale between Two Dipoles in (nm)” parameter. Typical values are 1 nm between dipoles, for rough calculations or very smooth objects. And 2 nm between dipoles, for very accurate calculations or objects with sharp corners. A good method of investigation is to start with 0.5nm between dipoles, run the calculation, switch to 1nm, then 2nm and see if the answer changes substantially. If it is still changing in going from 1nm to 2 nm, you probably need to increase the number of dipoles to get an accurate answer.

   If you are not concerned with being massively accurate, please restrict your calculations to 1nm between dipoles.

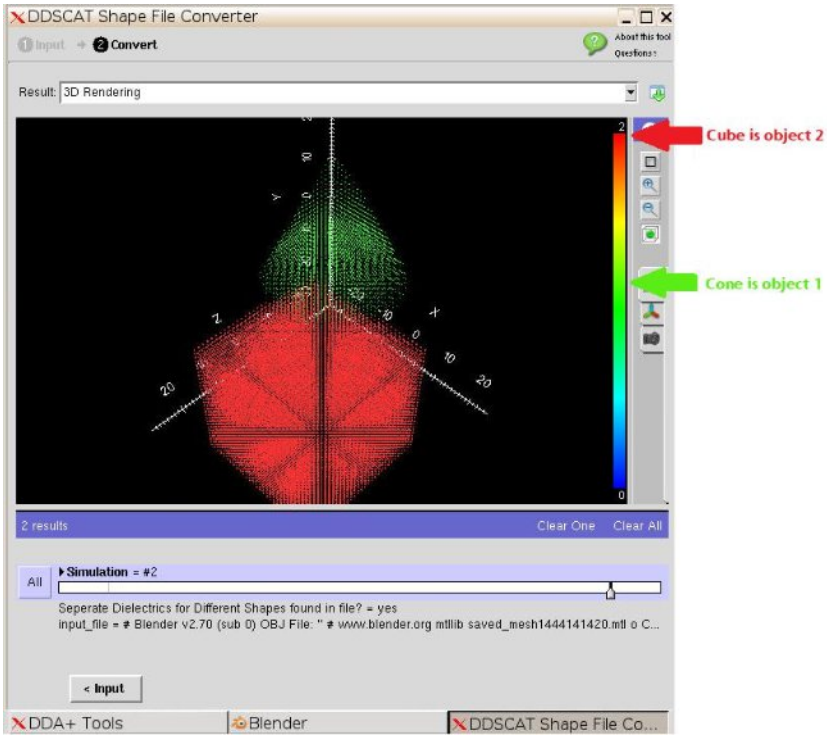
5) The next three boxes are all optional, but will provide significant outputs (including a 3D display of the output) if selected.

   A) The first checkbox creates an additional output of the converted shape as a .dx filetype for specifying volumes. This can be used in other programs not contained in this workflow, such as the University of Illinois' Visual Molecular Dynamics (VMD) program. A dropdown allowing specification of Angstroms between dipoles will also appear if this box is checked.

   B) The second checkbox will generate a 3D preview of the actual discrete dipole object the final calculation will run on. You should ensure that this object completely matches what you intended in Blender before proceeding. Possible problems usually stem from a failure to correctly define all faces in Blender before exporting the object. Note the panel on the right-hand side which has some basic 3D viewer tools for view manipulation.



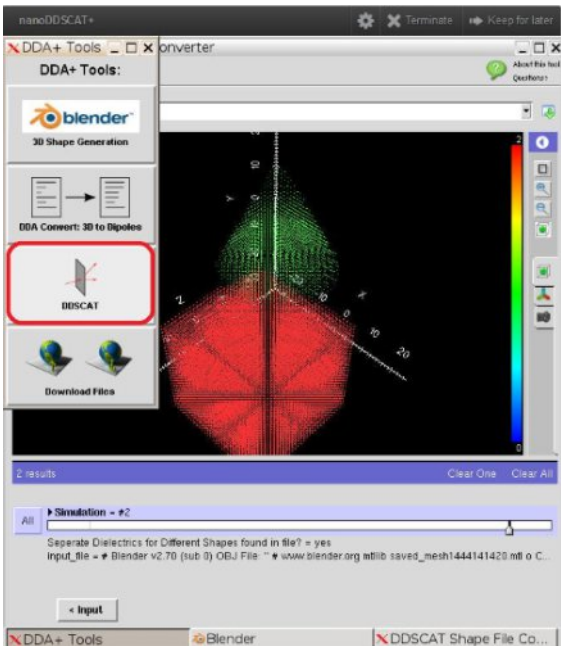
C) The third checkbox is only significant if you had multiple objects in your file and you want to assign different materials to each shape during the DDSCAT simulation. The program will automatically assume different objects are composed of the same material unless this box is checked. The 3D rendering will be colored respectively to show the different objects that were recognized. Knowing the object numbering will become important soon when we specify which compositions each material has. This can be determined by looking at the color bar on the right of the image and noting the order of the colors.

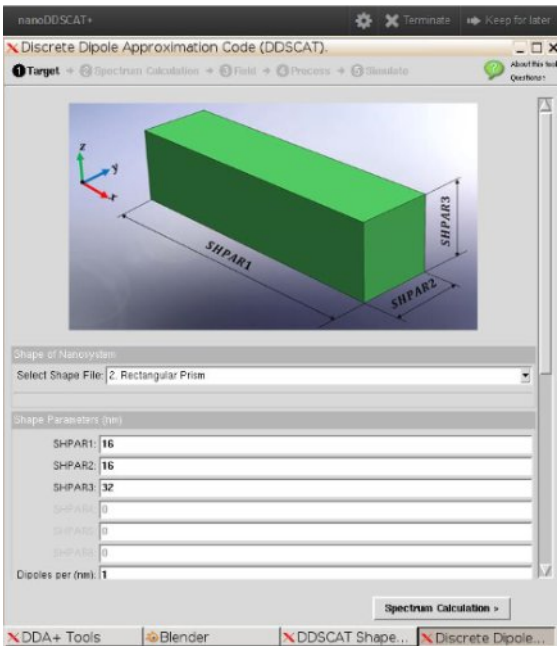


By default, overlapping objects will have the overlapped volume allocated to the smallest object. Checking the third box also opens up a 4th checkbox which allows for the ability to have the algorithm flipped and to allocate overlapped volume to the largest object.

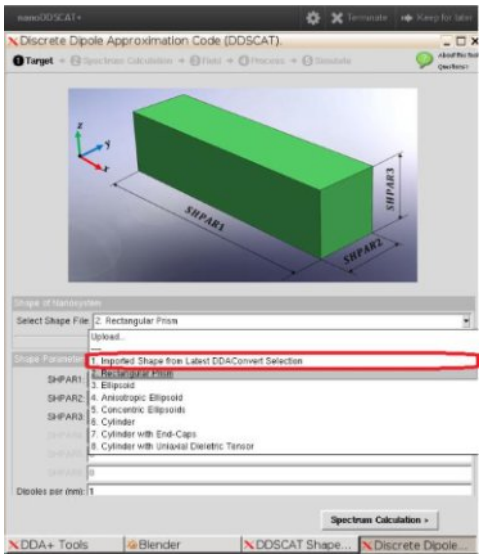
nanoDDSCAT+ (part 3/3, DDSCAT Main):

Now you are ready to run the actual calculation. To do this, navigate back to the main menu and select the third program, DDSCAT.





1) While the program has a few built-in shapes, in the shape file dialogue, you should select “Imported Shape from Latest DDAConvert Selection”. If the previous step was done successfully, then it should upload your shape file to run the calculation on.



2) Next in the target rotations tab you select import light polarization from Blender session. This should set the propagation and polarization of the light as was defined in Blender visually. The target rotations tab allows one to rotate the object relative to the incident

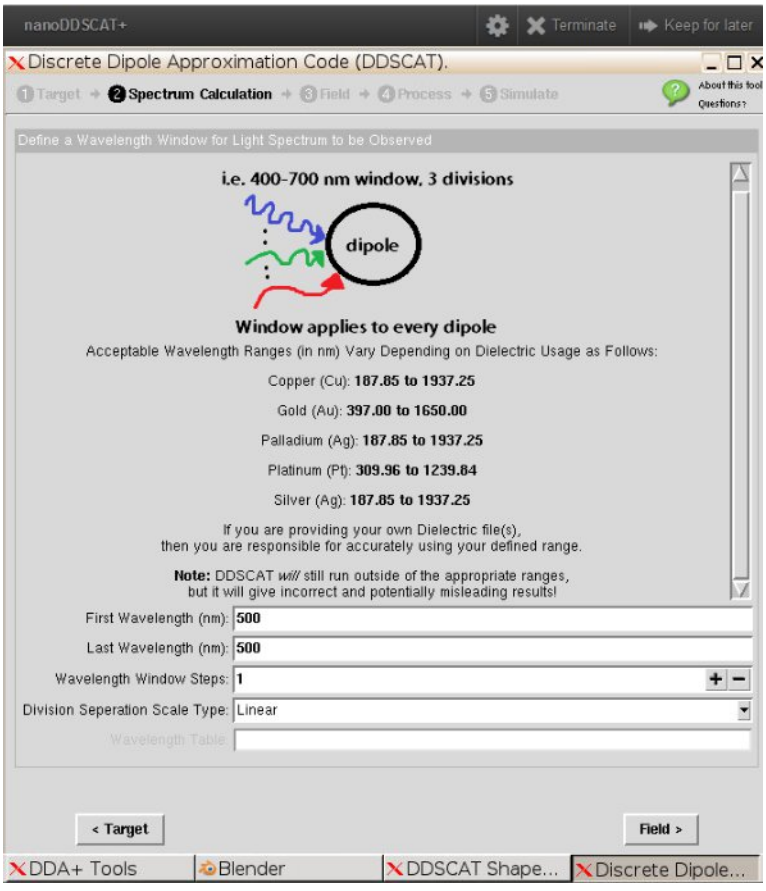
light. By default, the light propagates along the x direction. Since the light is fixed, rotating the object will change the angle between the electric field vector of the light and the object, and thus change the types of "modes" which are excited by the light.

3) Do not change the light polarization from linear y (propagation along x, magnetic field along z) or this will scramble everything relative to what you defined in Blender.

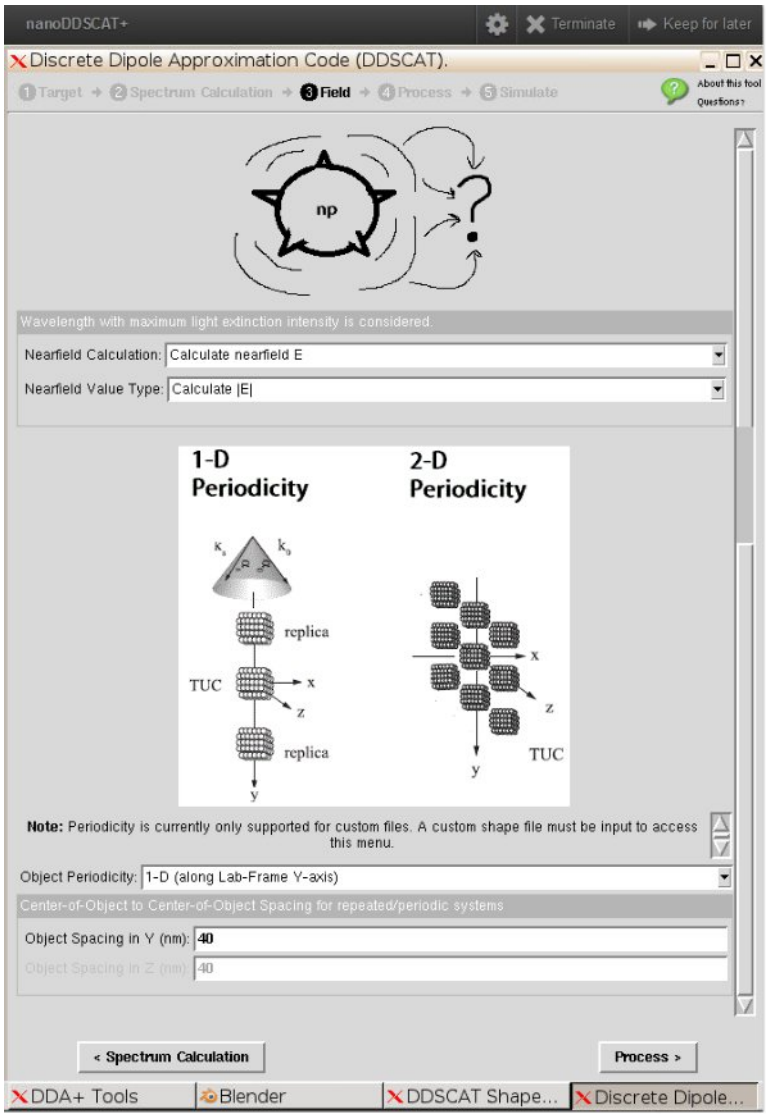
4) For number of dielectric materials to use, select one, unless you produced multiple objects in blender and selected separate dielectrics for objects in the previous step with the DDAConverter tool. At this point you can select any of the preset dielectrics and compare if you wish. Try out different options to see the result!

5) The refractive index for vacuum is 1.0. The refractive index for water is 1.33.

6) On page 2 – "Spectrum Calculation", you may want to select a fairly wide range of frequencies (wavelengths) in order to find any resonances of your object. Having more steps will generate a "smoother" curve, but each extra step means an additional calculation at that wavelength. We suggest that you try to find a happy medium between runtimes and accuracy. Most likely, you will want to start with fewer steps for a broad range (i.e. 10 steps for every 100nm). Following which, you can then subset the wavelength range to the region of interest and increase the step size.



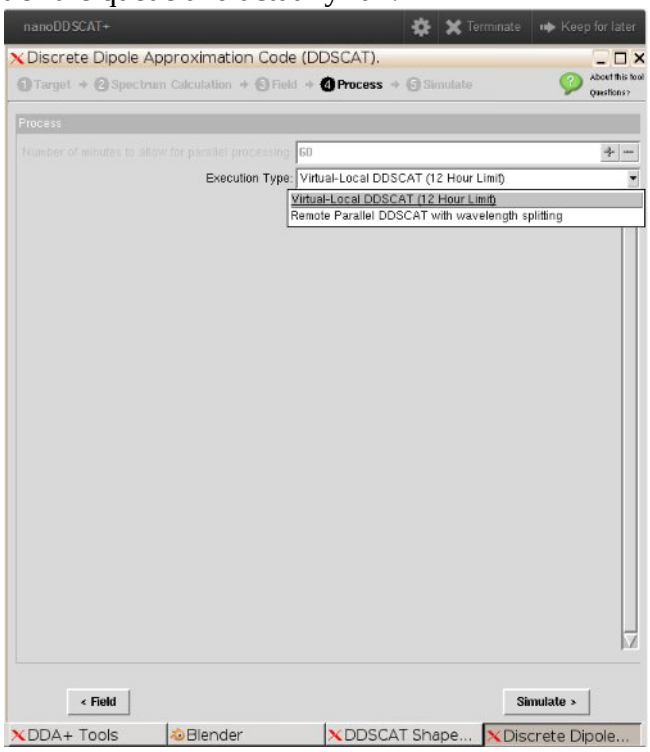
7) On page 3 – “Field”, select calculate Nearfield E, then if desired select calculate |E|^2. This will calculate the field in the vicinity of the particle (or rather its magnitude, if using |E|^2).



(Optional)

8) Repeat the object infinitely in 1-D or 2-D for use by the simulation.

9) On page 4 – “Process”, if you are not using the built-in shapes then you will likely want to select Remote Parallel DDSCAT, rather than Virtual-Local. The reason for this is that calculations of arbitrary geometries usually take substantially longer to converge than simple shapes. For this reason nanoHUB provides us with a cluster to run such calculations on that will run much faster than the local machine. The local machine only allows simulations to run for approximately 12 hours. By default nanoHUB allows remote jobs to run for 1 week before terminating a session, so a job that takes longer than a week would require special permission. Typically jobs on single objects will almost never take more than a day, even at very high resolutions, but jobs involving large arrays of objects can take significantly longer. In terms of defining how many minutes to send the remote job for, the results will display how long a simulation took after it has completed. This can give you a better idea for the future how many minutes you should try to use. Asking for more minutes than needed can result in longer wait times before the job will be taken out of the queue and actually run.



Results:

In the result tab there will be several files which you can look at and download, including downloading images or text data of the 3D plots. To download, click the green arrow in the top right-hand corner (shown below). Absorption and scattering represent the absorption and scattering spectra respectively. Extinction is the sum of both of these. For fun you can click on the electric field cutplanes tab. This will plot the electric field in the vicinity of the object. The maximum of the extinction spectrum is the wavelength that will be used for the 3D plots and this wavelength value is reported in the Simulation Status log.