Investigation of flexibility in Myosin V using a new 3D mechanical model MAHDI HAGHSHENAS-JARYANI, Department of Mechanical Engineering, University of Texas at Arlington — This paper presents the development of a three dimensional rigid multibody model for the simulation and analysis of motor protein locomotion. The interesting aspect of this model is that it retains the mass properties, in contrast to the commonly used models which omit mass properties at the nano scale. The disproportionate size of the small mass of Myosin V relative to the large viscous friction forces requires a small integration step size that leads to a long simulation run time; however, the proposed model can be numerically integrated in a reasonable amount of time. This paper discusses modeling flexibility in the protein as an extension of the original rigid body model. Empirical studies have shown that Myosin V's neck domain can be considered as three pairs of tandem elements called IQ motifs which can bending at junctures between them. Therefore, each neck is modeled by three rigid bodies connected by ball-and-socket joints together, rather than single rigid body has been used in the previous works. Euler parameters are used to model the orientation of bodies in order to eliminate singularities in the description of orientation. In order to accomplish this, the equations of motion are reduced to minimal form using changing holonomic and non-holonomic constraints applied to the model which represent the normalization of the Euler parameters as well as contact and impact non-penetration conditions. The differences between the dynamic behavior of the new mechanical model, with flexible neck domains, and the original rigid body model are compared using simulation results.

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