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A model of the kinetic cycle of single cytoplasmic MANORANJAN P. SINGH, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697, USA, ROOP MALLIK, STEVEN P. GROSS, Department of Developmental and Cell Biology, University of California Irvine, Irvine, CA 92697, USA, CLARE YU, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697, USA — We use Monte Carlo simulations to model molecular motor function at the single molecule level. For kinesin, we show that the simulations of the kinetic cycle reproduces accurately the dependence of velocity on ATP concentration and applied load, described by Michaelis-Menten kinetics. More importantly, the Monte Carlo approach allows us to implement nonlinear models of more complicated branching enzymatic pathways, like those found in enzymes such as cytoplasmic dynein. Our dynein simulations reproduce the main features of recent single molecule experiments that found a discrete distribution of dynein step sizes depending on load and ATP concentration. The theory relates dynein's chemical/enzymatic properties to its mechanical force production. It proposes the existence of negative cooperativity of ATP binding at secondary binding sites, which is required to reproduce the experimentally observed step distribution and improves dynein's ATP economy by suppressing small steps under high-ATP/ no-load conditions.

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