G-CSC - Kolloquium

Biomolecules in a structured solvent - a nonlocal electrostatics treatment

Prof. Dr. A. Hildebrandt, Bioinformatik, Universität Mainz

Abstract

The successful development of new drugs is one of science's most difficult tasks today. Even under optimal circumstances, it takes years to finish, has a very low probability of success, and is immensely expensive. In this talk, I want to show how molecular modeling techniques can help to make drug design cheaper, faster, and more reliable.

In particular, I will focus on the accurate computation of electrostatic effects which play an important role in the energetics of biomolecules. Many of those effects are dominated by the shielding effect of the water that is always present in biochemical reactions. Therefore, a highly accurate computation of electrostatic potentials of biomolecules in water is an important precursor for many applications in bioinformatics, like the mentioned computer aided development of inhibitors for disease related enzymes.

In the literature, nonlocal extensions of classical macroscopic electrostatics have been proposed to capture the effects of the water on the electric potential. We propose a reformulation of the resulting equations, which we can be addressed numerically. The method has been shown to yield very accurate results on small systems like mono- or polyatomic ions and initial results on selected proteins are highly promising.