Supplementary Information for "Buckling instability in ordered bacterial colonies"

Denis Boyer, William Mather, Octavio Mondragón-Palomino, Sirio Orozco-Fuentes, Tal Danino, Jeff Hasty, Lev S. Tsimring

Continuum model parameter matching with DES

In order to provide a quantitative connection between discrete-element simulations and continuum model, we need to relate the material constants of DES rods and the parameters of the continuum model. Some parameters are straightforward to relate: the volumetric growth rate a coincides with the rate α of the exponential growth of rod length between divisions. Similarly, the friction coefficient μ in the continuum model is equal to the friction coefficient of individual rods and the bottom. Finding elastic constants of the cellular "medium" is somewhat less trivial. However, we can estimate analytically the elastic constants λ_{ij}, ξ for a nematic close packing of spherocylinders with mean length ℓ and diameter d. In our DES model we assume that rods interact via Hookian springs connecting the points of the minimal distance between the axes of two rods, if the distance is less than the cell diameter d, with the inter-particle force $F_{ij} = K_n \chi_{ij}$ where χ_{ij} is the cell diameter d minus the minimal distance between the axes.

To compute the normal elastic modulus λ_{xx}, we consider a rectangular box of height L_x and width L_y filled with particles with mean length l nematically ordered along vertical x axis. Initially the particles do not overlap with each other. After a normal displacement Δ of the upper wall down along x direction, the mean overlap per particle is $\chi = \Delta/N_x$, where $N_x = L_x/\ell$ is the mean number of rods per column in a box of height L_x. The force per contact is $K_n\chi$, then the normal stress is

$$\sigma_{xx} = -\frac{K_n \chi L_x N_y}{L_x L_y} = \frac{K_n l}{d L_x}\Delta$$

where $N_y = L_y/d$ is the number of columns of rods in the sample of width L_y. On the other hand,

$$\sigma_{xx} = \lambda_{xx} \frac{\Delta}{L_x}$$

From equating these two expressions we get the relationship between λ_{xx} and K_n, $\lambda_{xx} = K_n \ell/d$. A similar calculation yields $\lambda_{yy} = K_n d/\ell$.

It is easy to see that for our system of sliding rods, the shear moduli $\lambda_{xy}, \lambda_{yx}$ are zeros, because the ordered stack of rods with no static friction forces among rods has no shear rigidity and a shear strain produces no shear stress.

The bending constant ξ can be computed by considering the increase in energy of a parallel set of spherocylinders that are then bent into a radial geometry with a curvature radius R. In the calculation, all rods have diameter d and length ℓ. In the bent geometry, the center $\vec{\zeta}$ of a rod is parameterized by coordinates r, θ (θ assumed small), and Δy, associated with Cartesian coordinates $(r \sin(\theta), r \cos(\theta) + \Delta y)$. The corresponding tangential unit vector $\hat{t}$ along the rod axis is $(\cos(\theta), -\sin(\theta))$.

We consider two columns of rods that are bent along two circles with radius R but different centers (different Δy), see Fig. S4. We assumed $\Delta y = 0$ and $\Delta y = -d$ for the two sets rods, such that there is no overlap between the rods for $R \to \infty$, but this can be relaxed.

The energy for two touching spherocylinders shown in Fig. S4 is proportional to the square of the overlap χ_{12}. The overlap for two rods with centers $\vec{\zeta}_1$, $\vec{\zeta}_2$ and respective tangential unit vectors $\hat{t}_1$, $\hat{t}_2$ is defined to be

$$\chi_{12} = \max \left[0, \ \max \left(d - \left| (\vec{\zeta}_1 + s_1 \hat{t}_1) - (\vec{\zeta}_2 + s_2 \hat{t}_2) \right| \ : \ |s_1| \leq (\ell - d)/2, |s_2| \leq (\ell - d)/2 \ \right) \ \right] \tag{1}$$

To obtain the mean energy per rod we have to average the square of the overlap χ_{12} over all possible values of angle θ_2 (for a given θ_1) for which there is non-zero overlap. Similarly, we can compute the mean square overlap $\langle {\chi_{12}}^2 \rangle$ for the contact between the rod at $\Delta y = 0$ and a rod at $\Delta y = d$. Using standard techniques, we find an asymptotic expression for the mean square overlap between a rod and its upper and lower neighboring rods for small ℓ/R:

$$\left\langle {\chi_{12}}^2 \right\rangle_{\text{total}} \approx \frac{(\ell - d)^4}{60 R^2} \tag{2}$$

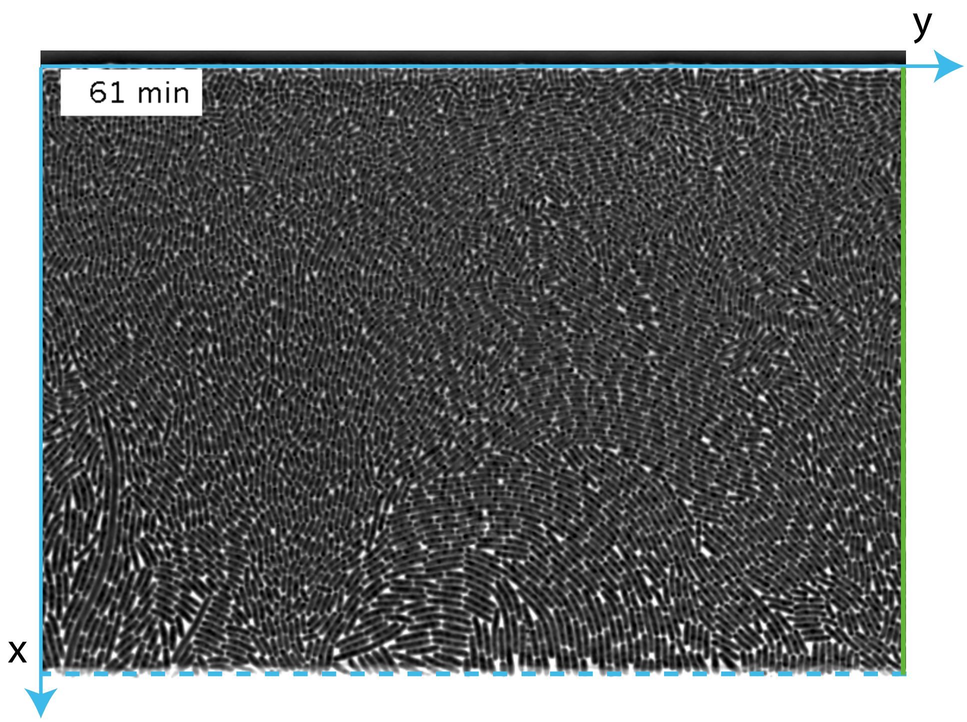
Supposing that the interaction energy between rods is Hookean, we obtain the bending energy per rod $E_b = K_n \langle {\chi_{12}}^2 \rangle_{\text{total}} /2$. After dividing the energy by the area of the rod

($\approx d\,\ell$) to compute the bending energy per unit area, we then find the bending constant

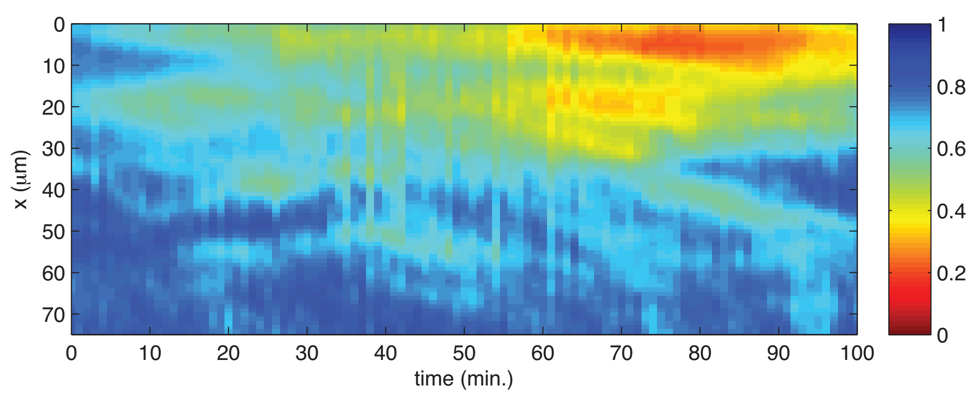
$$\xi = \frac{K_n(\ell - d)^4}{120 d\,\ell} \tag{3}$$

which scales approximately as ℓ^3/d for $\ell \gg d$. Note that $\xi = 0$ when $\ell = d$, i.e. when the rods degenerate into spheres, as expected.

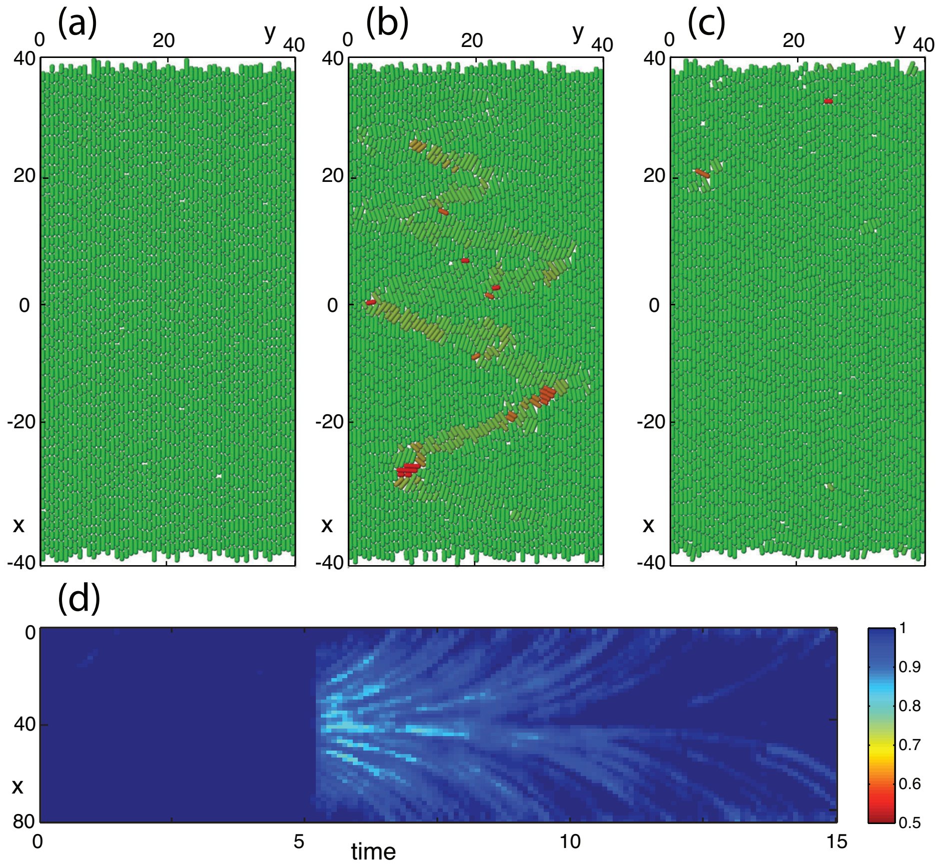
Supplementary Figures



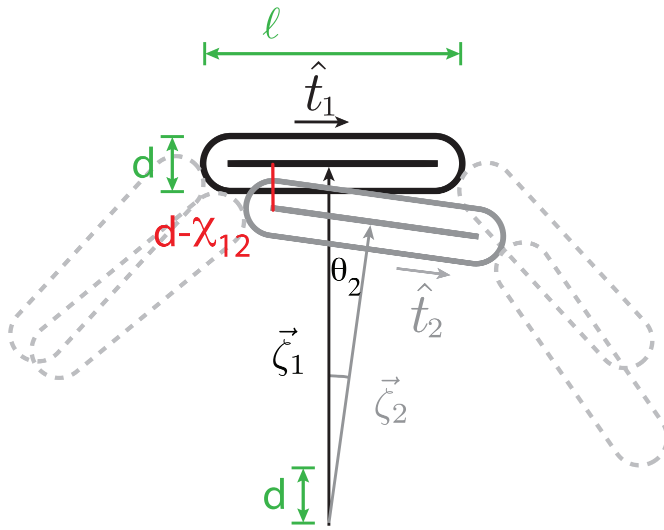
Supplementary Figure S1: A snapshots from the experimental run in a 100×150 μm^2 side trap in which buckling instability was observed. The dashed blue line shows the open side of the trap.



Supplementary Figure S2: Space-time diagram of the local order parameter η averaged over the width of the trap for the run illustrated by Fig. S1



Supplementary Figure S3: (a-c) Three still frames from a simulation of a growing colony in a 40×80 open trap at times (a) $t = 5$, (b) $t = 6$, (c) $t = 15$. The growth rate $a = 0.5$, mean aspect ratio of cells at division is $A = 4$, and the bottom friction $\mu = 5$ was turned on at $t = 5$. Coloring of the rods indicates rod's angle with respect to x-axis: green $\phi = 0$, red $\phi = \pm\pi/2$. (d) Space-time diagrams of the magnitude of the order parameter averaged over the y dimension for the simulation exemplified in Fig. S3a-c



Supplementary Figure S4: Schematic of the bending geometry used for the calculation of ξ. We show the interaction between two rods (additional rods shown as dashed lines) with centers $\vec{\zeta}_1$, $\vec{\zeta}_2$, and respective tangential unit vectors $\hat{t}_1$, $\hat{t}_2$. The rod centers are shown such that $\theta_1 = 0$. Rods 1 and 2 interact through a contact force that depends on the overlap distance χ_{12}. The red line indicates the minimal distance between the axes of rods 1 and 2 for this configuration.

Supplementary Movies

Movie S1. Development of a bacterial colony in a $100 \times 90\mu m^3$ side trap.

Movie S2. Development of a bacterial colony in a $150 \times 100\mu m^3$ side trap.

Movie S3. DES simulation of a population of growing and dividing rods in a 40×80 open trap. The mean aspect ratio of rods at division time is $A = 6$, growth rate $a = 0.71$, bottom friction $\mu = 20$ is turned on at $t = 20$. Rods are colored according to their orientation.

Movie S4. DES simulation of a population of growing and dividing rods in a 40×80 open trap. The mean aspect ratio of rods at division time is $A = 4$, growth rate $a = 0.5$, bottom friction $\mu = 10$ is turned on at $t = 50$. Rods are colored according to their orientation.

Movie S5. DES simulation of a population of growing and dividing rods in a 40×80 side trap. The mean aspect ratio of rods at division time is $A = 6$ near the open boundary, and $A = 3$ near the back wall. The growth rate $a = 1$ near the open boundary, and $a = 0.5$ near the back wall. The coefficient of bottom friction $\mu = 13.5$. Rods are colored according to their orientation.

Movie S6. DES simulation of a population of growing and dividing rods in a 40×80 side trap. The mean aspect ratio of rods at division time is $A = 4$ everywhere. The growth rate $a = 1$ everywhere. The coefficient of bottom friction $\mu = 13.5$. Rods are colored according to their orientation.