Supplementary Information (SI) for Soft Matter.

ELECTRONIC SUPPLEMENTARY MATERIAL
Kinetically arrested periodic clusters in active filament arrays

Sony Karayat[a], Prashant Purohit[b], L Mahadevan[c], Arvind Gopinath[d,‡], Raghunath Chelakkot[a,‡]

A Model and analysis of array dynamics

A.1 Mean-field model for filament deformation in the pre-contacting stage

During the initial evolution of the array, but before the onset of clustering, the deformation of each individual filament is set by the active compressive follower force and restoring elastic force. Once the filaments deform significantly, contact between adjacent filaments ensues, and filament-filament steric interactions start to play a role. Here, we obtain a continuum model for the initial period when filaments do not experience steric contact forces but do experience viscous drag as a result of their motion in the ambient fluidic medium. Our aim is to study the linear stability of these equations and thereby to understand the process and conditions under which initially vertical filaments become unstable and deform.

Our reference state is a stationary filament of length ℓ that is vertically aligned in the y direction and can deform in the $x-y$ plane. Therefore, the position of each material point comprising the filament is defined by its x and y components, measured here with respect to a laboratory-fixed origin. Let us define laboratory-fixed unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. The filaments are anchored along a line parallel to $\mathbf{e}_1$ (along the x axis), and each filament is initially aligned parallel to $\mathbf{e}_2$ (parallel to the y axis). In addition to their Cartesian position, the material points along the filament can also be located using an arc-length parameter s.

Clearly, $0 \leq s \leq \ell$ is based on the reference state where the anchored end (base) corresponds to $s = 0$, and the free end is $s = \ell$. In the deformed state, let the segment of length ds located between $s + ds$ and s in the reference state map to a deformed segment of length ds'. The stretch function $\lambda(s) \equiv ds'/ds$ quantifies the axial stretch so that $\lambda(s) = 1$ when the filament is inextensible. We specify the shape of the filament using the angle made by the local tangent at s with the x axis, $\theta(s)$. The tangent and normal vectors may then be written as

$$\mathbf{n}(s) = -\sin\theta \mathbf{e}_1 + \cos\theta \mathbf{e}_2$$

and

$$\mathbf{t}(s) = \cos\theta \mathbf{e}_1 + \sin\theta \mathbf{e}_2$$

respectively. For planar deformation without torsion,

$$d\mathbf{n}/ds = -\theta' \mathbf{t}(s), \quad d\mathbf{t}/ds = \theta' \mathbf{n}(s).$$

The local curvature is θ', the subscript (prime) here denoting differentiation with respect to s. The force resultant in the filament can be expressed as

$$\mathbf{F}(s) = \overline{T}(s)\mathbf{t}(s) + \overline{N}(s)\mathbf{n}(s).$$

The active follower forces per unit length that act on the filament can be written as $\mathbf{f}_a(s) = -f_a \mathbf{t}(s)$.

[a] Department of Physics, Indian Institute of Technology Bombay, Mumbai, India.
[b] Department of Mechanical Engineering, School of Engineering and Applied Sciences, University of Pennsylvania, Philadelphia, PA, USA
[c] Department of Physics, Department of Organismic and Evolutionary Biology, and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA.
[d] Department of Bioengineering, University of California Merced, Merced, CA, USA
‡ Corresponding authors: agopinath@ucmerced.edu, raghu@phy.iitb.ac.in

Each filament moves in an ambient Newtonian fluid that helps dissipate active energy. We restrict the analysis to small Reynolds numbers and use a local description of the drag on the filament corresponding to the freely draining limit. The friction viscous drag force per unit length is

$$\mathbf{f}_v(s) = -(\xi_{\|} u_{\|} \mathbf{t} + \xi_{\perp} u_{\perp} \mathbf{n})$$

where $\xi_{\|}$ and $\xi_{\perp}$ are the effective viscous resistances per unit length for the motion of the filament along its local tangent and normal vectors, respectively, and $u_{\|}$ and $u_{\perp}$ are the components of the local velocity of the centerline. Since the filaments are not in contact at this pre-clustering stage, there are no contact (steric) interactions between filaments, and so the associated force $\mathbf{f}_c(s) = \mathbf{0}$. Imposing filament inextensibility $\lambda(s) = 1$ (valid in the pre-clustering stage), and expressing the local velocity of the centerline in terms of shape changes allows us to eliminate N from the equations. The final form of the equations for θ and T are

$$0 = T'' + (\theta''\theta')' - \frac{1}{\gamma}\theta' \left(-\theta''' + T\theta'\right), \tag{1}$$

$$0 = -\theta'''' + (T\theta')' - \dot{\theta} + \gamma\theta' (T' + \theta''\theta' - \beta). \tag{2}$$

where $\gamma = \xi_{\perp}/\xi_{\|}$. Here, we scaled forces by κ/ℓ^2 and lengths by ℓ. For a pinned head (no translation, and free rotation), the boundary conditions are

$$T'(0,t) - \beta = 0, \quad \theta'''(0,t) = \theta'(0,t) = 0 \tag{3}$$

The boundary conditions at the tail end are

$$\theta'(1,t) = \theta''(1,t) = T(1,t) = 0. \tag{4}$$

Our base state is a straight horizontal filament: $\theta(s) = \theta_0 = 0$ with a static tension field given by $T(s) = \beta(s-1) \equiv T_0(s)$.

A.2 Equations for static filaments in the cluster stabilized by contact forces

In our Brownian dynamics simulation, the beads comprising the filaments fluctuate over time. Thermal (stochastic) forces affect the position of each bead comprising the filament. Additionally, time-dependent inter-bead contact forces also cause fluctuations in position. However, when averaged over appropriately long time scales, the shape of a filament in the interior of a cluster is approximately static. In this setting, the average viscous drag forces acting on the beads may be neglected so that $\mathbf{f}_v(s) = \mathbf{0}$.

Focusing on such a trapped filament, we express the effective frictional contact forces acting along the centerline (backbone) in the (dimensional) form

$$\mathbf{f}_c(s) = \overline{f}_{cT}(s)\,\mathbf{t}(s) + \overline{f}_{cN}(s)\,\mathbf{n}(s).$$

At each location s, a force balance provides the relationship

$$\mathbf{F}' - f_a \mathbf{t}(s) + \mathbf{f}_c(s) = \mathbf{0}$$

where, at leading order, we have

$$\mathbf{F}' = (\overline{T}' - \overline{N}\theta')\mathbf{t} + (\overline{N}' + \overline{T}\theta')\mathbf{n}.$$

Balancing moments acting on an infinitesimal element located about s provides the relationship $\mathbf{M}' + \lambda(\mathbf{t} \times \mathbf{F}) + \mathbf{M}_N^c = 0$ where $\mathbf{M}_N^c$ is an effective torque from steric interaction with adjacent filaments. Local internal

f	β	Δ	Θ_1	Θ_2
10	29.66	2	29.74	29.48
10	29.66	3	22.51	21.65
10	29.66	4	16.65	16.43
15	44.49	2	27.71	27.69
15	44.49	3	23.52	25.86
15	44.49	4	18.37	15.92
20	59.32	2	23.03	30.17
20	59.32	3	20.27	18.13
20	59.32	4	19.22	16.92

Table A1: Averaged values of Θ_1 and Θ_2 measured for each pair (f, Δ) are shown in this table. We also list the activity parameter β corresponding to each value of f. Higher values of β correspond to stronger activity effects. A perfectly symmetric cluster implies $\Theta_1 = \Theta_2$. Here differences between the two arise from the effects of noise, imperfect jamming at the colloidal scale, and effects due to intermittent impacts from filaments oscillating between clusters.

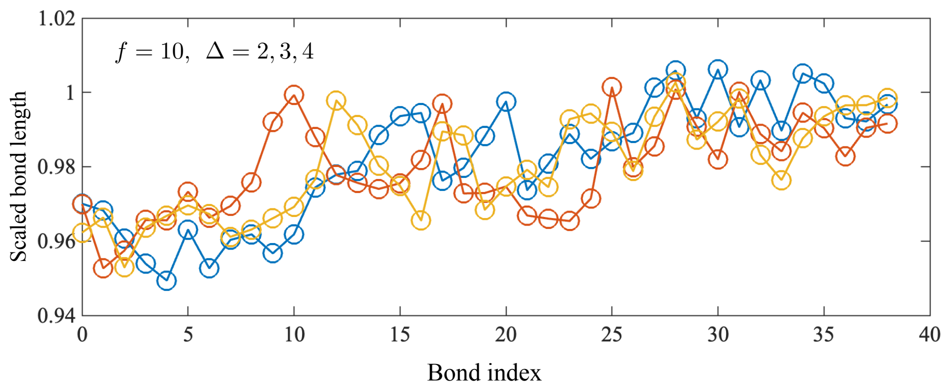

Figure A1: Scaled bond length between successive colloid beads as a function of the bond index (number). Parameters used in the simulation are indicated in the figure.

elastic moments are related to the local curvature via the bending stiffness κ, $\mathbf{M} = \kappa\theta'(\mathbf{t}\times\mathbf{n})$, and the normal forces satisfy to leading order $\overline{N} = -\left(\kappa\lambda^{-1}\right)\theta''$. Scaling forces by κ/ℓ^2 and lengths by ℓ, we combine these relationships and obtain expressions for the contact forces required for maintain a static shape in the interior of the cluster,

$$f_N^c = \left(\lambda^{-1}\theta''' - \lambda'\lambda^{-2}\theta''\right) - T\theta' \quad (5)$$

$$f_T^c = -T' - \theta''\lambda^{-1}\theta' + \beta. \quad (6)$$

Here, T and N are scaled (coarse-grained) internal force components, and f_T^c and f_T^c are scaled (coarse-grained) contact force densities. We note that contact forces may be discontinuous and attain values as required to keep the interior filaments stationary. The maximum value of contact forces increases for a larger number of filaments within a cluster, that is, for thicker clusters.

For an inextensible filament, equations (5) and (6) can be simplified using $\lambda(s) = 1$ and $\lambda'(s) = 0$. This choice is motivated by our simulation results that demonstrate that filament extensional strains are small to negligible (see Figure A1).

B ESM Movie descriptions

- **ESM Movie 1:** The formation of kinetically arrested thick clusters of tightly packed active filaments at moderate activity ($\beta = 44.49$) and the inter-filament spacing $\Delta = 2$.
- **ESM Movie 2:** The formation of kinetically arrested clusters of active filaments at large spacing, $\Delta = 2$ and at moderate activity ($\beta = 44.49$).
- **ESM Movie 3:** The formation of kinetically arrested clusters of active filaments at large spacing, $\Delta = 4$ and when the activity is approximately equal to the critical value for individual filaments to be neutrally stable. ($\beta = 29.96$).
- **ESM Movie 3:** Spatiotemporal evolution of the active torque calculated as described in the main text. The active force density is $f = 20$ ($\beta = 59.32$) and the inter-filament spacing $\Delta = 2$.
- **ESM Movie 4:** Spatiotemporal evolution of the elastic bending moment calculated as described in the main text. The active force density is $f = 20$ ($\beta = 59.32$) and the inter-filament spacing $\Delta = 2$.
- **ESM Movie 5:** Spatiotemporal evolution of the contact torque due to the interaction between filaments within arrested clusters and contact interactions between the cluster and inter-cluster filaments. The active force density is $f = 20$ ($\beta = 59.32$) and the inter-filament spacing $\Delta = 2$.