Geometric Problems and Algorithms in Computer-Aided Molecular Design

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Abstract: Computer-Aided Molecular Design describes a research area covering all kinds of computer applications in the design of molecules having desired properties. It is widely applied for the design of bioactive molecules like pharmaceuticals or agricultural products. From the computer scientists perspective, computer-aided
molecular design contains a large variety of computational problems, often geometric and/or combinatorial in nature. In the introductory part of this talk, a short overview of these problems is given.

The main focus in this talk will be on protein-ligand docking. The aim of a docking calculation is to predict, whether two molecules bind to each other (i.e. form an energetically favorable complex). If they do so, one is interested in the geometry of the molecular complex and in the binding energy. The most prominent variant is protein-ligand docking. Here the first molecule is a protein while the second molecule is a small compound. Since most drug targets are proteins and most drugs are small compounds, software for protein-ligand docking is extensively used in pharmaceutical research. Since 1993, we are developing the software package FlexX which belongs to the most widely used codes for protein-ligand docking. An outline of the underlying models, the applied algorithms as well as some examples will be presented.

References:

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