CELLmicrocosmos X

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1   Introduction

The CELLmicrocosmos project represents a prototype of a static virtual cell environment combining different cytological levels. Ten years of development, starting from an initial cell animation, leading over a first educational interactive prototype, proceeding with a number of cell modeling projects. Today, approaches have been presented at the molecular, mesoscopic as well as functional level [1].

Integrative Bioinformatics combines different computer technology-related research areas to support life science research. Here, a major vision of bioinformatics is addressed: the creation of a virtual cell. The CELLmicrocosmos project combines the knowledge of more than ten databases with the objective to create a three-dimensional virtual cell environment integrating three cytological levels; the mesoscopic, the molecular and the functional level. Using the CellExplorer with the PathwayIntegration (CmPI)), virtual cell environments – directly or indirectly derived from microscopic data – are combined with protein-related networks by using localization information acquired from different well-known databases [2], [3]. In addition, these cell models can be extended by published data-based PDB membranes generated with the MembraneEditor (CmME) [4].

2   From Mesoscopic to Molecular Level

The right image shows the journey from the molecular to the mesoscopic level. Starting from the mesoscopic perspective, showing the complete cell model
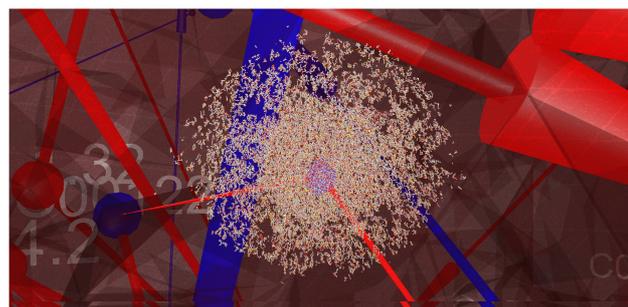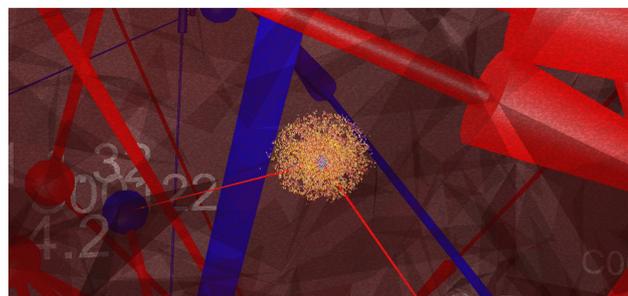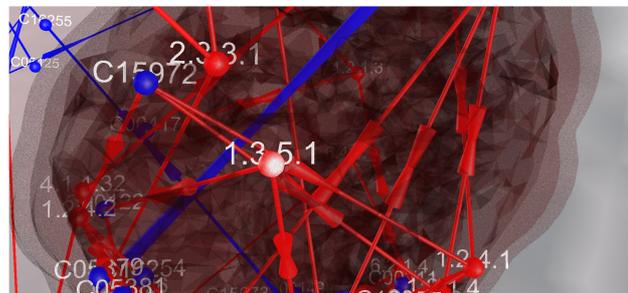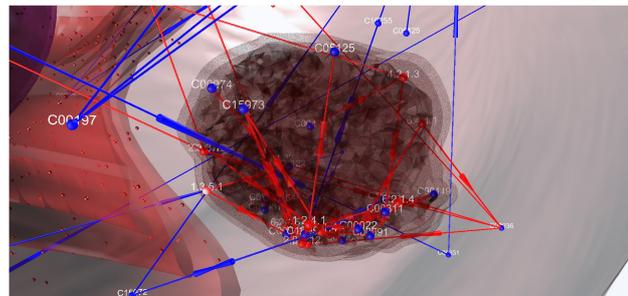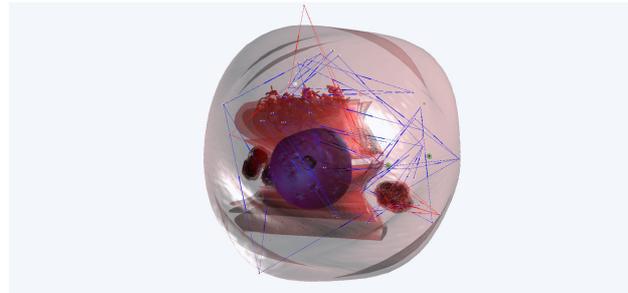
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associated with two metabolic pathways from KEGG, the citrate cycle and the glycolysis, the user navigates towards the mitochondrion. The metabolic pathways were localized by using CmPI [3].

The mitochondrion model was associated with a texture of a mitochondrial PDB membrane model surrounding a protein which is part of the citrate cycle. Finally, the molecular structure is combined with the surface of the mitochondrion by using a novel technique we have recently introduced as Membrane Mapping [5].

3   Outlook

CmX is a small plug-in which can be used to combine the CellExplorer and the MembraneEditor to enable a smooth workflow, bridging the gap between the mesoscopic and molecular level. After the full release of the CellExplorer, CmX will also be freely available.

Now, the resulting projects can be used as a starting point for a collaborative project, providing a visual framework to combine and present different levels of cytological knowledge.

4   Acknowledgments

5   References

[1] B. Sommer. CELLmicrocosmos-Integrative cell modeling at the molecular, mesoscopic and functional level. Doctorate Thesis, Bielefeld University, Bielefeld, Germany, 2012.

[2] B. Sommer, J. Künsemöller, N. Sand, A. Husemann, M. Rumming, and B. Kormeier. CELLmicrocosmos 4.1: an interactive approach to integrating spatially localized metabolic networks into a virtual 3D cell environment. in *BIOSTEC BIOINFORMATICS 2010*, 2010:90–95.

[3] B. Sommer, B. Kormeier, P. S. Demenkov, P. Arrigo, K. Hippe, Ö. Ates, A. V. Kochetov, V. A. Ivanisenko, N. A. Kolchanov, and R. Hofestädt. Subcellular Localization Charts: A new visual methodology for the semi-automatic localization of protein-related data sets. Journal of Bioinformatics and Computational Biology, 11(1):1340005, 2013.

[4] B. Sommer, T. Dingersen, C. Gamroth, S. E. Schneider, S. Rubert, J. Krüger, and K. J. Dietz. CELLmicrocosmos 2.2 MembraneEditor: a modular interactive shape-based software approach to solve heterogeneous Membrane Packing Problems. Journal of Chemical Information and Modeling, 5(51):1165–1182, 2011.

[5] T. Waltemate, B. Sommer, and M. Botsch. Membrane Mapping: Combining Mesoscopic and Molecular Cell Visualization. Vienna, Austria, 2014:89–96.