

Blender Molecular Visualization Tutorial II

By Björn Sommer, in part based on ePMV Tutorials.
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Blender with ePMV:

<http://epmv.scripps.edu/download-install-free/perhost>

Actual Version of Blender:

<http://www.blender.org>

Preparations

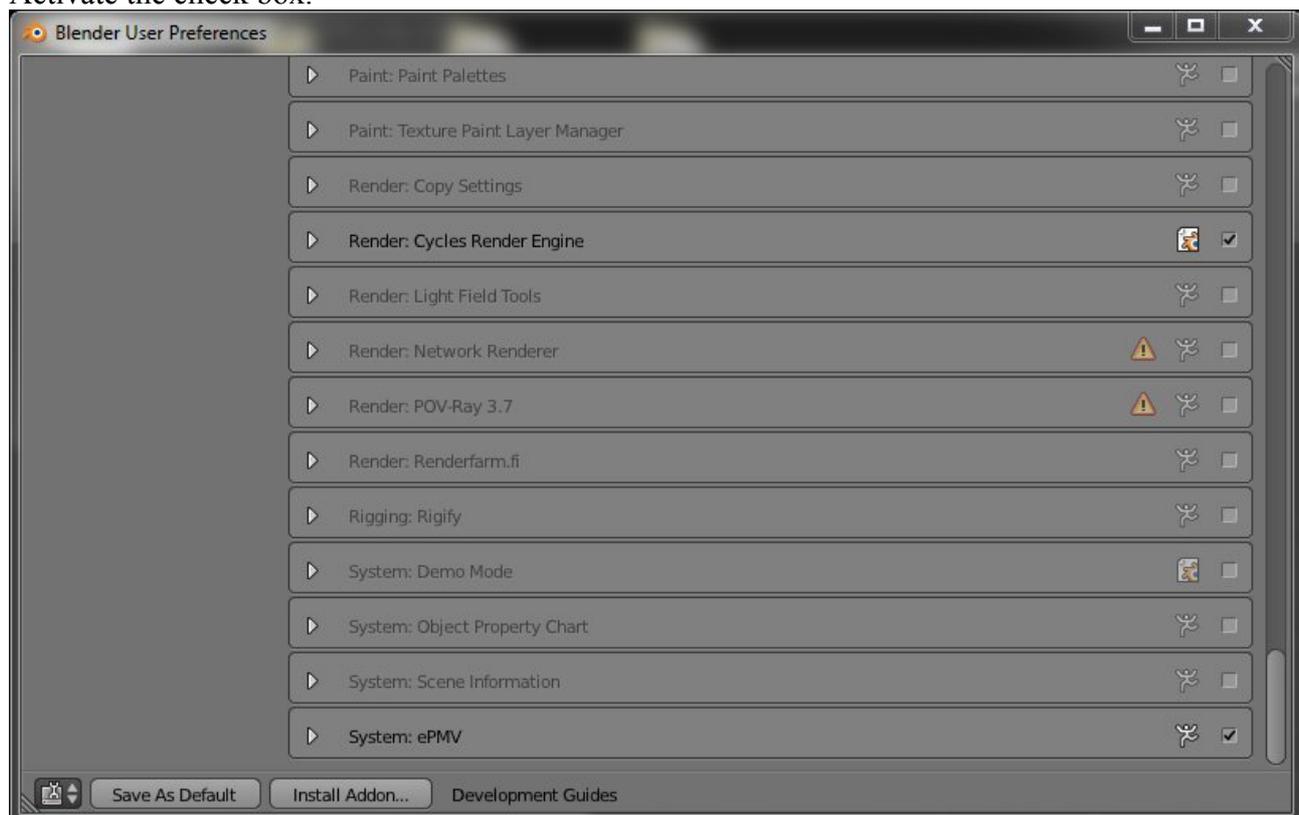
If not already done, download the ePMV-Blender version stated above and start it.

Now the ePMV-Plugin has to be activated. Do this in

File → User Preferences → Addons:

System: ePMV

Activate the check box.



Now you are ready to use ePMV.

ePMV

Press the ePMV-Button  at the end of the Menu row

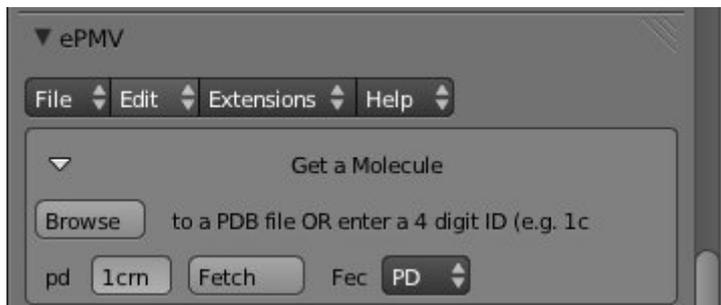


The ePMV menu is shown:



Load and edit a PDB file

1. Just use this dialog to load a file:



2. You can choose a file locally by pressing the "Browse" button or you can directly fetch the file from the PDB database by entering the identifier into the text box and pressing "Fetch"
3. Now you can test a lot of options shown in
 1. Preset Presentations
 2. Backbone Presentations
 3. Surface Presentations (here you can also select Metaballs)
 4. Color by
4. Note:
Not all configurations work with every molecule, but sometimes you just have to wait for a longer time until all atoms are loaded

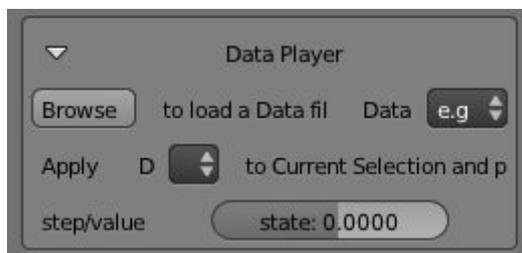
Load and edit a volumetric file

This tutorial is based on:

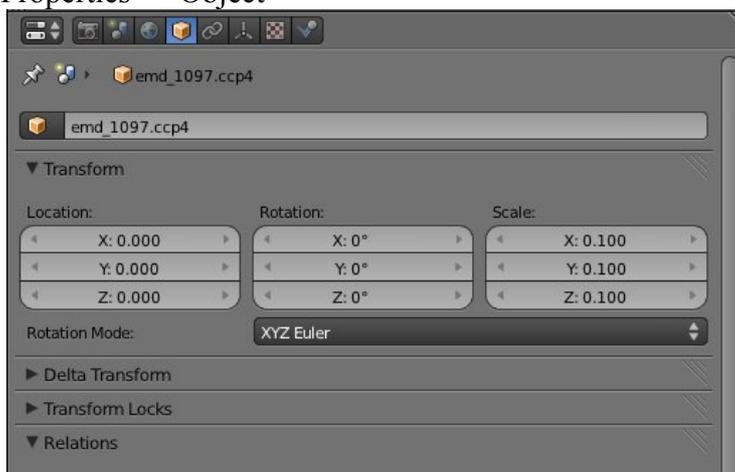
<http://epmv.scripps.edu/documentation/tutorials/written-tutorials/general-epmv-tutorials>

In this case we'll load a *emd_1097.ccp4* of a **Nuclear Pore Complex (NPC)** derived from single-particle Electron Microscopy

1. Visit the [Electron Microscopy Data Base](#)
2. Click *Basic Search*
3. Type *nuclear* into the Title box on the search page and hit the [start search] button
4. Click on entry *1097*
5. Click *Map Information*
6. Click to download then unzip *emd_1097.map.gz*
7. CHANGE *emd_1097.map* to *emd_1097.ccp4* (bug in PMV doesn't recognize the .map tag)
8. Open ePMV
9. Unfold DataPLayer

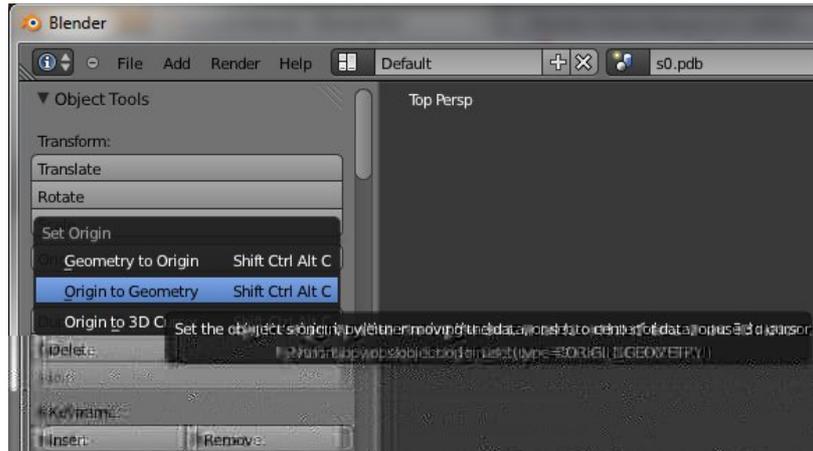


10. In Data Player panel, Browse to your .ccp4 file to load it
11. Since the EMDB file should be formatted with proper headers, the map should load at a correct scale compared to any molecules in the scene (often shockingly large)
 1. It's wise to confirm this scale simply by making a scale bar with a cube that is the length of your EMDB molecule (find dimensions of that molecule with a web search or by asking your content expert)
12. Zoom out to see your nuclear pore complex surface map.
13. You will see now that it is a problem in Blender to show the whole molecule.
 1. Click the Molecule (*emd_1097.ccp4*), e.g. in the Outliner
 2. Go to Properties → Object

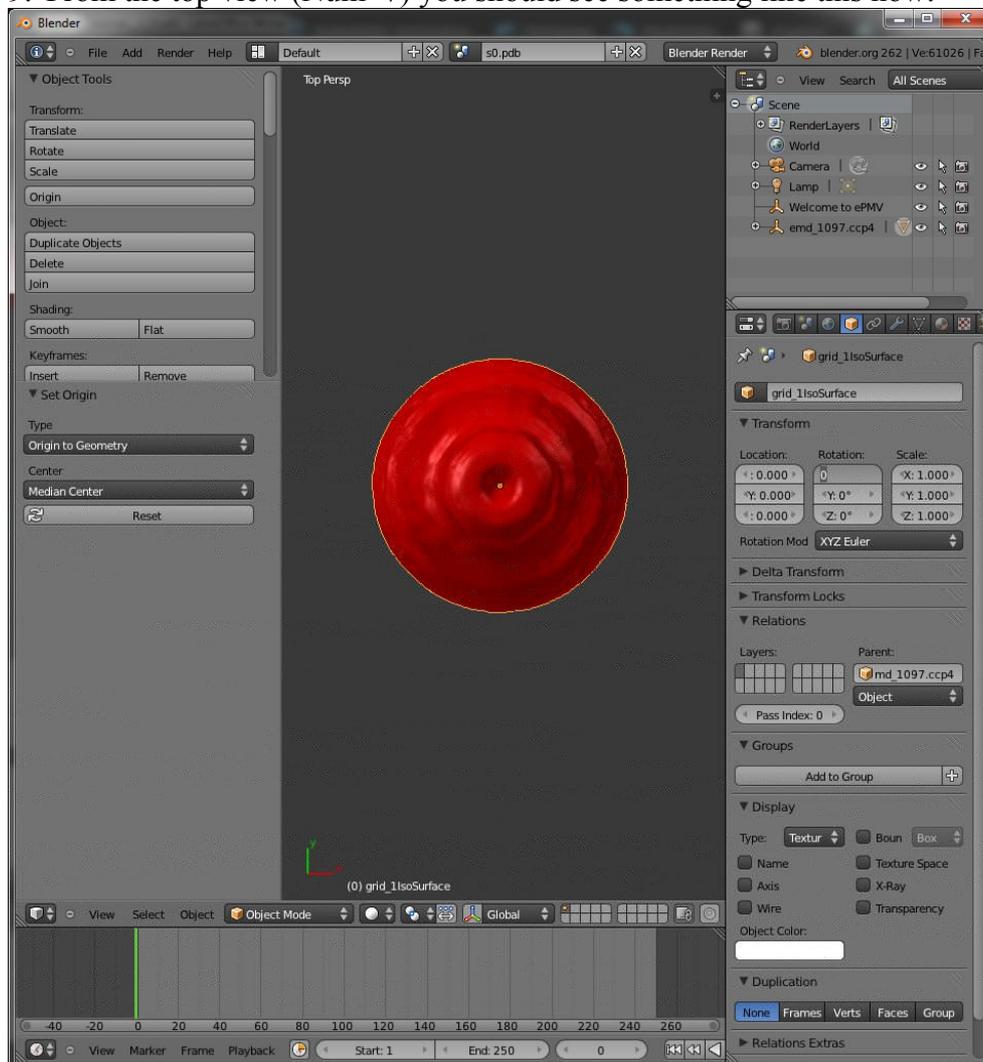


3. Change the scaling of the object from 1 to 0.1
4. There is a problem with the origin of the object. Therefore, it should be centered by using the following options:
5. Go to the Object Tools (usually at the left top)
6. Click "Origin to Geometry"

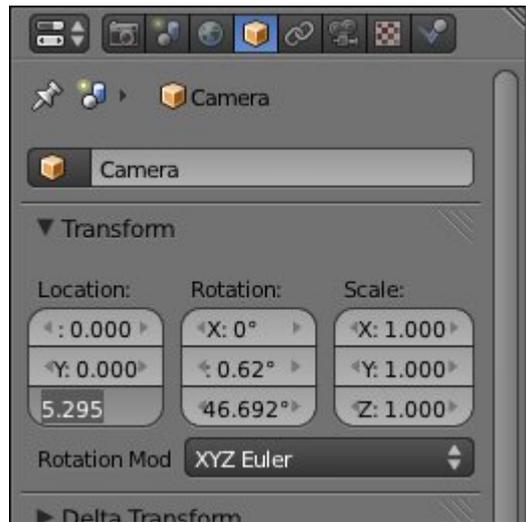
- Now the origin of the molecule has moved into its center and we can align it to the center of the universe



- Now make sure in the previously used Object Rollout that the object is centered at Position (0,0,0)
- From the top view (Num+7) you should see something like this now:



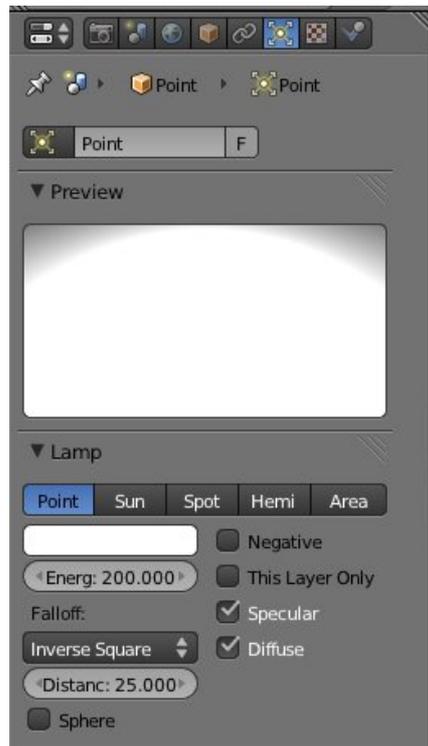
- First, make a rendering (F12). You should see, that the camera position has to be changed and that the light is to dim
- First, change the camera position using the methods you learned in Tutorial 1
- Move the camera for example by using the Object Rollout of the Properties



13. The camera should be positioned to enable the top view of the complete object, e.g. at $Z=300.00$
14. Now the problem will emerge that the object is not shown at all or only a small part of the object
15. Therefore, go to the Object Data menu of the Properties
16. Search there for Lens → Clipping → End
17. Change this setting to 1000

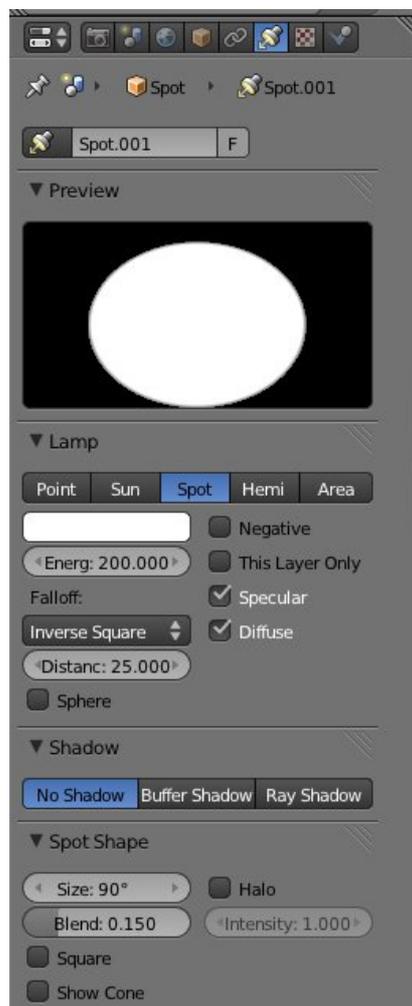


18. Now, the complete object should be shown
19. But if we make a rendering, everything will be dark or dim
20. Now, change the light or create a new one, e.g. a point light
21. Go to Properties → Object Data and change the light intensity to 200

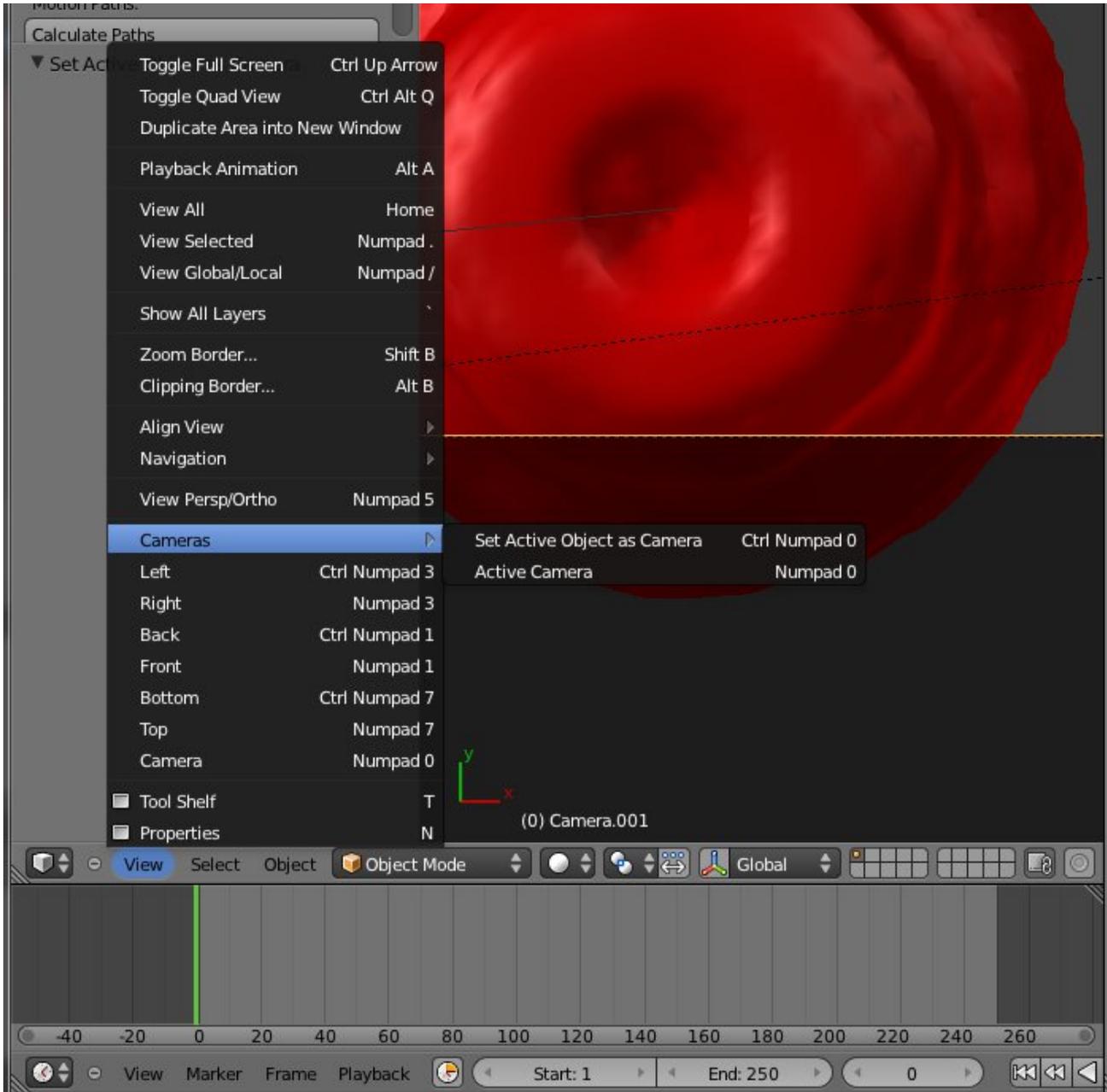


22. change the position of the point light to e.g. (0,0,150)

23. another option is to create a spot at the same position, here the properties are shown (make sure to increase also here the energy and to switch of the shadows to “No Shadow”)



24. Create a second camera and look for an interesting position (do not forget to change the clipping plane as shown before)
25. Keep this camera selected
26. In the 3D View menu bar, go to Cameras → Set Active Object as Camera (`Ctrl Numpad 0`): now the selected camera is rendered and shown each time the user presses NUM+0



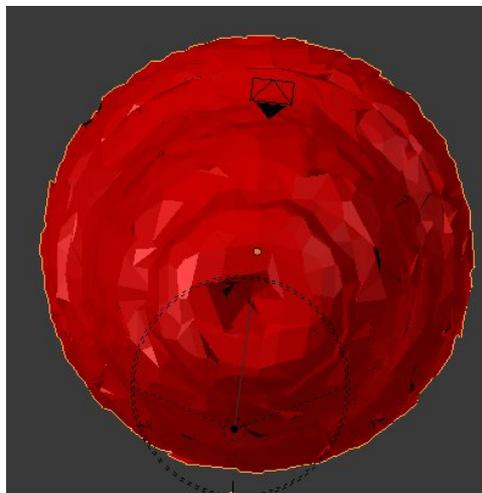
14. You can play around now with this nuclear core complex

Distribute an Object on the Surface of another Object

1. First the Object created in the last tutorial has to be simplified, because it has a quite complex mesh
2. Expand the Object “emd_1097.ccp4” in the Outliner and select the mesh object “grid_1IsoSurface”
3. Go to the Properties → Object Modifiers and add the Modifier “Remesh” and enter an Octree Depth of 5

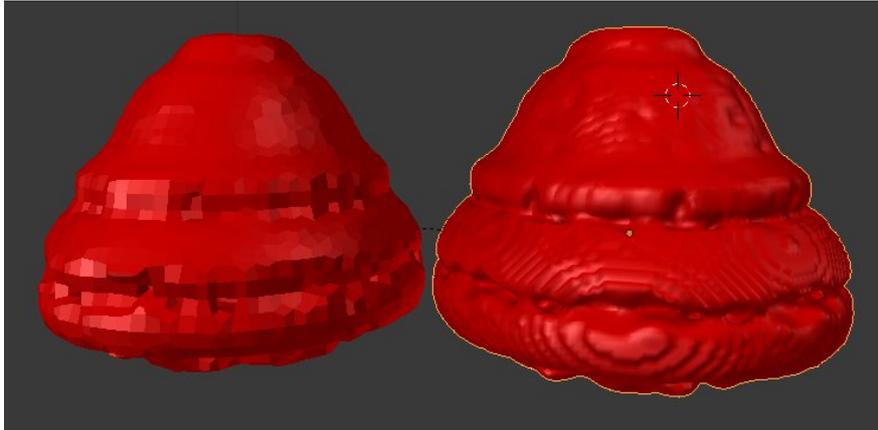


4. the mesh should look like this now:



5. It may be better to choose the Mode “Smooth” in the Remesh Rollout

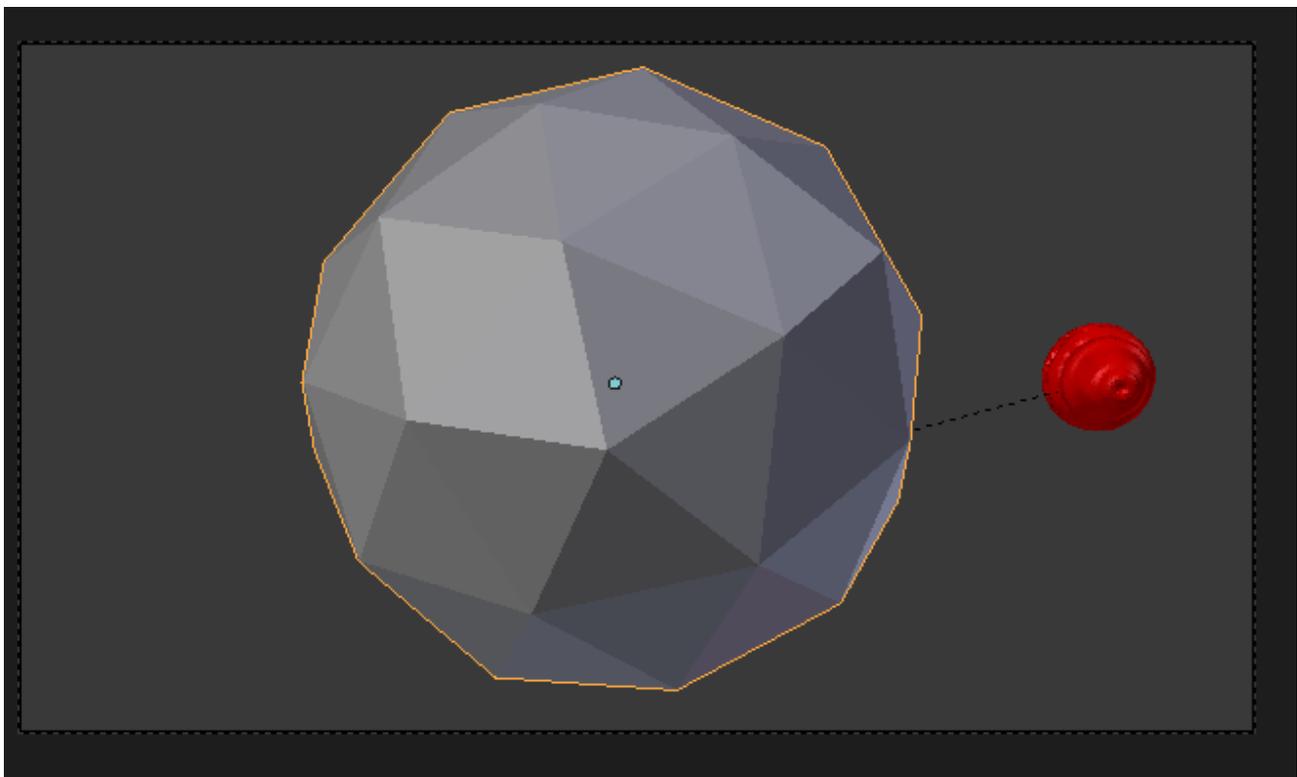
6. You may want to make a copy now by pressing  before making further changes



7. Hide this object afterwards, for rendering as well as for the viewport



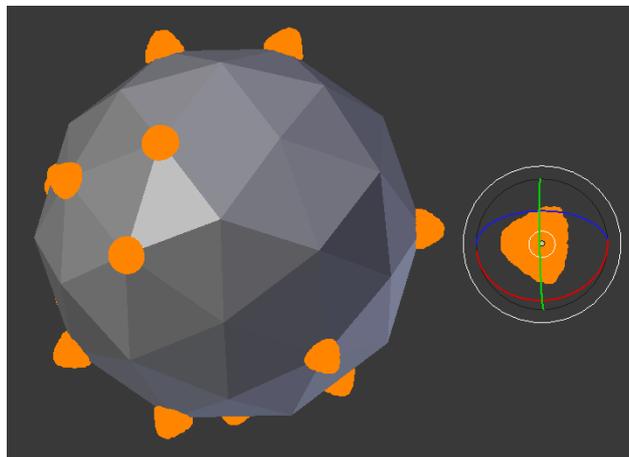
8. Now we re-select our original object, and press “Apply” in the Remesh modifier panel
9. Now the mesh of the object is simplified; this is the object – the Nuclear Pore – we want to distribute on a Sphere, symbolizing the Nucleus
10. Now we create an Mesh → Icosphere, this is the object, on which surface the Nuclear Pore will be distributed
11. Scale this Icosphere to be something like 10 times the size of the pore and use a camera to show the whole scene – the pore should be placed in the neighborhood of the Icosphere



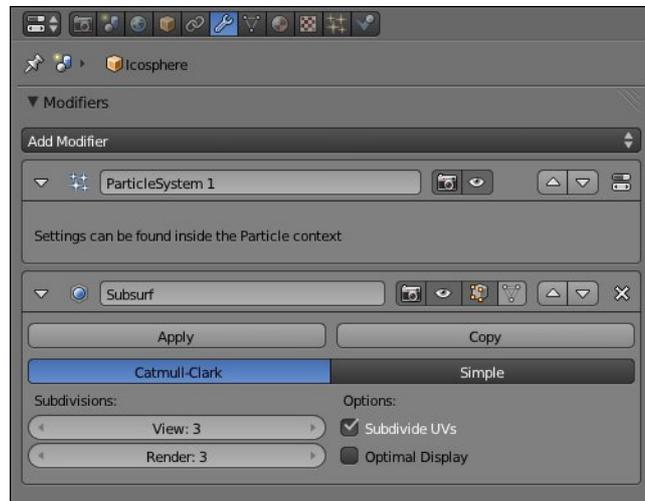
12. Now we need a modifier to distribute the Pore on the Icospheres surface

1. Select the Icosphere
2. In the Properties go to the Particles dialog

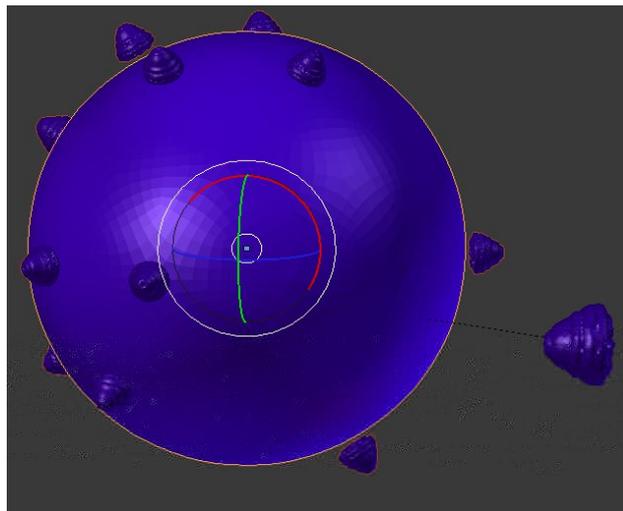
3. Add a new Particle System by pressing “+”
4. The Particle System is quite complex, therefore we have to change some settings, before the final solution is found
5. Select in the Category “Emission”
 1. Number: 20; this will be the number of distributed object shown on the surface of the sphere
 2. Select under “Emit From”: “Verts”
 3. Deselect the check box “Random”
6. Select in the Category “Physics”
 1. “None”, deactivating Physics – we do not need this here
7. Select in the Category “Render”
 1. Parent: Icosphere; yes, this is the distribution object, the Nucleus
 2. Select the Option “Object”
 3. And now select as Dupli Object your Nuclear Pore, something like grid_1 isoSurface
 4. You do not see anything? Yes, you have to activate the check box “Unborn” (because we do not use any real physics-driven system I guess)
 5. Now, you should see 20 Pores distributed on the surface – but those are quite strange: instead pointing towards the inner of the Nucleus, they seem to point somewhere else; we have to correct this
13. We originally selected the parent object for the pore; therefore we have to correct the rotation of this object now
 1. Select the original object; we can not fix this problem by just changing the rotation in Object Mode, because this transformations are not applied to the pore
 2. Change to Edit Mode
 3. Make sure, before selecting the object, that also the backface is taken into account during the selection, by selecting 
 4. As you used to do in Tutorial 1, use CTRL and the left mouse button to select the whole object – make sure everything is selected by rotating the view around the object
 5. Now select the Rotate Mode and change the rotation until the pores on the surface are correctly positioned



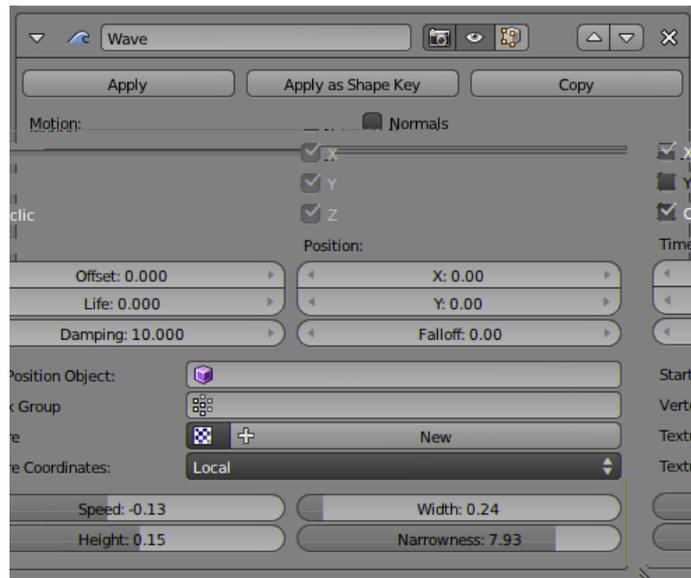
6. The major work is done, so let us put some new maps on the surface of the nucleus as well as the pores – remember, dark blue might be a good option and you can also add multiple textures, e.g. you can combine the texture “Noise” with “Musgrave”
7. But the surface of the Icosphere does not look really organic, so let us add a new Modifier: “Subsurf”, using 3 subdivisions for the surface



8. But now we will have to face a small problem: the Icosphere shrunk, so the pores are flying!



9. Let us solve this problem by returning selecting the original pore, changing again to edit mode by pressing TAB and this time translating the pore along its Y position until the distributed pores are moving into the nucleus
10. Finally, let us add the “Wave” modifier to the Nucleus and play around with it:



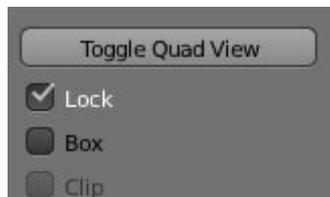
11. Because we modeled a nucleus, let us finish by adding the secondary nucleus wall:
 1. just select the nucleus
 2. be sure you are in Object Mode
 3. Press SHIFT+D
 4. place the duplicate in the middle
 5. go to its modifiers and hide the Particle System completely, because for the inner layer we do not need again the pores: 
 6. change the scale of the inner membrane only a small bit, so that you can see the difference when rendering it
12. We are done!
13. Another option is – not discussed here – is the distribution of objects along a path: <http://blendersushi.blogspot.de/2011/08/grease-scatter-objects-alternative-way.html>

Additional Blender Functions

stores the actual scene as the default scenario; this is started each time is pressed
To lock the camera to a specific object, use the “Lock to Object” Selection from the View Rollout (toggle this Rollout with)



Also in this Rollout, the QuadView can be toggled:



Activate Lock to prevent that the perspective of the three orthogonal view can be changed

Additional Options/Future Topics

Background Mode → start Blender from Command Line

Stereoscopic Script for Blender:

<http://www.noeol.de/s3d/>

Keyframes for Meshes → different from regular Key frames, search for the editor and add “Shape Keys“ (this tutorial section still has to be improved)