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MULTIBODY MINIMUM-ENERGY TRAJECTORY WITH APPLICATION TO PROTEIN FOLDING

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This work considers the optimal control of open-chain multibody systems being actuated with control forces which impact the system's motion directly. The goal is to find a dynamically feasible minimum-energy trajectory of system conformations from an initial to a desired final conformation. The optimal control problem and its constraints are integrated in a discrete version of the equation of motion allowing the minimization of system potential energy with respect to a discrete state and control trajectory. This work is centered on a specific type of open-chain multibody system where the overall system dynamic is described essentially by bodies torsion. The body orientation are described with respect to a body-fixed frame, where its local displacements and global multibody conformation are controlled using an elastic band. The coupling between to optimal conformations is described as an elastic grid of replicas of possibly conformations. The grid elastic forces are used to control system's motion directly, reflecting the influence of the system potential energy field on its conformation, using the Nudged-Elastic Band method. Here the equations of motion of the multibody grid are solved by using the augmented Lagrangean method and sparse matrix solver. In this context, if a feasible minimum-energy trajectory of system exists it is as a stationary state on the multibody grid moments. A typical example of this type of mechanism is a protein, since peptide planes remain relatively rigid during protein dynamics and its overall dynamics is described by their backbone dihedral angles. These are open-chain systems defined using relatively rigid components, possibly deformable, linked together using revolute joints. The method described in this work will be evaluated for protein folding. In this contribution we tested the presented method to find a transition state pathway, between two saddle conformations.