CELLmicrocosmos 2.2 MembraneEditor – Modeling Membranes for MD Simulations

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The CELLmicrocosmos 2.2 MembraneEditor (CmME) is a freely available software tool which enables the fast and easy modeling of heterogeneous biological membranes. It is based on the PDB format and uses a shape-based approach to distribute lipids along a two-dimensional plane. The theoretical description was presented as the 2.5-D Knapsack Packing Problem [1]. The membrane generation is supported by different lipid packing algorithms optimized for special application cases. CmME supports the semi-automatic placement of proteins based on PDBTM and OPM [2,3] as well as the use of custom PDB files. The generation of stacked membrane bi-layers or mono-layers is possible as well as the definition of microdomains.

Currently we are developing a plugin providing an interface between the MembraneEditor and GROMACS [4]. This interface should simplify the first steps into the field of molecular dynamic simulations (MD). The GMX-Plugin is able to connect CmME via ssh to a computer cluster and run the MD simulation with GROMACS, using the starting structure from CmME [5]. Different all atom and coarse-grained membrane simulations are currently being analyzed.

In addition, we are currently working on a plugin solving three-dimensional packing problems, which enables the generation of ellipsoid vesicles.

The alpha version of the Vesicle Builder, the source code of the MembraneEditor as well as its Java WebStart application are located at:

http://Cm2.CELLmicrocosmos.org

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