CELLmicrocosmos

The Vesicle Builder -
A Plugin for the CELLmicrocosmos MembraneEditor

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Background

The CELLmicrocosmos 2.2 MembraneEditor (CmME) is a Java Webstart software developed to solve heterogeneous Membrane Packing Problems [SDG+11]. It was originally designed to conveniently generate rectangular membrane structures in PDB format [BWF+00]. These membranes are especially needed for *in silico* experiments with molecular simulation software like Gromacs [HKV+08]. CmME supports the generation of microdomains as well as the integration of multiple layers.

It features an algorithm-plugin-interface which can be used to generate custom algorithms. This interface was the basis for the development of the first version of the Vesicle Builder, enabling the creation of ellipsoid heterogeneous single-/double-layered membranes.

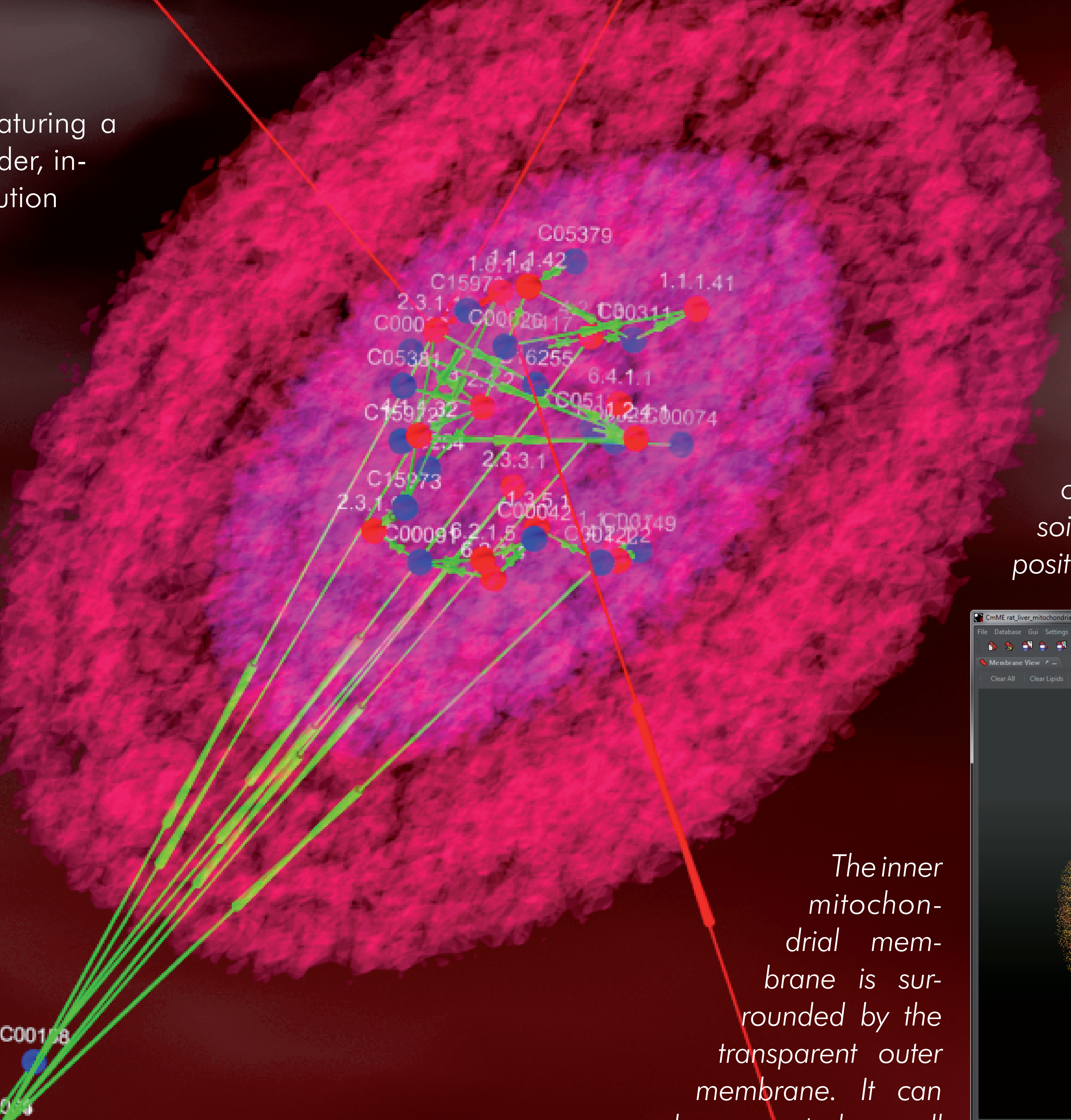
Application Case

A simple double-layered mitochondrion model featuring a length of 0,05 μm was created with the Vesicle Builder, including two bilayers based on published lipid distribution values [SDG+11].

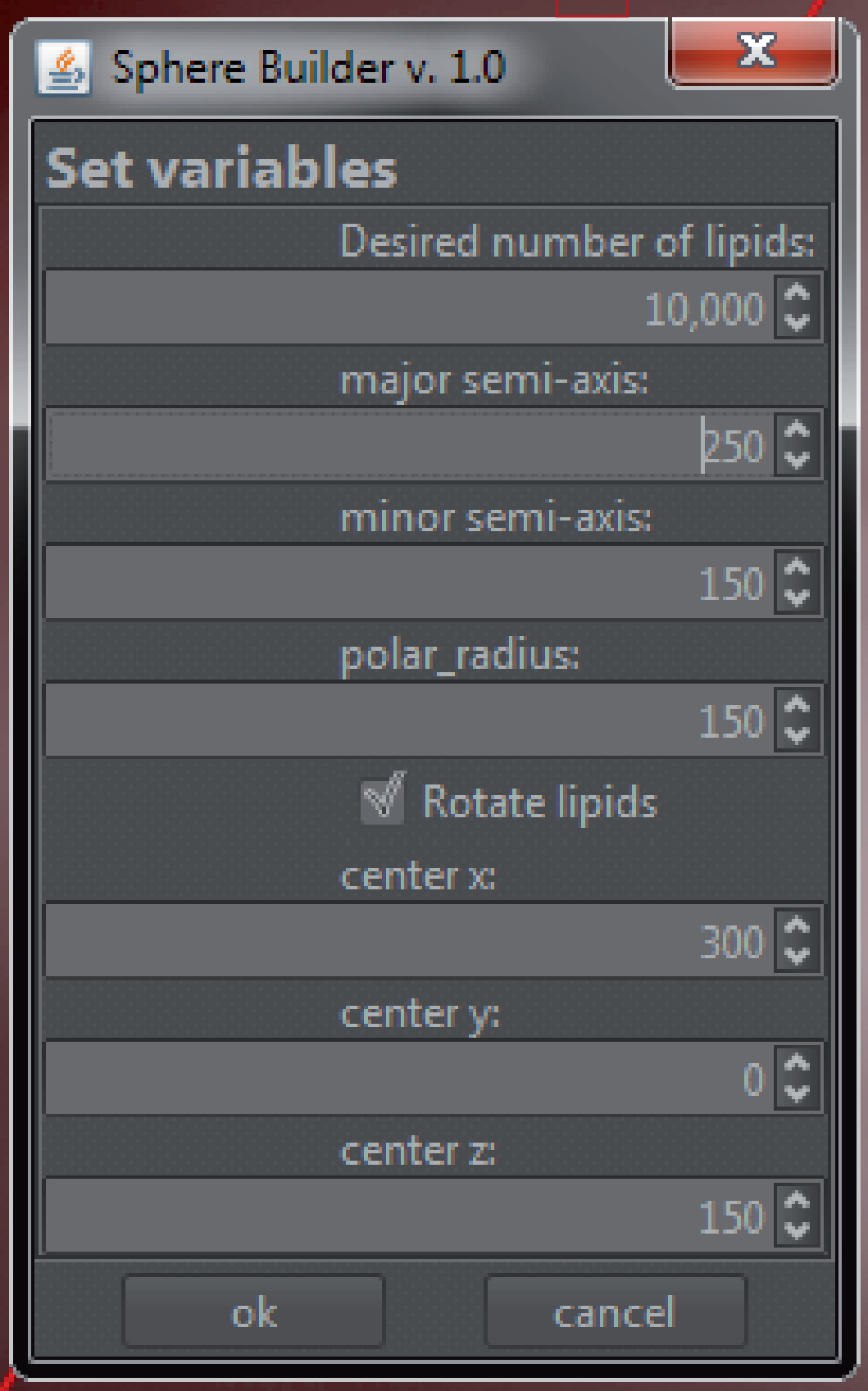
The generated structures were exported to PDB and directly visualized with Jmol [J12], which was then used to generate the Van-der-Waals-Surface and to export the three-dimensional mesh to VRML97.

This model was prepared for the CELLmicrocosmos 4.2 PathwayIntegration (CmPI) where it was integrated into a virtual cell and correlated with the Citrate Cycle (hsa00020) and the Glycolysis from KEGG [KGS+12].

This model was exported by CmPI to VRML97 and rendered with Autodesk® 3ds Max®.

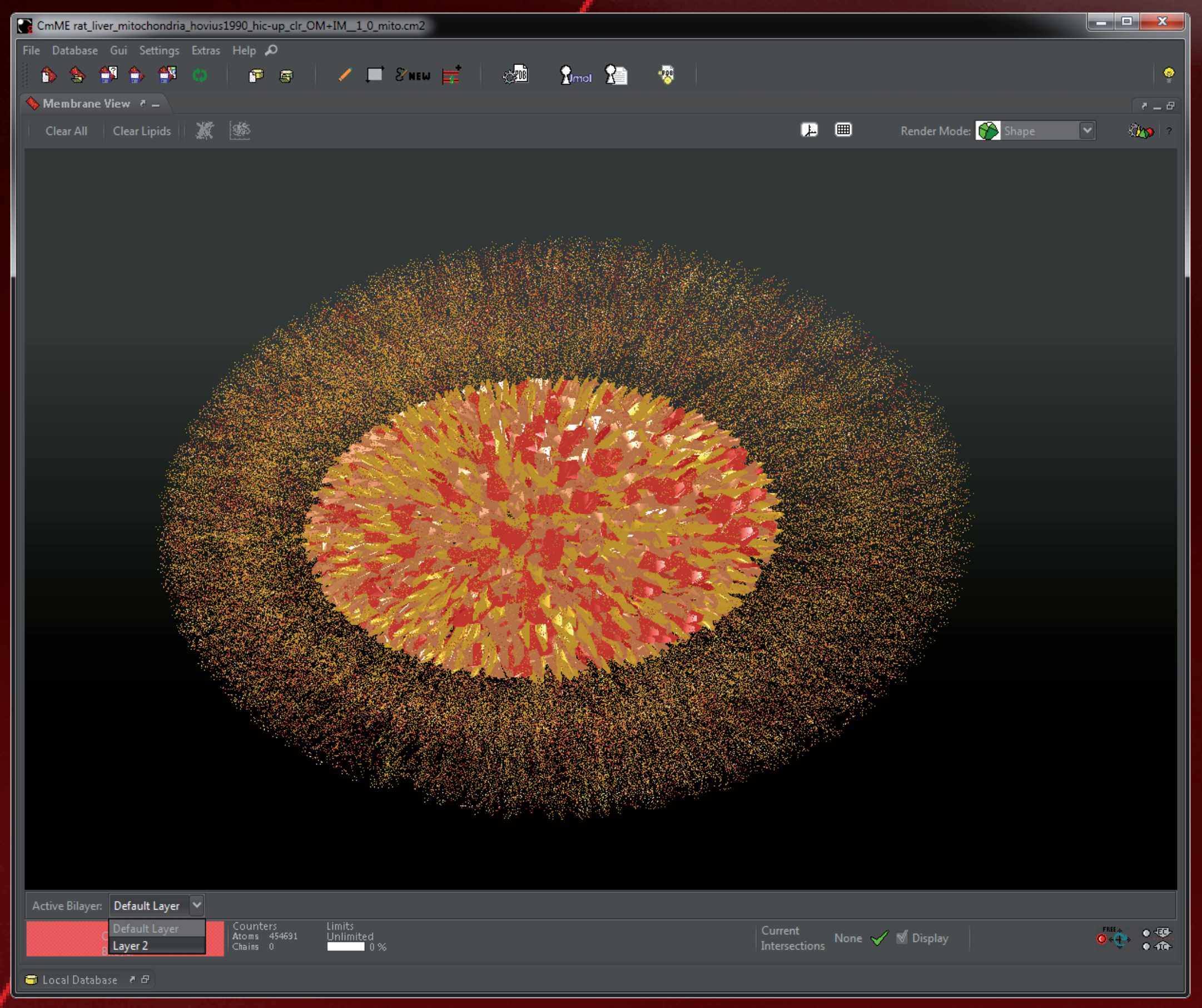


Based on the CmME-Plugin-Interface, the new Vesicle Builder version 1.0 was created, independently from the original source code.



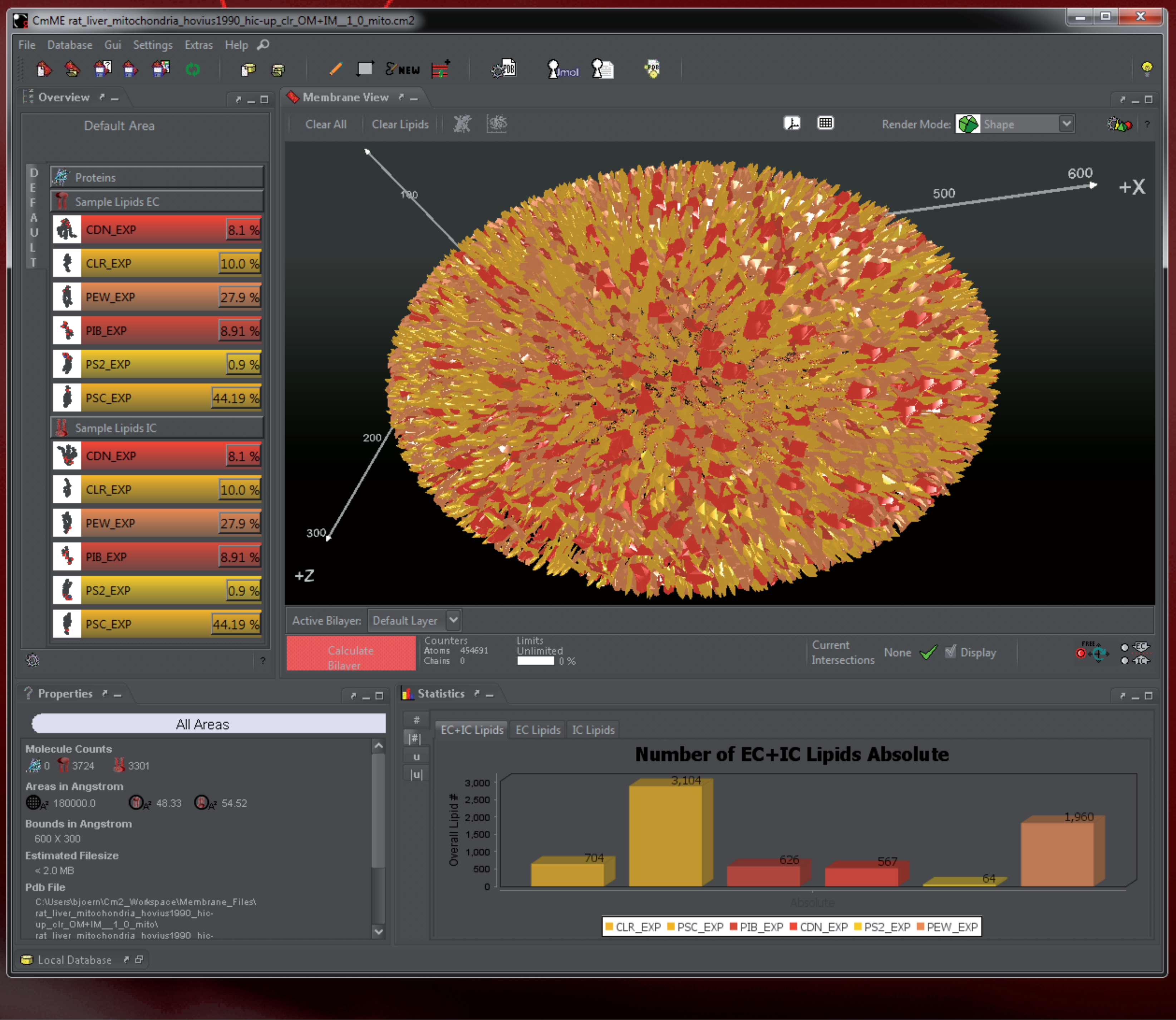
Desired number of lipids: 10,000
major semi-axis: 250
minor semi-axis: 150
polar_radius: 150
☑ Rotate lipids
center x: 300
center y: 0
center z: 150

This image shows the GUI of the Vesicle Builder which can be used to change the ellipsoid shape and the position of the vesicle.



Counters Atoms 454691 Chains 0
Limits Unlimited 0 %
Current Intersections None ✓ ☑ Display

The inner mitochondrial membrane is surrounded by the transparent outer membrane. It can be generated as well as edited independently.



Sample Lipids EC		Sample Lipids IC	
CDN_EXP	8.1 %	CDN_EXP	8.1 %
CLR_EXP	10.0 %	CLR_EXP	10.0 %
PEW_EXP	27.9 %	PEW_EXP	27.9 %
PIB_EXP	8.91 %	PIB_EXP	8.91 %
PS2_EXP	0.9 %	PS2_EXP	0.9 %
PSC_EXP	44.19 %	PSC_EXP	44.19 %

Active Bilayer: Default Layer
Counters Atoms 454691 Chains 0
Limits Unlimited 0 %
Current Intersections None ✓ ☑ Display

Molecule Counts: 0 3724 3301
Areas in Angstrom: 180000.0 48.33 54.52
Bounds in Angstrom: 600 X 300
Estimated Filesize: < 2.0 MB
Pdb File: C:\Users\bjoern\Cm2_Workspace\Membrane_Files\rat_liver_mitochondria_hovius1990_hic-up_clr_OM+IM__1_0_mito\rat_liver_mitochondria_hovius1990_hic-

The percental distribution can be defined prior to membrane generation. The statistics show the accuracy of the resulting membrane distribution. The shape-based visualization enables the modeling of large membranes.

Java Webstart

Cm2.CELLmicrocosmos.org

References

[BWF+00] Berman H M, Westbrook J, Feng Z, Gilliland G, Bhat T N, Weissig H, Shindyalov I N, Bourne P E: The Protein Data Bank. *Nucleic Acids Res.* 28:235–242, 2000. | [HKV+08] Hess B, Kutzner C, van der Spoel D, Lindahl E: GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. *J. Chem. Theory Comput.* 4:435-47, 2008. | Jmol: An Open-source Java Viewer for Chemical Structures in 3D. *http://jmol.sourceforge.net*, 2012. | [KGS+12] Kanehisa M, Goto S, Sato Y, Furumichi M, Tanabe M: KEGG for Integration and Interpretation of Large-scale Molecular Data Sets. *Nucleic Acids Res.* 40:D109–D114, 2012. | [SDG+11] Sommer B, Dingersen T, Gamroth C, Schneider SE, Rubert S, Krüger J, Dietz K-J: CELLmicrocosmos 2.2 MembraneEditor: A Modular Interactive Shape-Based Software Approach To Solve Heterogeneous Membrane Packing Problems. *J. Chem. Inf. Model.* 5:1165–1182, 2011.