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Building a three-dimensional model of kinesin stepping on a microtubule MATTHEW MURROW, JUTTA LUETTMER-STRATHMANN, Department of Physics, The University of Akron, Akron, OH 44325-4001 — The motor protein kinesin plays an integral role in cell function, transporting, for example, vesicles and proteins. Kinesins are composed of two heads, two neck linkers, and a coil connecting these parts to the carried cargo. Kinesin molecules, upon ATP binding, have been shown experimentally to walk along tubulin-based protein structures called microtubules in a hand-over-hand stepping motion, carrying their cargo eight nanometers per step. A number of kinesin models for computer simulations have been developed but none are able to replicate the observed stepping efficiency. Atomistic models provide insight into details of the moving motor protein but are computationally too expensive to simulate stepping. Abstract models are more efficient but can be difficult to relate to the biological system. The goal of this work is to build a coarse-grained 3D protein model of the kinesin-microtubule complex that can be simulated economically and replicate the stepping efficiency of the motor protein. To this end we are developing an interaction site model for the protein heads and neck-linker domain that will be combined with an existing microtubule model for Brownian dynamics simulations.

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