Electronic Supplementary Information for: Self-propelled Worm-like Filaments: Spontaneous Spiral Formation, Structure, and Dynamics

Rolf E. Isele-Holder, Jens Elgeti, and Gerhard Gompper Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulations, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

DESCRIPTION OF THE VIDEOS

The three videos in the ESI show example simulations of a filament with the same bending rigidity $\xi_P/L = 0.2$ from the three different filament regimes: the polymer regimes (S1.mpeg, Pe = 200), the weak spiral regime (S2.mpeg, Pe = 1000), and the strong spiral regime (S3.mpeg, Pe = 5000). The filament is in grayscales with the leading tip colored black. The camera moves with the filament; the red points indicate a spatially fixed reference system as a guidy to the eye.

DETAILS OF THE SIMULATION SETUP

Details of the simulation setup of the free-swimming filaments are summarized in Table I.

$\xi_P/L = \kappa/(k_B T L)$	N	$Pe = f_p/(k_BTL^2)$	$\Delta t/\tau$	t_e/ au	t_s/τ
100	25	0 - 20000	8.00×10^{-10}	0.0512	5.12
		50000	2.00×10^{-10}	0.0256	2.56
		100000	1.00×10^{-10}	0.0128	1.28
40 - 20	25	0-2000	6.40×10^{-9}	0.0512	5.12
		5000	3.20×10^{-9}	0.0512	5.12
		10000	1.60×10^{-9}	0.0512	5.12
		20000	8.00×10^{-10}	0.0512	5.12
		50000	$2.00{ imes}10^{-10}$	0.0256	2.56
		100000	1.00×10^{-10}	0.0128	1.28
10	50	0 - 10000	8.00×10^{-10}	0.0512	5.12
		20000	4.00×10^{-10}	0.0512	5.12
		50000	1.00×10^{-10}	0.0256	2.56
		100000	5.00×10^{-11}	0.0128	1.28
4	50	0 - 100000	8.00×10^{-10}	0.0512	5.12
2 - 0.2	100	0-20000	1.00×10^{-10}	0.0512	5.12
		50000	5.00×10^{-11}	0.0256	2.56
		100000	2.50×10^{-11}	0.0128	1.28
0.14 - 0.1	200	0-50000	2.50×10^{-11}	0.0128	1.28
		100000	2.50×10^{-11}	0.0064	0.64

TABLE I. Details of the simulation settings. ξ_P/L is the persitence length divided by the filament length, Pe is the *Peclet* number, k_BT is the thermal energy, κ is the bending rigidity of the filament, N is the number of bonds, f_p is the propulsive force per unit length of the polymer, τ is the time that the filament requires to diffuse its own body length, Δt is the timestep of the integrator, t_e is the equilibration time at the beginning of the simulation that is discarded in the analysis, and t_s is the simulation time during which data for the analysis is collected.