

Advanced Tutorial: Taking Functionalization Workbench Results to nanoDDSCAT+

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Getting Started

This is a tutorial for an advanced function building off of the material available in the two tools:

“Functionalization Workbench”

(<https://nanohub.org/tools/partsub/>)

“nanoDDSCAT+”

(<https://nanohub.org/tools/ddaplus/>)

Tutorials can be found respectively at:

(https://nanohub.org/resources/23407/download/inorganicBuilder_tutorial_NANO.pdf)

(https://nanohub.org/resources/22905/download/ddaplus_tutorial.pdf)

Rendering the STL Volume Files of All Molecules Used

- 1) The first assumption will be that you have created a functionalized particle using the Functionalization Workbench, leaving you with a VMD session looking something like this:

The image shows two overlapping windows from a molecular simulation environment. The left window is titled "InorganicBuilder" and contains a control panel for building a surface structure. The right window is titled "VMD Main" and shows a 3D visualization of the molecule with a table of its components.

InorganicBuilder Window:

- Surface Molecule: Select loaded molecule
- PSF: /home/nanohub/sobh1/vmdNEW/vmd2/vmd/Au Browse
- PDB: /home/nanohub/sobh1/vmdNEW/vmd2/vmd/Au Browse
- Output file (.pdb, .psf): CombinedStructSurf Reset Device
- Get Surface Atom Types: AU Draw Surface Atoms
- Structures: Add Structure Remove Structure Pack Struts as STL
- 0 Peg Attachment 1 custom
- 1 PEG attachment 2 custom
- Periodic Settings of Surface with Structures:
 - Build Periodic in: X Y Z
 - Hex box:
 - Box dimensions (Angstrom): X: 4.0782 Y: 4.0782 Z: 4.0782
 - Periodic Directions (Degrees): Alpha: 90 Beta: 90 Gamma: 90
- Buttons: Build Structures Run NAMD Cancel

VMD Main Window:

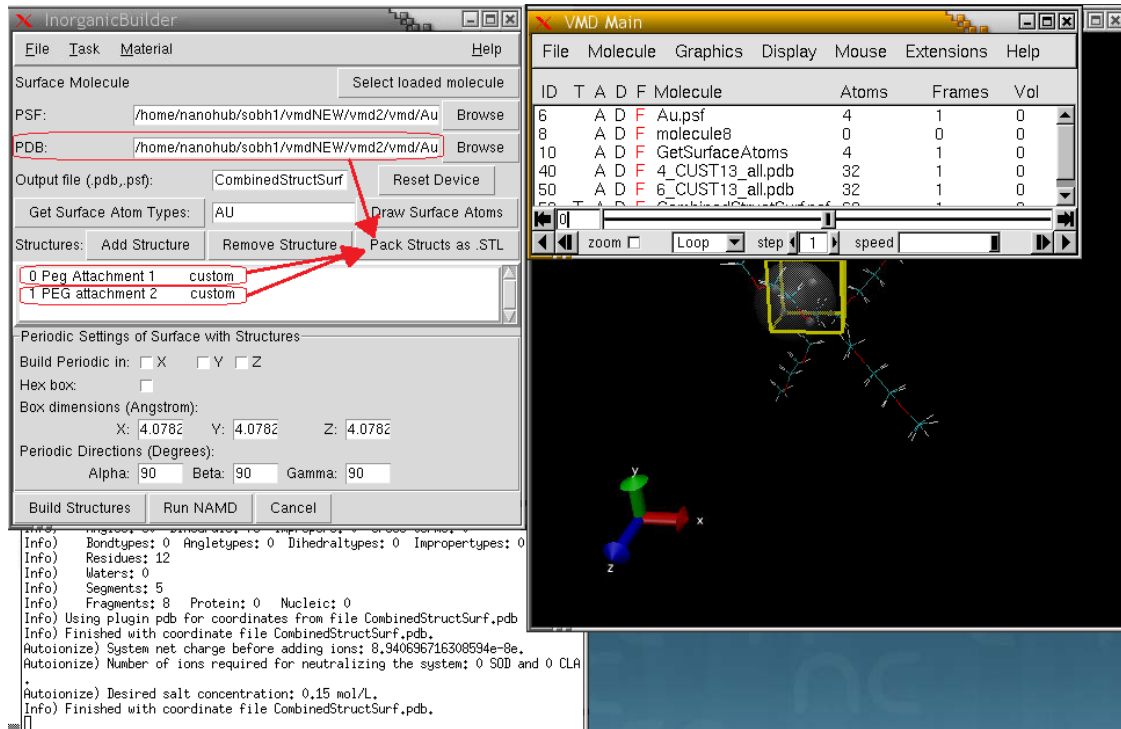
ID	T	A	D	F	Molecule	Atoms	Frames	Vol
6	A	D	F		Au.psf	4	1	0
8	A	D	F		molecule8	0	0	0
10	A	D	F		GetSurfaceAtoms	4	1	0
40	A	D	F		4_CUST13_all.pdb	32	1	0
50	A	D	F		6_CUST13_all.pdb	32	1	0

The VMD window also shows a 3D visualization of the molecule with a yellow box highlighting a specific region. The bottom of the VMD window shows a 3D coordinate system with x, y, and z axes.

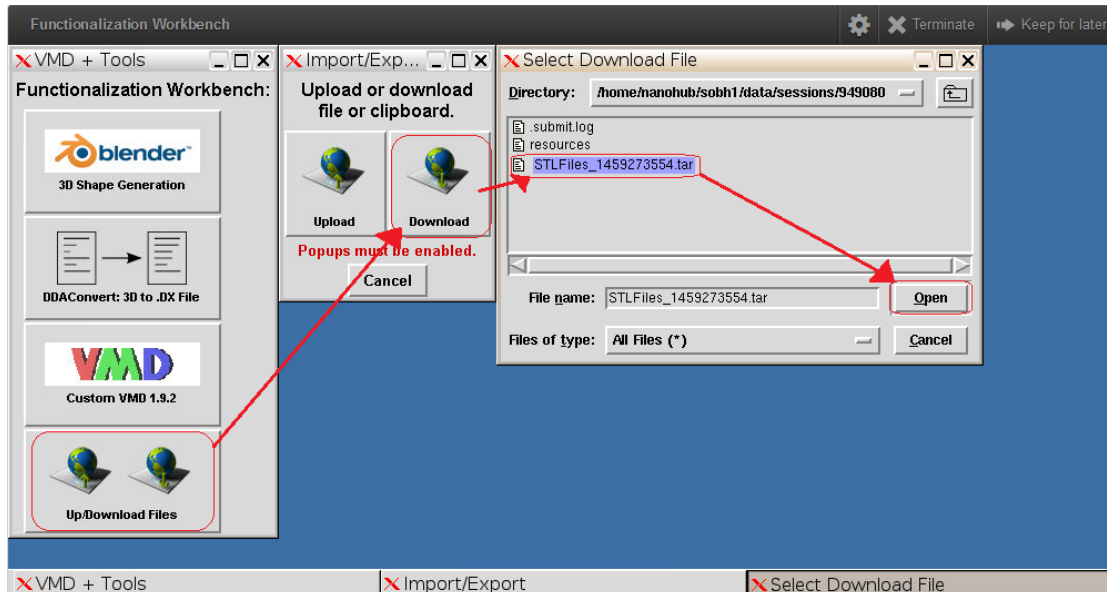
Terminal Output (bottom of InorganicBuilder):

```
Info) Bondtypes: 0 Angletypes: 0 Dihedraltypes: 0 Improptypes: 0
Info) Residues: 12
Info) Waters: 0
Info) Segments: 5
Info) Fragments: 8 Protein: 0 Nucleic: 0
Info) Using plugin pdb for coordinates from file CombinedStructSurf.pdb
Info) Finished with coordinate file CombinedStructSurf.pdb.
Autoionize) System net charge before adding ions: 8.940696716308594e-06.
Autoionize) Number of ions required for neutralizing the system: 0 500 and 0 CLR
Autoionize) Desired salt concentration: 0.15 mol/L.
Info) Finished with coordinate file CombinedStructSurf.pdb.
```

- 2) Note the new “Pack Structs as .STL” button. Clicking this button will automatically export all the relevant pieces of the structure constructed as separate volume files. It does not matter whether the structure has been built or not, the routine simply exports the base molecule used as well as the intermediary structures that the user has added:

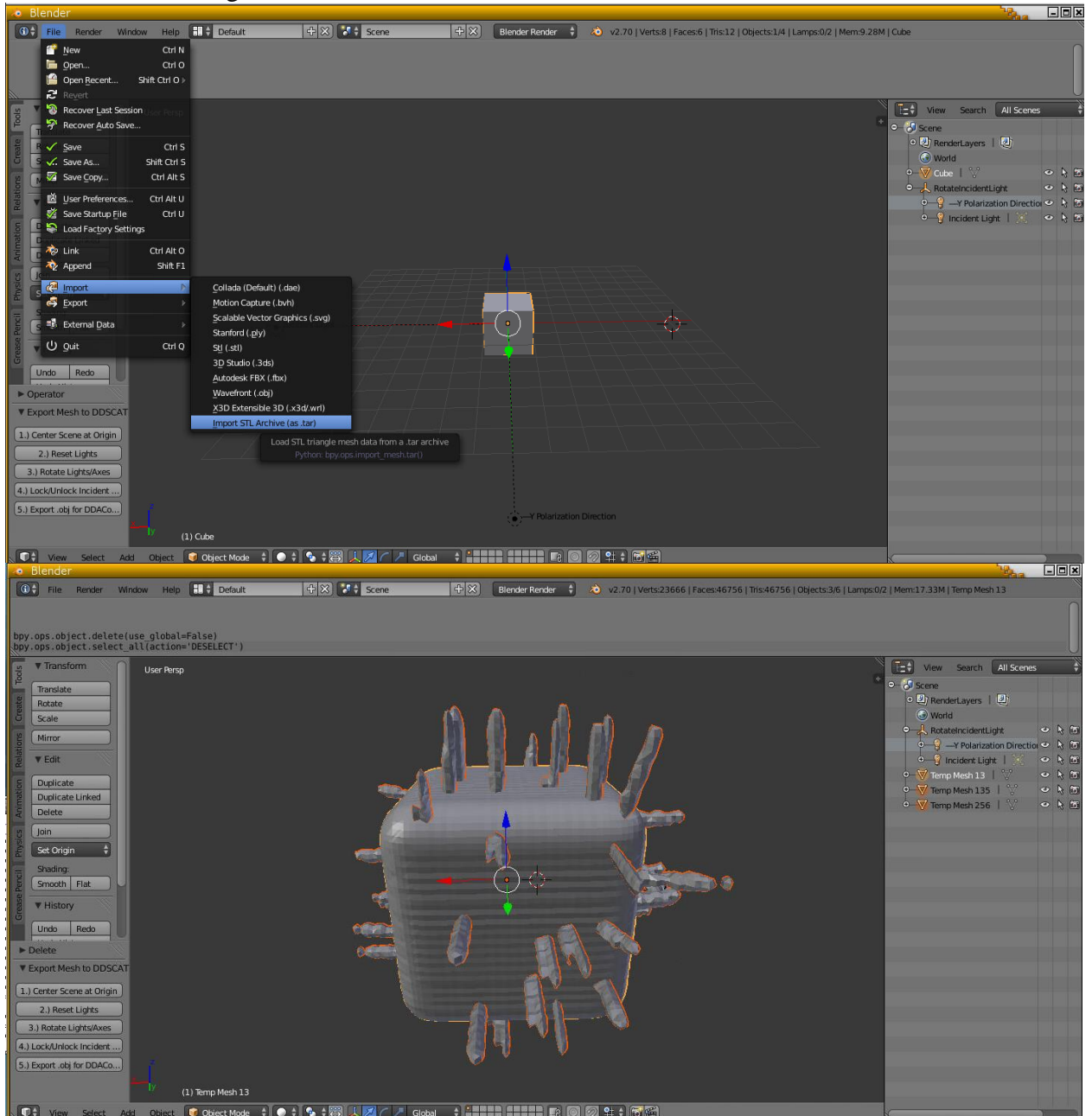


- 3) The STL files are saved as a .TAR archive in order to facilitate downloading all the files at once. This can be downloaded locally through the Upload/Download feature in the Workflow toolbar:



Loading the STL Files into nanoDDSCAT+

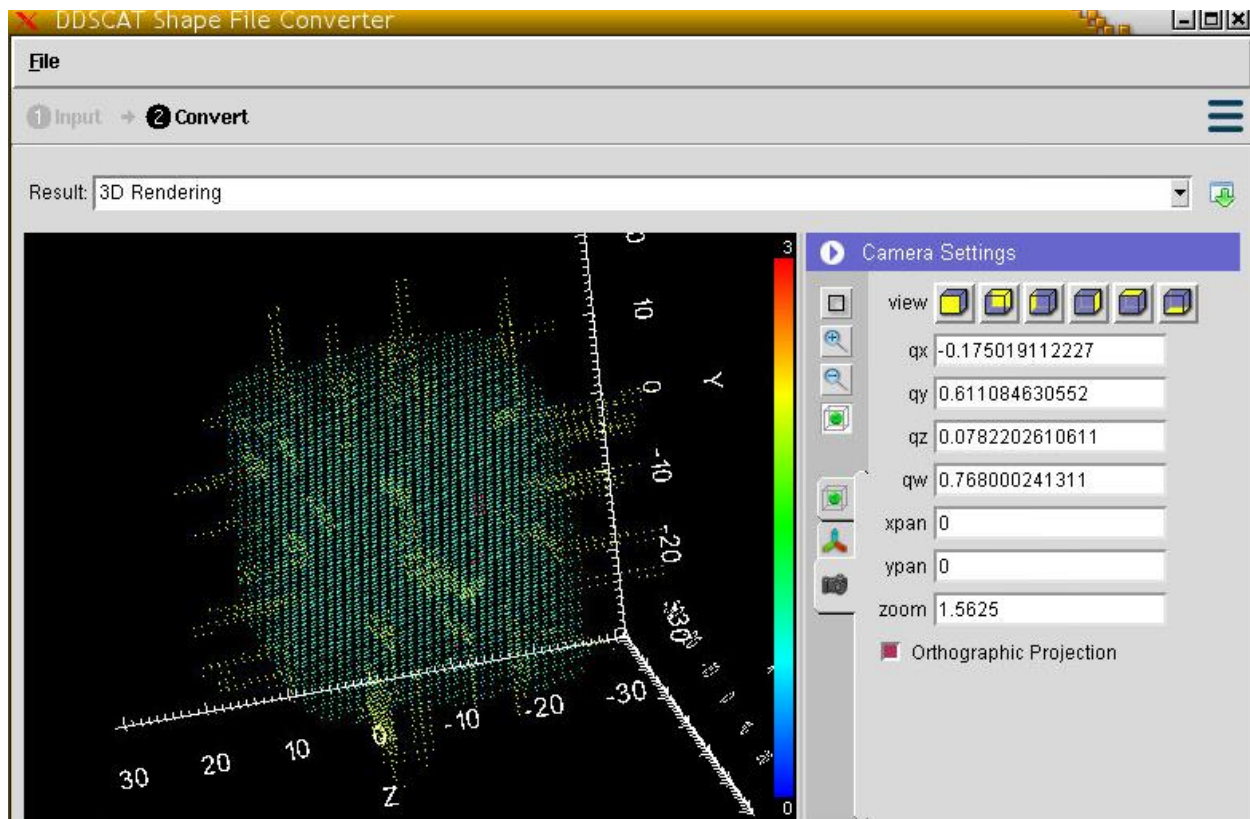
- 1) Upload the .TAR package as-is into a nanoDDSCAT+ session using the Upload/Download button in the Workflow toolbar.
- 2) Open up Blender and under File>Import> select “Import STL Archive (as .tar)”. Then, select to open the .TAR file you uploaded and the volumes should immediately appear in the viewer for editing.



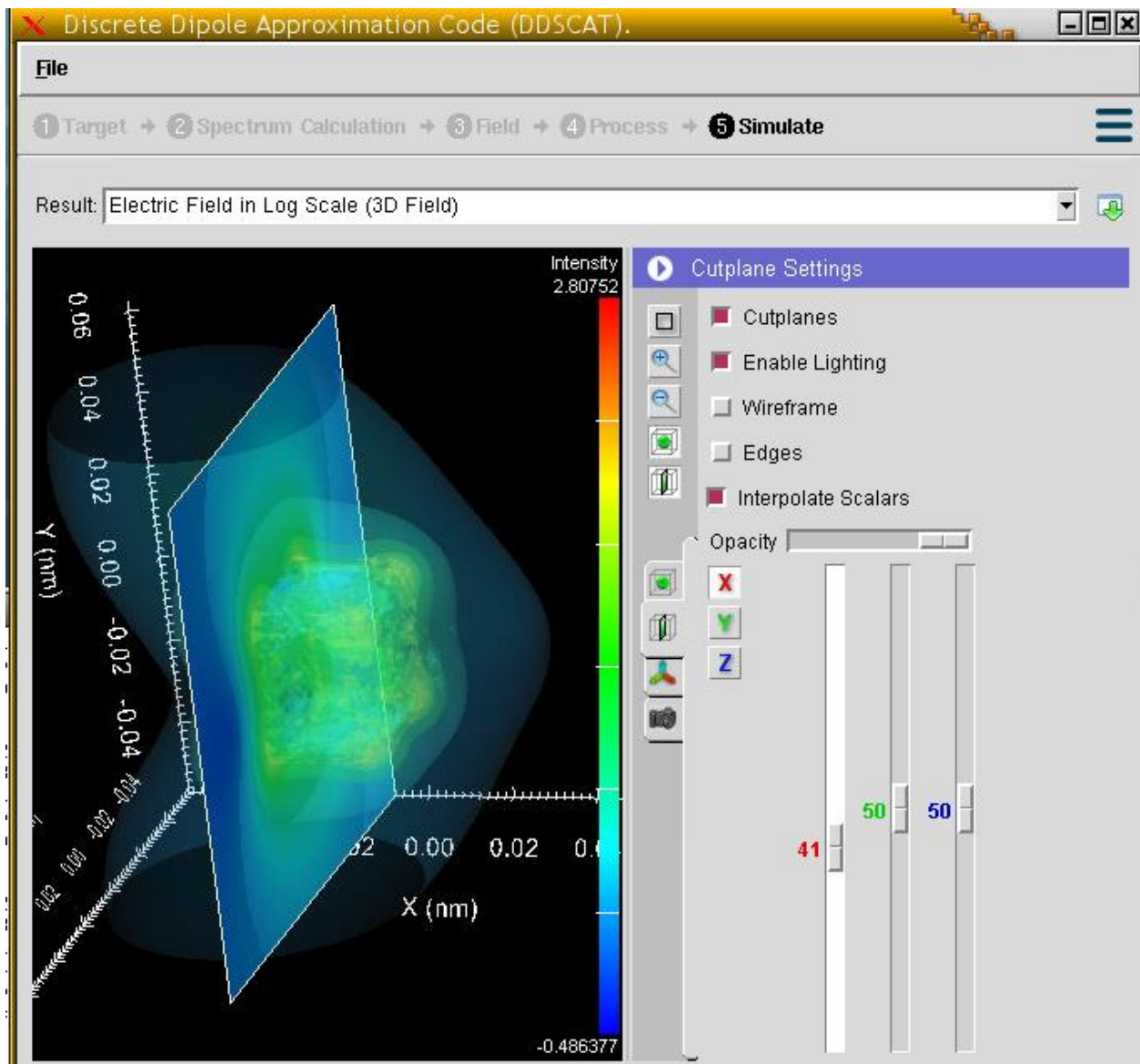
- 3) Continue through the workflow for nanoDDSCAT+ as usual. Every STL volume for each intermediary piece of the functionalized particle from Functionalization Workbench can/will be considered as a separate volume (if this option is selected in DDAConvert).

Note about nanoDDSCAT+ simulation with molecular volumes:

- Refractive indices for the various materials (i.e. PEG) can be found online and approximated as a single value. Input these values using the Constant Dielectric option for each respective shape in nanoDDSCAT. For example, a simple internet search for “average refractive index of Polyethylene Glycol” yields several pages from www.sigmaaldrich.com giving approximate indices of PEG as ranging from 1.460 to 1.467 so here we would likely use 1.4635 as PEG’s refractive index.
- Instead of creating an MD setup with water molecules, one can just set the ambient refractive index in nanoDDSCAT to be 1.33



(Discretization of Functionalized particle as points)



(Electric Field generated by nanoDDSCAT on the discretized model)