Over a decade applying robotics-inspired algorithms to the study of biomolecules

Relying on the analogy between problems in robotics and structural biology, methods originally developed to compute robot motions have been extended and applied to the simulation of molecular systems. In this talk, I will give an overview of works carried out at LAAS-CNRS (Toulouse) in this area. Then, I will focus on two particular topics: 1) The conformational sampling and motion simulation of loop regions in proteins. 2) The exploration of the energy landscape of highly-flexible biomolecules, such as peptides and intrinsically disordered proteins.