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Probing the Effects of Cargo Loads in Single-Molecule Kinesin Mechanochemistry[1] B.D. JACOBSON, S.J. KOCH, S.R. ATLAS, Department of Physics and Astronomy, University of New Mexico — The influence of cargo loading on the dynamics of motor proteins such as kinesin is key to understanding fundamental aspects of their kinetic cycles and mechanochemistry. Kinetic models offer insight into these complex processes which occur on time scales up to seconds, and coupled with experimental data, they are a powerful tool in generating an increasingly fine-grained understanding of the chemical and mechanical mechanisms involved in kinesin procession, as well as the prospect of direct coupling to atomistic-scale simulations [1]. Here we present a kinetic model of single-molecule kinesin to study the effects of external forces due to intracellular cargo transport on chemical and mechanical rate constants. We use a simulated annealing algorithm that optimizes rate constants to fit published experimental data on kinesin speed and processivity, and kinetic Monte Carlo to compare predicted values with independent experimental measurements. We also discuss the application of sensitivity analysis to provide additional insight into the critical transitions and states of the processing protein under load.
[1] B. D. Jacobson, L. J. Herskowitz, S. J. Koch and S. R. Atlas, Investigation of kinesin processivity via simulated annealing, Biophys. J., submitted (2013).

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