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“Parametrization and Graph Algorithms for Multibody Configurational Problems”

ABSTRACT: Configurations (positions and orientations, also called conformations in biochemistry) of multibody systems are of great practical and theoretical interests, with important scientific and engineering applications in diverse fields such as computational structural biology, computer simulation, and robotics. In practice, it is very challenging to effectively compute valid system configurations and motions, since multibody systems generally have many degrees of freedom and complicated constraints such as no collision for physical objects and low energy for protein conformations. An important, but largely overlooked, issue is system parametrization: a given constraint can have very different formulations in terms of different parameters, which may affect the solvability of the constraint, the structure of the system configuration space, and the complexity of configuration and motion generation problems.

In this talk, we will present our newly developed simplex-based parameters and algorithms that have achieved orders of magnitude improvement over existing work. We will also briefly describe graph based algorithms that were originally developed in the robotics community but have been successfully adapted for the computational study of many configurational problems, such as protein and RNA folding, ligand binding, and simulation of animal group behaviors.