The Chair of Applied Dynamics at the Friedrich-Alexander-University Erlangen-Nuremberg has an immediate offer for a

Bachelor's / Project thesis

on

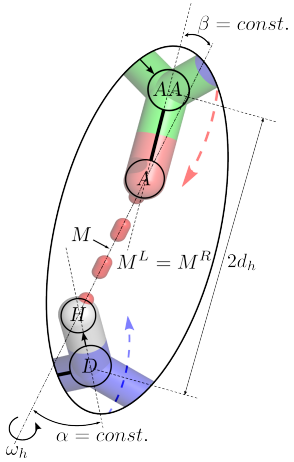
Geometric modeling of hydrophobic interactions to sample molecular conformations

Proteins and RNAs are dynamic macromolecules that move between different conformational states to perform their biological function. Non-covalent interactions such as hydrogen bonds and hydrophobic forces can stabilize native conformations and are often conserved across states. In order to maintain such interactions throughout sampling, they can be geometrically modelled as holonomic constraints, which define coordinated kinematic substructures or rigid bodies within the molecule.
This thesis focuses on geometrically modeling such non-covalent interactions. Existing software tools in Python and C++ already model hydrogen bonds as five-valued constraints, only allowing the rotation about the bond axis. The goal is to model hydrophobic interactions in a similar fashion, restricting two degrees of freedom. Extensions to additional non-covalent interactions like ion-coordination or halogenide bonds are possible. The work includes

- literature research on descriptions of hydrophobic interactions
- identifying hydrophobic interactions in molecular structures
- implementation of associated rigidity analysis in C++
- application to examples and validation with existing competitive software tools

Necessary qualifications

- programming experience in Python and C++
- lecture 'Dynamics of rigid bodies' or equivalent
- interest in computational biology
- basic knowledge in biochemistry (not mandatory)



Geometric modeling of hydrogen bond interaction via five holonomic constraints.

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