Background: Only a few programs support membrane computation and/or modeling. They enable the user to create very simple structured membrane layers and usually assume a high level of knowledge. Much work need to be invested, before the sophisticated work dealing with algorithms can begin. The CELLmicrocosmos 2 project develops a tool providing a user-optimized, modular and scalable concept for the computation of membrane (bi-)layers: The MembraneEditor (CmME).

Results: To accelerate the membrane generation process, the computation is geometry-based, supporting fast to more complex membrane generations. CmME is based on the integration of two different types of PDB [1] models: Lipid models, provided for example by the HIC-UP database [2], are integrated with editable percental distribution values and algorithms. Proteins are inserted and aligned manually into the bilayer by a user interface. The resulting membrane is exported in PDB format. Compatibility with other programs is provided by extensive export settings. High lipid densities are possible through advanced packing algorithms. A Plugin-Interface supports the development of applied distribution algorithms.

Conclusions: CmME has been extended and tested to meet the requirements of different PDB visualization programs as well as molecular dynamics (MD) simulation environments like Gromacs [3]. The documentation and a Java Webstart version, requiring only an internet connection and Java 6, are accessible at:

http://Cm2.CELLmicrocosmos.org

Workshop: The workshop will focus at different application areas:
- How to model and visualize different Membrane Compositions.
- How to choose the appropriate algorithm.
- How to generate MD compatible membranes.
- How to develop own algorithms using the Plugin-Interface.

Outlook: The support of multilayers, an automatization process for protein placement and access to the atomic level for the membrane algorithms will be integrated to meet the advanced requirements of the simulation community. In the near future, exported membranes additionally could be integrated into virtual cell environments.

References: