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Simulation of λ-phage DNA in microchannels using a coarse-grained MD method VASILEIOS SYMEONIDIS, GEORGE KARNIADAKIS, BRUCE CASWELL, Brown University — In this work we present Dissipative Particle Dynamics (DPD) simulations of polymers subject to the Marko-Siggia wormlike chain (WLC) spring law. We demonstrate the advantages of Lowe's DPD method, which simulates high Schmidt numbers for the solvent, and contrast it with the velocity-Verlet scheme. Shear flow results for the wormlike chain (WLC) simulating single DNA molecules compare well with average extensions from experiments, irrespective of the number of beads. However, coarse-graining with more than a few beads degrades the agreement of the autocorrelation of the extension.

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