Supplemental Material

Flow-induced nonequilibrium self-assembly in suspensions of stiff, apolar, active filaments

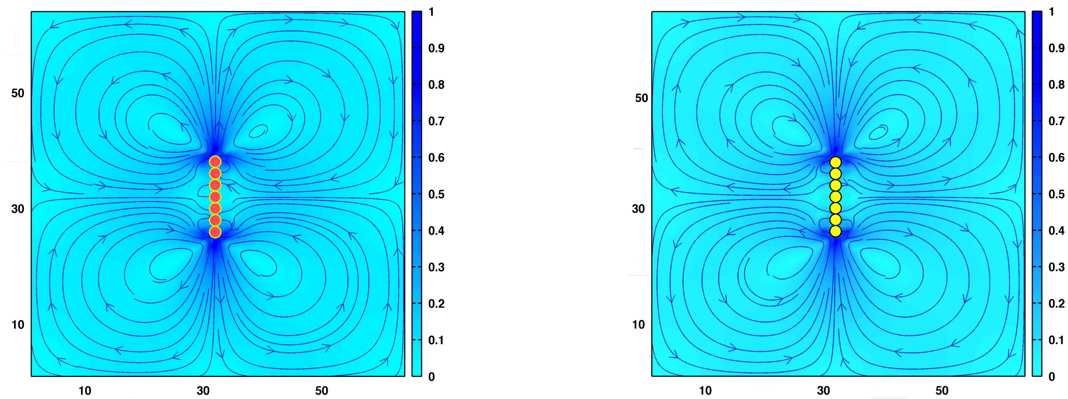
Ankita Pandey,[1] P. B. Sunil Kumar,[1] and R. Adhikari[2]

[1] *Indian Institute of Technology, Madras, Chennai 600036, India*

[2] *The Institute of Mathematical Sciences, CIT Campus, Chennai 600113, India*

(Dated: September 15, 2016)

FLOW FIELD GENERATED BY A SINGLE FILAMENT

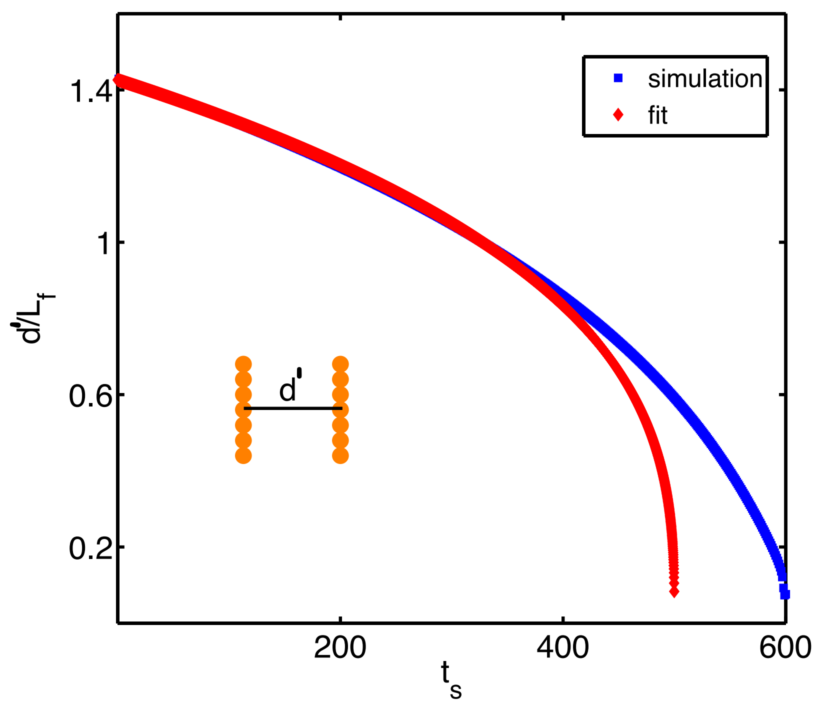


SI Fig. 1.(Colour online) (a) Flow field generated by an extensile filament. (b) Flow field generated by a contractile filament. For these simulations, box size is 64×64×1, stiffness 0.4 and viscosity 1/12 in reduced units. The background colour indicates the magnitude of the velocity normalised by its maximum.

In the case of an extensile filament, the flow field is pointing outwards along the filament axis, and inwards along the normal of the filament (see SI Fig.1(a)). For a contractile filament, the flow field points inwards along the filament axis and outwards along normal of the filament, see SI Fig.1(b). The LBM flow is computed with periodic boundary conditions. Streamlines under periodic boundary conditions must either be closed or should wrap around the periodic boundaries. Hence, we observe four closed lobes as expected and shown in the above SI Fig.(1). This symmetric flow field ensures that an isolated straight filament produces active flows but does not actively translate or rotate and is, thus, individually apolar. However, as we show, translational and rotational motion is possible in the combined flow of two or more stiff, apolar filaments. This inherently collective and non-equilibrium source of motion, when constrained by the anisotropic excluded volume interaction between filaments, leads to non-trivial states of aggregation in suspension.

ATTRACTION DUE TO HYDRODYNAMIC FLOW

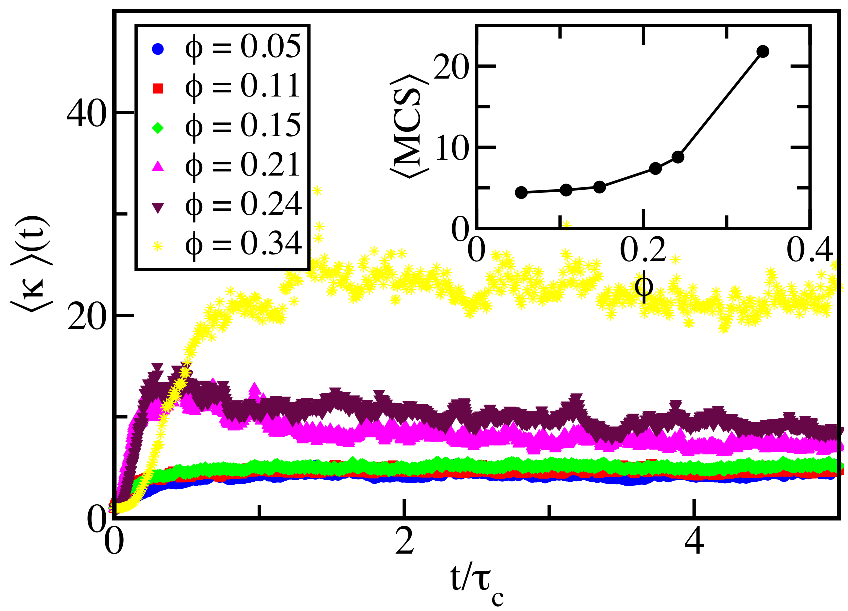
Here we provide a qualitative description of a quantitative calculation of the attraction between filaments that follows from Eq. (23) of the main text. Every bead in the filament produces an active flow. At distances large compared to the size $L = (N-1)b_0$ the dominant component of the hydrodynamic flow is that of a stresslet. The stresslet produces a velocity that decays as $1/r^2$ with distance. Thus, the rate of change of position of a distant particle in such a flow varies inverse squarely with position. Integrating this, the position itself varies as the cube root of time. Since stresslet flow has both converging and diverging streamlines, the distance can either increase or decrease. This depends on both the sign of the stresslets and their relative orientation. Extensile stresslets attract when they are parallel but repel when they are perpendicular. Contractile stresslets attract when they are perpendicular but repel when they are parallel. In all of these cases, their relative distance varies as the cube root of time. In SI Fig.(2), we compare the measured dependence of the relative distance on time from simulation with the expected cube root variation for extensile filaments in perpendicular orientation. The agreement between the far-field prediction and the measured value is excellent for early times but deteriorates at late times when the filaments are within the distance L and the near-field components of the flow begin to dominate.



SI Fig. 2. (Color online) Variation of distance d', scaled by the filament length $L_f = L$, as a function of scaled time $t_s = t\eta b_0/\kappa$ for a pair of parallel extensile filaments. The fit to $d'(t) \sim t^{1/3}$ is excellent for early times.

MEAN CLUSTER SIZE FOR CONTRACTILE FILAMENTS

To understand cluster dynamics in contractile filaments, we calculate mean cluster size with time for contractile filaments. As shown in SI Fig. 3, for all densities, the cluster size grows quickly in time τ_c and saturates afterwards, unlike in an extensile system where cluster grows monotonically with time till most of the filaments are in one cluster. There is a rapid initial growth of the mean size for a duration τ_c followed by saturation at later times. We estimate τ_c from the intersection of a pair of straight lines that best fit the data. There is an initial very quick growing regime where filaments come together to form small clusters and



SI Fig. 3.(Colour online) Growth of mean cluster size as a function of time in contractile filaments suspensions, at different volume fractions. The initial quick growth, on a time scale τ_c, forms many small clusters followed by a saturation. Inset shows time averaged mean cluster size variation with volume fraction ϕ. Mean cluster size grows with volume fraction ϕ.

soon saturates. In contractile filaments, clustering happens at short time scale $\tau_c \ll \tau_e$, and system attains steady state. As we increase volume fraction ϕ, contractile filaments show aggregate state of asters, clusters and percolated network (see main text Fig. 4). The mean cluster size grows with volume fraction ϕ, as shown in inset of SI Fig. 3.

MOVIE TITLES AND CAPTIONS

Movie M1: extensile-rotating-dimers.avi

Extensile filament pairs attract laterally in their mutual hydrodynamic flow. The lateral attraction drives parallel filaments towards each other till steric forces prevent further motion. Development of small shear flow along the filament long axis becomes more prominent at later stages and breaks flow field symmetry which causes a small lateral motion, thus forming a stable rotating dimer. For this simulation, volume fraction $(\phi) = 0.01$, box size $= 64\times64\times1$, stiffness 0.4 and viscosity is 1/12 in reduced units. This simulation animation is viewable at this https URL: https://youtu.be/q_lZ5VWiDuU

Movie M2: extensile-aggregation-kinetics.avi

In extensile filaments, the lateral hydrodynamic attraction destabilises the homogeneous isotropic state of the suspension. Dimer pairs form rapidly and further aggregate to form k-mers. Asymptotically, the individual clusters collapse into a single dynamic cluster which translates and/or rotates. For this simulation, volume fraction (ϕ) = 0.05, simulation box size = 128×128×1, stiffness 0.4 and viscosity is 1/12 in reduced units. This simulation animation is viewable at this https URL: https://youtu.be/ijT-gkO26bE

Movie M3: contractile-T-shape-dimers.avi

Contractile filament pairs attract perpendicularly in their mutual flow. The perpendicular attraction, combined with steric repulsion, drives contractile filaments to form T-shaped dimers which translate and rotate. For this simulation, volume fraction (ϕ) = 0.01, box size = 64×64×1, stiffness 0.4 and viscosity is 1/12 in reduced units. This simulation movie is viewable at this https URL: https://youtu.be/fOH-RtLmxAw

Movie M4: contractile-self-assembly-asters.avi

At the lowest volume fractions, filaments transiently cluster into star-shaped k-mers reminiscent of asters. These k-mers frequently break and reform while their centers of mass diffuse as shown in this Movie. Through this dynamics, the spatiotemporally averaged position and orientation become, respectively, uniform and isotropic. For this simulation, volume fraction (ϕ) = 0.15, simulation box size = 128×128×1, stiffness 0.4 and viscosity is 1/12 in reduced units. This simulation movie is viewable at this https URL: https://youtu.be/kzplqhX_Htk

Movie M5: contractile-complete-clustering.avi

With an increase in volume fraction, the steric constraints limit the dynamic joining and breaking of k-mers and their diffusion. With further increase in volume fraction, this network gets sterically constrained to a great extent and thus shows greatly reduced positional and orientational dynamics. States that are initially inhomogeneous and have a preferred orientation are unstable and evolve, rapidly, into homogeneous, isotropic microstructured states shown in this Movie. For this simulation, volume fraction (ϕ) = 0.34, simulation box size = 128×128×1, stiffness 0.4 and viscosity is 1/12 in reduced units. This simulation movie is viewable at this https URL: https://youtu.be/nl4ohhwp1nQ