Abstract Submitted
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A symplectic integration method for elastic filaments TONY LADD, GAURAV MISRA, University of Florida — Elastic rods are a ubiquitous coarse-grained model of semi-flexible biopolymers such as DNA, actin, and microtubules. The Worm-Like Chain (WLC) is the standard numerical model for semi-flexible polymers, but it is only a linearized approximation to the dynamics of an elastic rod, valid for small deflections; typically the torsional motion is neglected as well. In the standard finite-difference and finite-element formulations of an elastic rod, the continuum equations of motion are discretized in space and time, but it is then difficult to ensure that the Hamiltonian structure of the exact equations is preserved. Here we discretize the Hamiltonian itself, expressed as a line integral over the contour of the filament. This discrete representation of the continuum filament can then be integrated by one of the explicit symplectic integrators frequently used in molecular dynamics. The model systematically approximates the continuum partial differential equations, but has the same level of computational complexity as molecular dynamics and is constraint free. Numerical tests show that the algorithm is much more stable than a finite-difference formulation and can be used for high aspect ratio filaments, such as actin. We present numerical results for the deterministic and stochastic motion of single filaments.

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