

Bio Visualisation with Blender and MembraneEditor Part 3

CELLmicrocosmos MembraneEditor

Konstanz Research School Chemical Biology (KoRS-CB) Workshop
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Forum:

<http://www.cellmicrocosmos.org/Cmforum/viewforum.php?f=63>

Actual Version of CELLmicrocosmos 2.2 MembraneEditor:

<http://Cm2.CELLmicrocosmos.org>

Target

This tutorial describes how create molecular membrane models with the CELLmicrocosmos 2.2 MembraneEditor.

Abbreviation

RMB Right Mouse Button

LMB Left Mouse Button

*! For using most of the shortcuts discussed in this tutorial, you have to be sure that the mouse cursor is **WITHIN** the view port of the 3D View !*

MembraneEditor

First make sure that you have installed the latest version of Java on your PC.

<http://java.com>

If you are using a 64 bit PC, make sure that you are also installing the 64 bit version of Java providing a much better performance than Java 32 bit! If you are using a Linux system, also the Open Java projects should work with the MembraneEditor, so you do not need the original Sun/Oracle Java.

Then, download and start the MembraneEditor from this website:

<http://Cm2.CELLmicrocosmos.org>

There are three options:

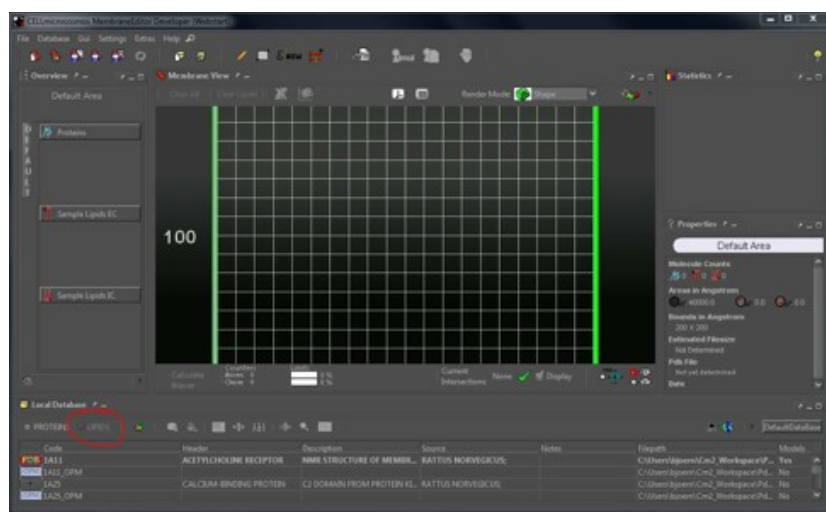
You can install the MembraneEditor via Java Webstart or download the self-executable Java file:

<http://www.cellmicrocosmos.org/index.php/start/startcm2>

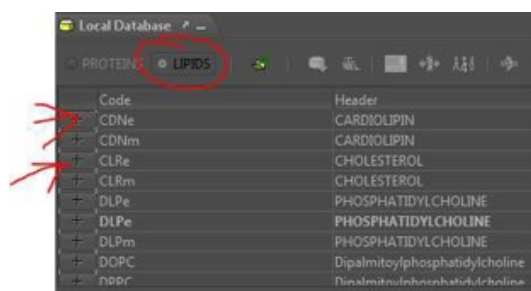
If you know how to handle Java development environments like Eclipse, the source code can be downloaded here:

<http://www.cellmicrocosmos.org/index.php/download/downloadcm2>

After the program is started you should see something like this:

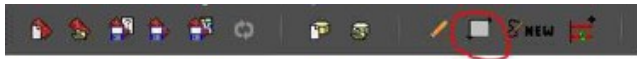


Click now on the following button “Lipids”:



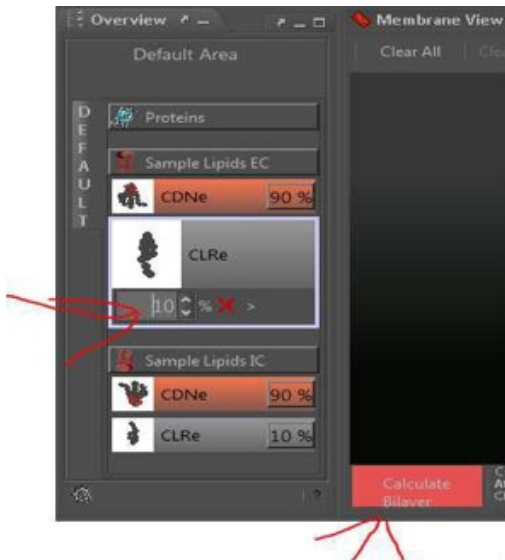
Here, the library with lipids is shown. Just press on the two buttons indicated by the arrows and add the lipids CDNe (Cardiolipin lipid) and CLRe (Cholesterol lipid) by selecting EC/IC (which means extracellular and intracellular side).

Before we continue, let us decrease the size of the membrane. At the moment, it is 200 x 200Ångström. So let us change it to 100 x 100Ångström. For this purpose, select this button:

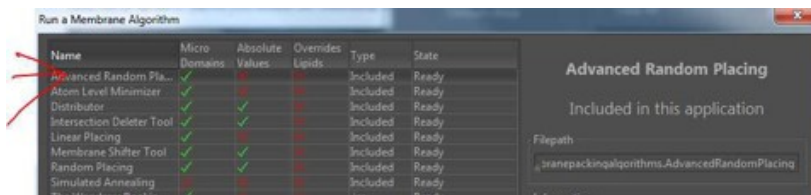


and change the size to 100 x100 in the following dialog and press “Accept”.

Before we start to generate the membrane, let us change the lipid distribution of the MembraneEditor to 90% CDNe to 10% CLRe:

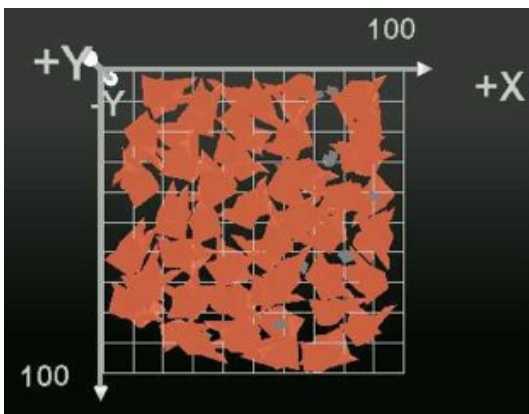


Now, let us generate the membrane by starting a Lipid Packing Algorithm. Click the big red button: Select the algorithm called “Advanced Random Placing”:

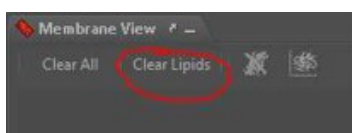




The following dialog appears. You may want to play around with the values. But you can also just click “OK” to start the algorithm.

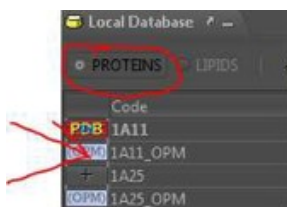


The result will be something like this:



Just a remark: if you are not satisfied with the result, you can just remove all lipids by clicking:

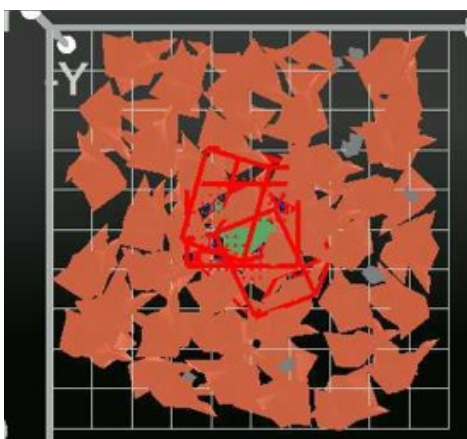
and then restart the algorithm.



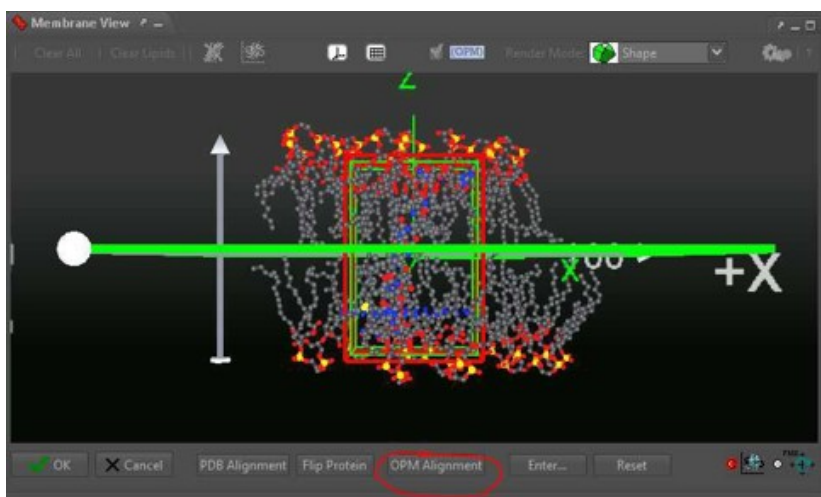
Now we have the lipids, just let us add a small protein. This time, select “Proteins” in the Local Database:

Choose the protein 1A11_OPM and place it into the membrane. You can just click on the OPM symbol, the protein is placed somewhere in the Membrane View, or you keep the button pressed on the OPM symbol until the Drag'n'Drop symbol appears and then you place it into the membrane.

Now, the protein is placed into the membrane:

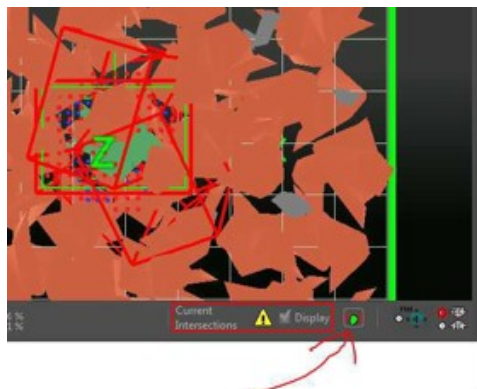


If you perform a RM onto the protein in the Membrane View and select “Align Molecule”, the following window appears:



Here, you see the atomic structures of the PDB files which are hidden in the regular view of the MembraneEditor. Make sure the OPM layers, indicated by a red layer on the top and a blue layer on the bottom, are placed like shown in the screen shot. If this is not the case, press the “OPM Alignment” button. Then click “okay”.

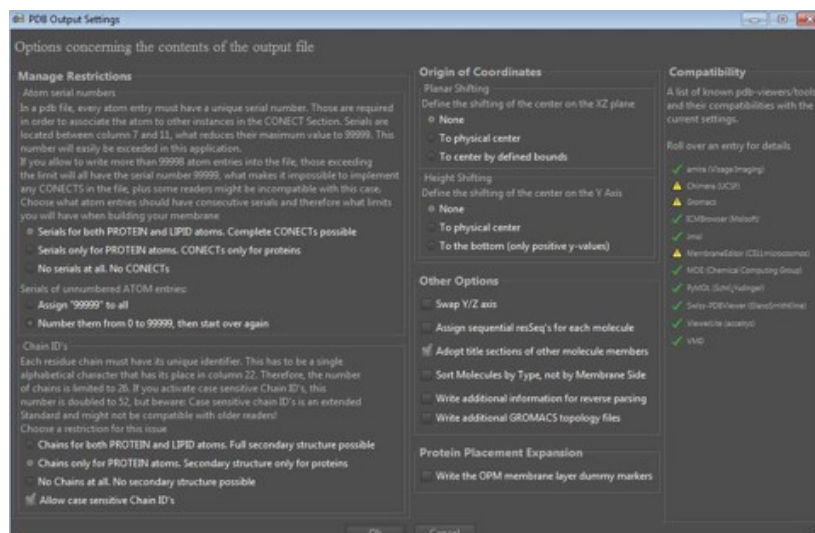
To remove now the intersections between the protein and the lipids, press this button:




Our membrane system is finished. Now, we need to export it to PDB. By clicking this symbol:



The following window appears:



Here, you can change a number of output settings for the PDB file which will be generated. If you want to use in the future different programs to import the PDB format, keep in mind that you can change here a lot of settings to change the compatibility.

The MembraneEditor comes with a very good documentation, just press “F1” to show it or press the button  to go directly to the page discussing the current topic.

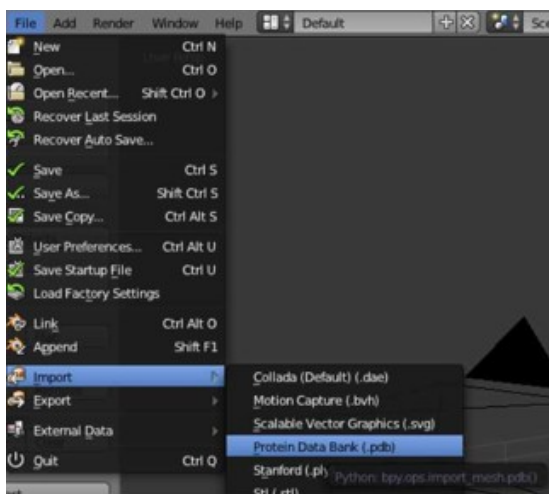
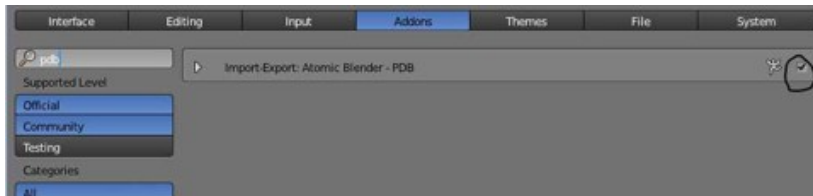


Now, two buttons are important. To preview the membrane in Jmol, just click this button
To export the PDB file, click this button. Do it, we will use this file in the next chapter.

Atomic Blender: The Standard PDB Importer for Blender

Now, we want to import the PDB file into Blender. For this purpose, Blender comes with a special plug-in which has to be activated.

Activate it
here: Atomic
Blender



Select now File → Import → Protein Data Bank (.pdb)

Okay, guess now which PDB file you will import? Yes, take the one from the MembraneEditor. In addition, in the appearing window you will see a lot of options, but use the basic options now:

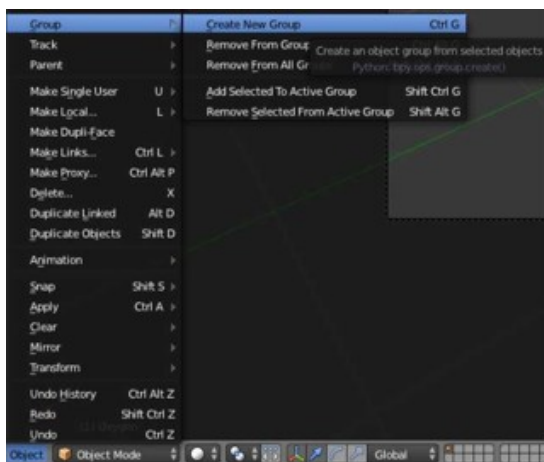


You will see now that Blender will need some time to import this structure. So if you generated the 100 x 100 membrane, it is a good idea to do it on a fast computer, such as an i7 with 8 GB Ram. If you find out that your computer is not fast enough, just generate a smaller membrane, let

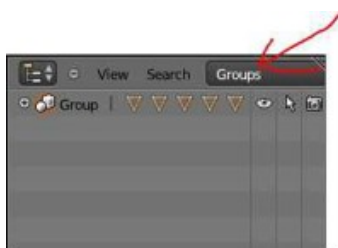
us say 50 x 50. This should solve the problem.

Directly after importing the structure it is a good idea to scale the membrane done to a size fitting to your environment. Just press “S” and scale it down.

In the Outliner, you see the different parts of the molecule. It might be a good idea to group them, so that it is no problem to select the whole molecule with one click. Select all segments part of the membrane by holding shift and LM all segment parts:



Then select Object → Group → Create New Group



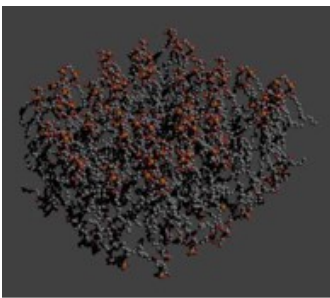
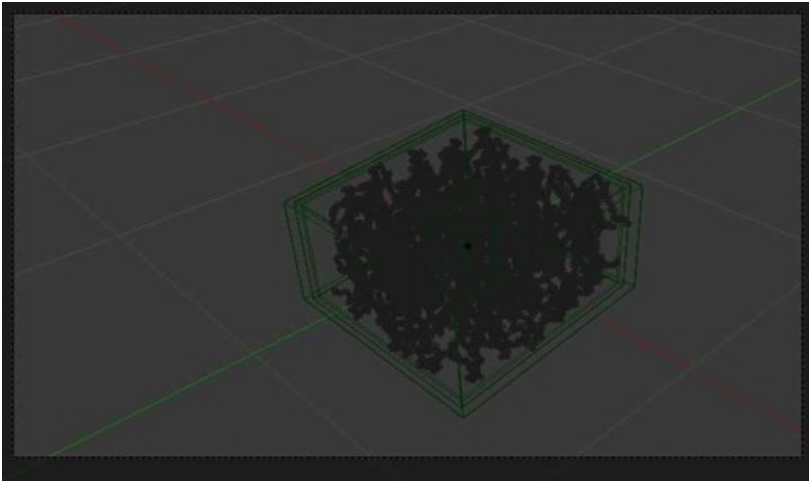
If you select now “Groups” in the Outliner:

You can select the whole membrane with one click.



Because the visualization of this many spheres needs a lot of performance, it would be a good idea to switch to Bounding Box mode.

It will look like this and the navigation will be much faster.



Now, do the rendering by pressing F12.

In the previous tutorials you have learnt a lot of ways to improve the visualization, do it, if you want to make a good visualization.