

# Supporting Material for How Fast Is Too Fast in Force-Probe Molecular Dynamics Simulations?

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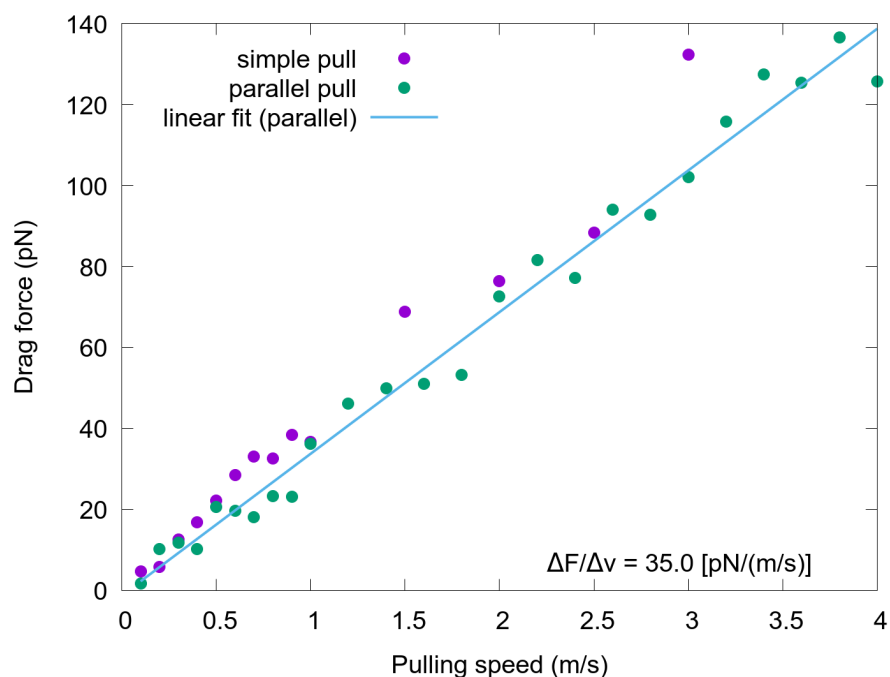


Figure S1: The raw data in determining water-spectrin repeat friction. Purple symbols refer to a simple center-of-mass pulling through the water box, allowing free rotation, while green ones feature a restraint force that keeps the spectrin repeats aligned with the long axis of the box. The linear fit is based on this latter data set, since this mimics the behavior of the system in a tandem construct more closely.

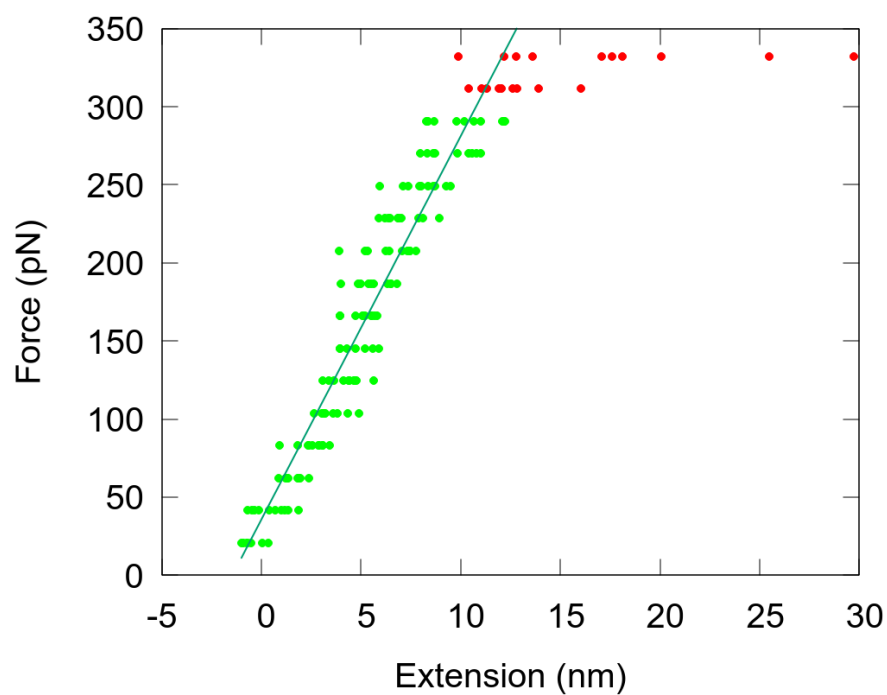


Figure S2: Force-extension curves of the tandem spectrin repeats determined from 160 constant-force pullings. Plotted are the changes in end-to-end distances after 5 ns of pulling of 10 different simulations. Green symbols correspond to forces deemed to produce a purely flexible response on this time scale, while red ones to forces that produce large, non-linear conformational changes. A linear fit based on the flexible response only is also shown.

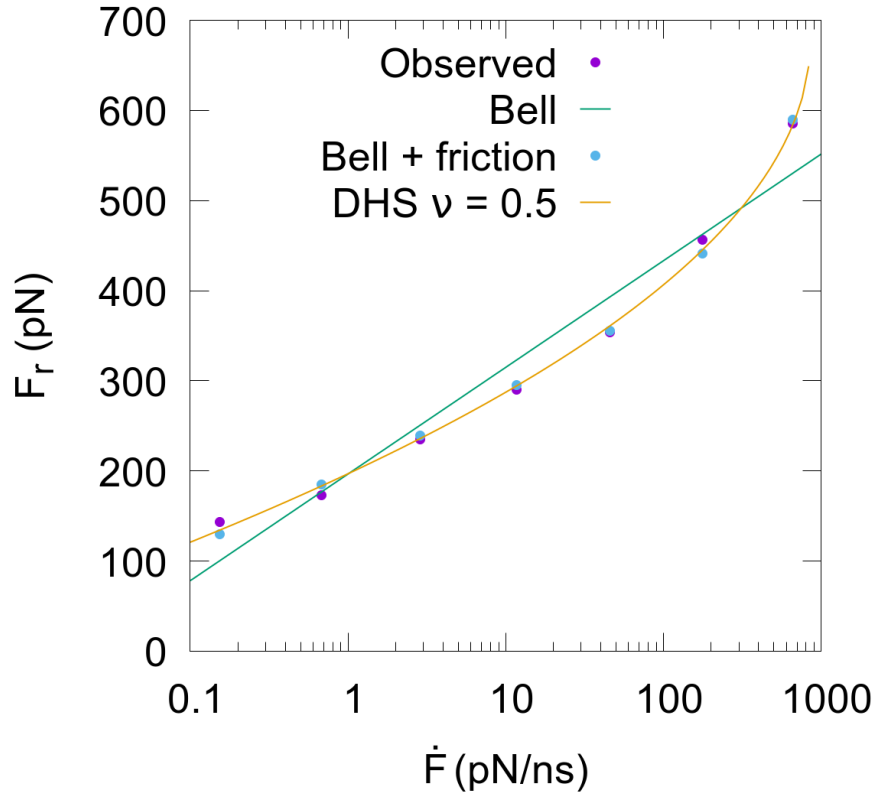


Figure S3: The dependence on the loading rate of the rupture forces. We either employ the simple Bell model, which in this case is inadequate, or improve on it through adding a linear term in friction (blue circles) or through the Dudko-Hummer-Szabo model.

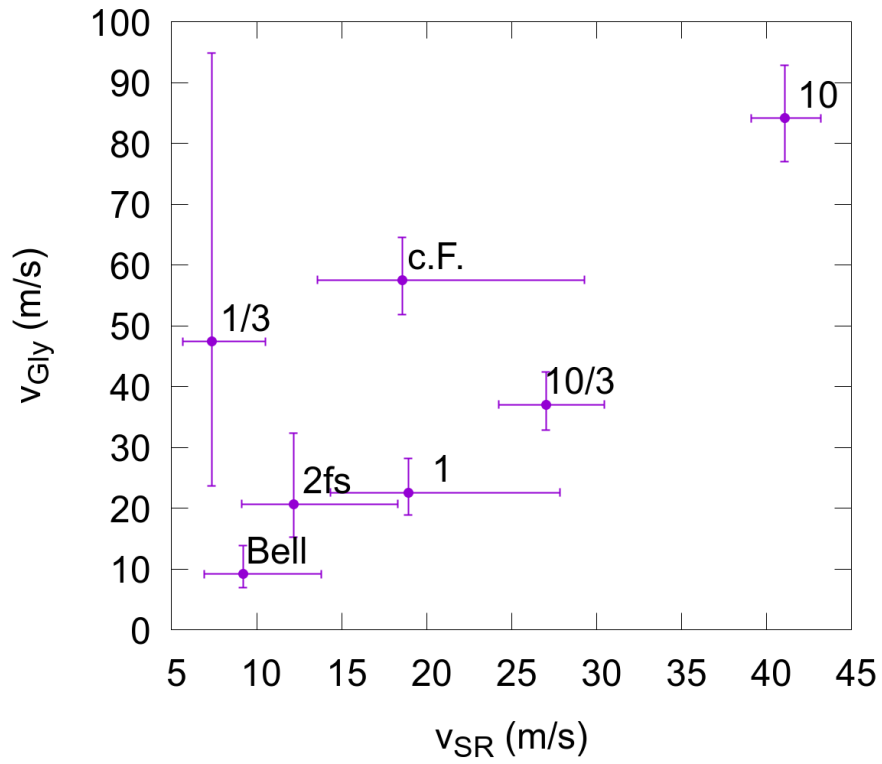


Figure S4: The speeds of propagation of the main text are validated against two different data sets: constant force pullings (“c. F.”, the same data as in Fig. S2) and in simulations without virtual sites (“2 fs”).