

Biomedical Engineering



Thesis Defense

Computationally Efficient Kinematics Analysis Methods in Biological Structures

By

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Abstract:

Open serial chains are mechanical links connected by joints. These chains have a fixed link and a free link, where the latter is referred to as the end effector. The links can move relative to each other about their joint axes. There exists a large body of knowledge that deals with the motion analysis (kinematics) of open serial chains. In this thesis, kinematics analyses tools are used to study biological structures that can be modeled as open serial chains. The advantages of using advanced kinematic tools are to make accurate model representations, avoid unnecessary use of confusing formulations, and significantly improve computational efficiency.

The biological structures investigated are the Human Lower Limb Kinematics and Protein Folding. In the case of the Human Lower Limb, the direct and inverse kinematics is mathematically described using the Zero Reference Position Notation (ZRPN) for six and nine degrees of freedom. This description has not been found in literature. In addition, joint torques are determined using a kineto-static analysis. Motion Analysis experiments of the human lower limb of subjects riding a bicycle were performed. The kinematics prediction correlates with experiments.

In the case of protein folding, the direct kinematics of proteins is mathematically described in the most computationally efficient form using the ZRPN. Then, the Kineto-Static Compliance Method is used to predict protein conformation (shape). This method replaces the need for dynamic analysis of open serial chains altogether and hence, it has a significant computational benefit. This methodology is based on the application of estimated driving forces and torques that move the current chain structure to a target structure. Forces are obtained from protein force field definitions found in the literature. The simulation has been proven to minimize joint torques and potential energy to obtain a final protein conformation.

Comparison between predicted and known structures showed a Root Mean Square Deviation (RMSD) of 0.2 or higher. If the input structure to the simulation is not close to the experimental protein conformation the RMSD values tend to be higher. The differences are due to model limitations and force field definitions.