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Coarse-grained model for a motor protein on a microtubule JUTTA LUETTMER-STRATHMANN, MANSOUR ALANAZI, Department of Physics, The University of Akron, Akron, OH 44325-4001 — The function of cells relies on the transport of substances within the cell. In eukaryotic cells, active transport by motor proteins moving on a substrate plays an important role. The goal of this work is to model a motor protein walking on a microtubule. For the microtubule, we employ a combined micromechanical/interaction site model from the literature. This allows us to calculate deformations of microtubules with finite element methods and map the results to an interaction site model that includes details about the microtubule structure, for example a seam along the length of the microtubule. The motor protein is represented by a coarse-grained model that was developed in earlier work. In this work, we perform Brownian dynamics simulations of the walker on a fixed microtubule substrate. Calculations of average displacements of the walker show that the efficiency is lower than in biological systems and can be improved by adjusting protein model parameters. In agreement with recent experimental observations, we also find that the protein walker does not cross the seam of the microtubule.

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