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Escape of a knot from a DNA molecule in flow[1] BENJAMIN RENNER, PATRICK DOYLE, Massachusetts Institute of Technology — Macroscale knots are an everyday occurrence when trying to unravel an unorganized flexible string (e.g. an iPhone cord taken out of your pocket). In nature, knots are found in proteins and viral capsid DNA, and the properties imbued by their topologies are thought to have biological significance. Unlike their macroscale counterparts, thermal fluctuations greatly influence the dynamics of polymer knots. Here, we use Brownian Dynamics simulations to study knot diffusion along a linear polymer chain. The model is parameterized to dsDNA, a model polymer used in previous simulation and experimental studies of knot dynamics. We have used this model to study the process of knot escape and transport along a dsDNA strand extended by an elongational flow. For a range of knot topologies and flow strengths, we show scalings that result in collapse of the data onto a master curve. We show a topologically mediated mode of transport coincides with observed differences in rates of knot transport, and we provide a simple mechanistic explanation for its effect. We anticipate these results will build on the growing body of fundamental studies of knotted polymers and inform future experimental study.

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