Distributed Collaborative Molecular Modelling

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The faithful and intuitive visualization of three-dimensional molecular structures and their properties, and the interaction with and simulation of the displayed molecular entities is one of the most important tasks when modelling molecular systems. Today, this is usually performed in large interdisciplinary teams that are often spread out over the globe. However, currently existing tools and applications are inherently single-user, with limited – or usually no – support for collaborative workflows. In our work, we investigate ways to assist drug designers with modern rendering techniques, resulting in greatly improved visual perception of three-dimensional molecular properties, and with 3D-internet [1] and collaboration techniques to unlock the potential of interdisciplinary, virtual cooperation.

We build on three areas of previous and ongoing research. First, we focus on the extension of the already existing molecular modelling framework BALL [2] with its graphical frontend BALLView [3] for collaborative use. We also analyze how to support the rendering of dynamic geometries and define efficient update protocols, since molecular objects and their annotations are frequently changing during a collaborative molecular modelling session. Furthermore, we concentrate on the integration of distributed information and the resolution of conflicting edit actions to the shared structural or annotation data.

[1] K. Sons, F. Klein, D. Rubinstein, S. Byelozyorov, P. Slusallek, Proc of 15th Int Conf on 3D Web Tec , **2010** , 175-184.
[2] A. Hildebrandt, A.K. Dehof, A. Rurainski, A. Bertsch, M. Schumann, N.C. Toussaint, A. Moll, D. Stockel, S. Nickels, S.C. Mueller, H.P. Lenhof, and O. Kohlbacher, *BMC Bioinformatics,* **2010**, *11*, 531
[3] A. Moll, A. Hildebrandt, H. Lenhof, and O. Kohlbacher, *Bioinformatics*, **2006**, *22*, 365–366.