CELLmicrocosmos – Membrane Modeling at the Molecular and Mesoscopic Level

Björn Sommer

Bio-/Medical Informatics Department, Bielefeld University, Bielefeld, Germany

bjoern@CELLmicrocosmos.org

The modeling of biological cells is an extremely complex and eclectic topic. Various cell modeling approaches exist. For example, it is possible to compute and simulate intracellular molecular interactions and – on the other side – to generate cell models based on microscopic images.

The combination of both approaches is a complex task for different reasons. One problem is the large variance in scale. Molecular Dynamic simulations (MD) usually operate on scales of a few Ångstrom, while the modeling of microscopy-based cell components takes scales of a hundreds to thousands of Nanometers into account.

CELLmicrocosmos introduces an Integrative Bioinformatics approach bridging the gap between molecular and mesoscopic modeling and visualization.

The CELLmicrocosmos 2.2 MembraneEditor (CmME) is a freely available software tool to model complex heterogeneous membranes based on the PDB format [1]. The membranes can be exported and used in conjunction with external MD packages like GROMACS [2]. CmME is a Java Web Start Application which can be downloaded from

http://Cm2.CELLmicrocosmos.org

CmME represents the molecular level, whereas the CELLmicrocosmos 1.1 CellExplorer (CmCX) operates on the mesoscopic level. It can be used to model abstract shape-based cell models or to import microscopy-based cell component structures, which could be acquired from the Cell-Centered Database [3]. The interactive cell environment can be used for educational as well as scientific purposes [4]. Potential future objectives and current developments of this work will be discussed.

Information about the team behind the different software tools can be found at

http://team.CELLmicrocosmos.org

[1] B. Sommer, T. Dingersen, C. Gamroth, S. Schneider, S. Rubert, J. Krüger, K.-J. Dietz, *J Chem Inf Model*, **2011**, *51*, 1165-1182.

[2] B. Hess, C. Kutzner, D. van der Spoel, E. Lindahl, *J Chem Theory Comput*, **2008**, *4*, 435-447.

[3] M. E. Martone, A. Gupta, M. Wong, X. Qian, G. Sosinsky, B. Ludäscher, M. H. Ellisman, *J. Struct. Biol.,* **2002**, *138*, 145–155.

[4] B. Sommer, J. Künsemöller, N. Sand, A. Husemann, M. Rumming, B. Kormeier, *BIOINFORMATICS 2010 – Proceedings of the 1st International Conference on Bioinformatics, Part of the 3rd International Joint Conference on Biomedical Engineering Systems and Technologies (BIOSTEC 2010)*, **2010**, 90–95.