Data-driven quantitative modeling of bacterial active nematics

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Active matter comprises individual units that convert energy into mechanical motion. In many examples, such as bacterial systems and biofilament assays, constituent units are elongated and can give rise to local nematic orientational order. Such ‘active nematics’ systems have attracted much attention from both theorists and experimentalists. However, despite intense research efforts, data-driven quantitative modeling has not been achieved, a situation mainly due to the lack of systematic experimental data and to the large number of parameters of current models. Here we introduce a new active nematics system made of swarming filamentous bacteria. We simultaneously measure orientation and velocity fields and show that the complex spatiotemporal dynamics of our system can be quantitatively reproduced by a new type of microscopic model for active suspensions whose important parameters are all estimated from comprehensive experimental data. This provides unprecedented access to key effective parameters and mechanisms governing active nematics. Our approach is applicable to different types of dense suspensions and shows a path towards more quantitative active matter research.

Significance Statement

Active nematics are non-equilibrium fluids consisting of elongated units driven at the individual scale. They spontaneously exhibit complex spatiotemporal dynamics, and have attracted the attention of scientists from many disciplines. Here, we introduce a novel experimental system (made of filamentous bacteria) and a new type of microscopic model for active nematics. Simultaneous measurements of orientation and velocity fields yield comprehensive experimental data that can be used to identify optimal values for all important parameters in the model. At these optimal parameters, the model quantitatively reproduces all experimentally measured features. This, in turn, reveals key processes governing active nematics. Our versatile approach successfully combines quantitative experiments and data-driven modeling; it can be used to study other dense active systems.

Examples of active matter can be found at diverse length-scales (1–6) from animal groups (7–11) to cell colonies and tissues (12–18), to \textit{in vitro} cytoskeletal extracts (19–26), and man-made microscopic objects (27–32). Energy input at the level of the individual constituents drives active matter systems out of thermal equilibrium and leads to a wide range of collective phenomena, including flocking (7, 19, 28, 29, 33, 34), swarming (12, 13), clustering (14, 27, 30, 32), two-dimensional long-range order (15, 35), giant number fluctuations (14, 15, 33, 35, 36), spontaneous flow (21, 24, 25, 37, 38), and synchronization (16).

Active matter systems consisting of elongated particles often lead to local nematic orientational order. This important active nematics class comprises experiments with vibrating granular rods (36), crawling cells (39–41), swarming sperms (42), filamentous bacteria (15) and motor-driven microtubules (20, 21, 24), which, together with theoretical work, have shown that the interplay between orientational order, active stress, particle and fluid flow leads to complex spatial-temporal dynamics and unusual fluctuations. The seminal work by the group of Dogic (21, 43) has been particularly influential. They experimentally observed spontaneous chaotic dynamics driven by topological defects, and their results triggered a large number of theoretical and modeling approaches. These are of two main types, particle-level ‘microscopic’ models (43–45) and continuous-level ‘hydrodynamic’ descriptions (46–53), with the latter usually written phenomenologically or by complementing equilibrium liquid crystal theories with minimal active terms. These studies provided important insights into the multi-faceted dynamics of active nematics, such as hydrodynamic instabilities, long-range correlations, anomalous fluctuations, defect dynamics, spatial and temporal chaos. However, these models generally contain a large number of parameters. This has made comparisons between models and experiments semi-quantitative at best.

Bacteria are widely used as model systems to study active matter (12–16). A recent study showed that elongated E. coli cells strongly confined between two glass plates can display the long-range nematic order and anomalous fluctuations typical of dry, dilute active nematics systems (15). However, so far, almost no bacterial system has been reported to exhibit the phenomenology of dense, wet active nematics as reported first by Dogic \textit{et al.}. One exception is a study of motile bacteria dispersed in a non-toxic lyotropic nematic liquid crystal (54, 55). When bacteria concentration is high enough, active stress destabilizes the ordered nematic state of this biosynthetic system, leading to a state where topological defects in the liquid crystal evolve chaotically in a manner closely


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Fig. 1. (A) Schematic illustration of a bacteria colony growing on agar; the active nematics dynamics studied here takes place in a millimeter-wide, few-micron thick region at the edge; our observation region is typically $277 \times 277 \mu m$. Mean cell length varies from 6 to $14 \mu m$, depending on antibiotic concentration. (B) raw image of our fluorescent cells (scale bar $30 \mu m$) in some experiment performed at $45 \mu g/mL$ drug level. (C,D) nematic order and velocity fields extracted from B. Black rods in C represent unit length director vector $\bar{u}$, and length of arrows in D is proportional to the local speed (scale bar $250 \mu m/s$). (E): colormaps coding the orientation of the nematic and velocity fields in C and D. The white symbols in C represent the $\pm \frac{\pi}{2}$ defects (see SI text and Fig. S2 for details about their orientation).

resembling that of the Dogic system. Here, we show that the typical phenomenology of wet, dense, active nematics can be experimentally realized in colonies of filamentous bacteria and show how to build a data-driven quantitatively-faithful theoretical description of it. To this aim, we introduce a new type of microscopic model for active suspensions and we use simultaneous experimental measurements of both orientation and velocity fields to estimate all its parameters.

**Experimental results**

Our experiments are carried out with *Serratia marcescens* bacteria. At the edge of growing colonies, 2-3 layers of cells actively swim by rotating flagella in a micrometer-thick millimeters-wide film of liquid on the agar surface (Fig. 1A). Apart from a narrow ($\sim 100 \mu m$) outer ring, the thickness of this quasi-2D suspension is very constant. No obvious spatial or temporal inhomogeneity is noticeable in measured fields. A sub-lethal level of antibiotic drug Cephalexin is added into the growth agar medium. The drug allows bacteria to grow but not to divide, leading to long cells. By varying the drug concentration, we can change the mean cell length by a factor of two, see Fig. S1A. Bacteria are labeled with a green fluorescent protein, which allows to record their motion under the microscope. In the dense, thin layer of interest, cells are almost always in close contact and nearly cover the whole surface. Our elongated cells are also frequently nematically aligned, as testified by the presence of $\pm \frac{1}{2}$ charge topological defects typical of 2D nematics (Fig. 1B). (Standard cells cultivated without antibiotic drug do not give rise to any significant local order.) Our images do not allow to distinguish the current polarity of each cell, i.e., in which direction it is currently swimming with respect to the fluid. In fact, the swimming of most bacteria is strongly hampered at such high density. Nevertheless, our cells move collectively, mainly advected by the fluid they have set in motion, in a spatiotemporally chaotic manner strongly reminiscent of other active nematics systems (21, 54) (Movies S1 and S2). From each image, we extract a nematic orientation field $\bar{u}(r, t)$ through a gradient-based method, and $v(r, t)$ the velocity field of cells in the laboratory frame using a standard particle image velocimetry technique (Fig. 1C,D, SI Appendix, Fig. S2). Movie S1 shows the typical evolution of the obtained coarse-grained orientation and velocity fields. This dynamics is fast. Typical correlation times are of the order of seconds (see below). In each experiment, we record images for 30 s, which is significantly shorter than the cell division time (20 min). Therefore, contributions of cell growth to active stress are negligible in our work (56, 57).

**Global measurements.** We first measure global statistical properties of our velocity and orientation fields. The average cell speed $v \equiv \langle |v(r, t)| \rangle_{r, t}$ varies between 20 and $50 \mu m/s$ from experiment to experiment but is approximately independent of the drug concentration (SI Appendix, Fig. S1B,C).

Next we compute spatial and temporal two-point correlation functions, which are defined and shown in Fig. 2A-D. The spatial/temporal separations corresponding to a correlation value of $1/e$ are identified as the correlation lengths and times. Symbols $L_v$, $L_n$, $t_v$, and $t_n$ respectively denote velocity and orientation correlation lengths, velocity and orientation correlation times. These quantities are typically of the order of tens of $\mu m$ and one second. When we increase the cell length with antibiotics, the correlation lengths $L_n$ and $L_v$ increase systematically (Fig. 2A,B). Such a systematic variation is only observed for correlation times $t_n$ if time is rescaled by the mean speed $v$ (Fig. 2C,D). Correlation functions from various experiments with different drug concentrations collapse onto each other when space and time are rescaled by correlation lengths and times (insets in Fig. 2A-D). Moreover, all these quantities are linearly related to each other. Strikingly, transforming correlation times into correlation lengths using the mean speed $v$, we find that $L_n$, $v \times t_n$, and $v \times t_v$ are all proportional to $L_v$ with approximately the same slope (Fig. 2E). This indicates that our experiments are characterized by a single lengthscale and the mean flow speed (58, 59). Because our bacteria are too closely packed to measure their length, we use $L_v$ and $v$ as “effective control parameters” of our experiments, with $L_v$ serving as a good proxy to the mean cell length, see SI Appendix, Fig. S1.

**Defect properties.** To go beyond the reduction of the complex spatiotemporal dynamics of our bacterial system to just a lengthscale and the mean speed, we now focus on the $\pm \frac{1}{2}$ topological defects of the orientation field. Their detailed structure and their dynamics offer unique access to the coupling between nematic order and flow, all information that we will show later to be crucial to determine model parameters.

We identify the location of $\pm \frac{1}{2}$ defects by contour integral of the director field (see Fig. 1C and Movie S1 for typical results). From the trajectories of defect cores, we measure...
\( v^\pm \), their velocity in the lab frame. We also measured the velocity of defects in the fluid frame, \( \Delta v^\pm = v^\pm - v_{\text{back}} \), where \( v_{\text{back}} \) is the fluid “backflow” velocity averaged over a small region surrounding the defect core (see SI Appendix, Fig. S2D). We finally determine the intrinsic orientation \( \vec{u}^\pm \) of defects. This is straightforward for the comet-shaped \( \pm \frac{1}{2} \) defects. For the \( \pm \frac{1}{2} \) defects, which are not polar but have a three-fold symmetry with three radial axes along which the nematic director is aligned, we choose the axis closest to the current orientation of \( v^- \) (see SI Appendix and SI Appendix, Fig. S2 for details).

As in other active nematics systems (21, 36, 41), defects are created in \( \pm \) pairs by bending of the ordered regions (Movie S1). Upon generation, \( \pm \frac{1}{2} \) defects typically quickly move away and less motile \( \pm \frac{1}{2} \) defects stay longer near the generation site. Pair of defects of opposite charge may also annihilate upon encounter. In a given experiment, generation and annihilation of defects balance each other so that their total number is approximately constant in time. The radial distribution functions of defect position, \( g(r) \), reveals that defects with the same sign repel from each other at short distances (Fig. 3A-C). For defects of opposite sign, \( g(r) \) has a short-scale peak reflecting the fact that defects are created in \( \pm \) pairs (43).

Restricting our analysis to “isolated” defects from now on, i.e. whose distance from nearest neighbors is larger than nematic correlation length \( L_n \), we observe that defects are essentially distributed randomly in space: no global translational nor orientational order is observed. Defect speed distributions, both in the lab and in the fluid frame, show that \( \pm \frac{1}{2} \) defects are more motile, but \( \pm \frac{1}{2} \) defects do not have a negligible speed, even in the fluid frame (Fig. 3E,G). We also find that the defect orientation \( \vec{u}^\pm \) is strongly correlated to their velocity orientation, and to the orientation of their velocity in the fluid frame. Essentially, all three vectors are aligned, even for the \( \pm \frac{1}{2} \) defects (Fig. 3H-K). Note that a small but finite velocity in the fluid frame \( \Delta v^- \) is at odds with usual statements about \( \pm \frac{1}{2} \) defects in active nematics, where they are treated as symmetric, force-free, diffusive objects (44, 53, 60). We elaborate on this point in Discussion section.

To further quantify the structure of defects, we average, over time and many defects, the orientation and velocity fields around their core, sitting in their intrinsic reference frame. The familiar mushroom-shape and three-fold symmetry of, respectively, the \( \pm \frac{1}{2} \) and \( \pm \frac{1}{2} \) defect are clearly observed (Fig. 4A,B). We also find that the speed of defects relative to the local flow speed at their core decreases with \( L_n \) while being also roughly independent of \( v \) (Fig. 5A). In the steady-state, the density of defects is statistically constant. From this steady density one can extract an inter-defect lengthscale \( L_d \), which behaves like all other correlation lengths, in agreement with previous work on wet active nematics (62, 63) (Fig. 5B). We also find that the speed of defects relative to the local flow speed at their core decreases with \( L_n \) while being also roughly independent of \( v \) (Fig. 5C,D, see a discussion of this below). Remarkably, the detailed spatial structure of defects does not vary significantly between experiments with different characteristic lengths: after rescaling spatial coordinates by defect core size, or, equivalently, correlation length, averaged director and velocity fields from different datasets overlap nicely. We further confirm this by comparing defect angular profiles at \( 0.6 R_\pm \) for different experiments (Figs. 5E-L).

**Quantitative modeling**

A microscopically faithful model of our dense, thin bacterial system where cells and their many flagella are in constant con-
All this also allows us to build an efficient, streamlined, but	
SI Appendix, Table S1 (red curves), corresponding to 6th column of	
Two-point pair correlation functions $g_4$ forcing. A dipole represents the local cell body orientation and active	
fluid film, and differs significantly from the common choice	
of non-swimming force dipoles immersed in an incompressible	
advected and rotated by the fluid. Our model thus consists	
crowded cells mostly exert force dipoles on the fluid, which is	
nearby cells prevent them to do so (see Movie S2). These	
Description of the numerical model. Recall that most cells in	
our dense system are not able to swim freely, simply because nearby cells prevent them to do so (see Movie S2). These
crowded cells mostly exert force dipoles on the fluid, which is then set in motion by their collective action. Cells, in turn, are	
advected and rotated by the fluid. Our model thus consists of non-swimming force dipoles immersed in an incompressible fluid, and differs significantly from the common choice of using a dynamic equation for a director field (64–69). As shown by a schematic diagram in SI Appendix, Fig. S3, each dipole represents the local cell body orientation and active forcing.

tact with each other and with the gel substrate is a formidable task well-beyond current numerical power. Besides, this would require the knowledge of many specific details that are unknown. Here we adopt a radically different approach: we treat the collisions and local interactions between cell bodies and their flagella at some effective level, where, we assume, they amount to a combination of steric repulsion and alignment. In addition, the far-field interactions and other effects due to the incompressible fluid surrounding bacteria are taken into account by solving the Stokes equation for the fluid flow. All this also allows us to build an efficient, streamlined, but comprehensive model in two space dimensions.

The fluid flow $\mathbf{v}(r,t)$ is the solution of the (2D) Stokes equation

$$\mu \nabla^2 \mathbf{v} + \nabla p - \alpha \mathbf{v} + \mathbf{F} = 0 \quad \text{with} \quad \nabla \cdot \mathbf{v} = 0$$

where $\mu$ is the fluid viscosity, $\alpha$ is the effective friction with the substrate, $p$ is the pressure enforcing the incompressibility condition, and $\mathbf{F}$ is the active force field exerted by dipoles on the fluid (64).

Our dipoles are point particles with position $\mathbf{r}_i$ and orientation $\hat{\mathbf{u}}_i$ (or, equivalently, unit orientation vector $\hat{\mathbf{u}}_i = (\cos(\theta_i), \sin(\theta_i))$. They locally align, are advected and rotated by the flow, and experience pairwise repulsion to keep their density homogeneous:

$$\dot{\mathbf{r}}_i = \mathbf{v}(\mathbf{r}_i) + C_s \sum_{j \neq i} \mathbf{r}_{ij}$$

$$\dot{\theta}_i = C_a \sum_{j \neq i} \sin[2(\theta_j - \theta_i)] + C_v \left( \nabla \times \mathbf{v} \right) \cdot \mathbf{z} + C_w \hat{\mathbf{u}}_i \times (\mathbf{E} \cdot \hat{\mathbf{u}}_i) \cdot \mathbf{z} + C_n \dot{\phi}_i,$$

where $\dot{\phi}_i$ is the fluid speed.

In Eq. (3), the first term on the right-hand side, with strength $C_a$, codes for the nematic alignment of dipole $i$ with all neighbors currently present within distance $R_{n}$. The next two terms govern how dipoles are rotated by the flow field $\mathbf{v}$, following Jeffrey’s classic work: both local vorticity $\nabla \times \mathbf{v}$ and local strain $\mathbf{E} = (\nabla \mathbf{v} + \nabla \mathbf{v}^T)/2$ are playing a role, but with coefficients $C_v$ and $C_w$ taking values a priori different from the classic ones calculated for perfect ellipsoids with no-slip boundaries (70). Finally, $C_n$ is a unit-variance, white, angular Gaussian noise. In Eq. (2), the right-hand side term $\mathbf{r}_{ij}$ represents a unit-range pairwise soft repulsion force between dipoles of strength $C_s$.

Note that self-propulsion is not included in Eq. (2) because our system is crowded.

The force field $\mathbf{F}$ in Eq. (1) is assumed to be dominated by the gradient of the active stress tensor field. (A small, residual contribution from the short-range repulsion force between neighboring dipoles exists, but can usually be neglected, see SI Appendix, Eq. S2 for details about this point.) The active stress tensor is itself assumed, as usual in wet active nematics studies (50, 51), to be proportional to the gradient of the orientation field:

$$\mathbf{F} = f_0 \nabla \cdot \hat{\mathbf{u}}$$

where $f_0$ is the typical strength of dipoles. In experiments, $\hat{\mathbf{u}}$ is the measured nematic orientation field. In the model, $\hat{\mathbf{u}}$ is the local coarse-grained orientation of our dipoles.

The full system constituted by Eqs. (1–4) can be seen as a minimal Vicsek-style model (71, 72) incorporating the main mechanisms at play in our bacterial active nematics. One thus expects a basic interplay between alignment and noise: if the alignment strength $C_a$, or the alignment range $R_n$, or the number density of dipoles $\rho_0$, or the noise strength $C_w$ is weak enough, local orientational (nematic) order can emerge. The global number density of dipoles $\rho_0$ and the noise strength $C_w$ have opposite effects. We checked that changing $\rho_0$ in the experimentally reasonable range [1.5, 4] (in simulation units) yields similar results. In the following, we fix $\rho_0 = 1.5$ to lighten the numerical task.

It is relatively easy to find parameter values such that the dynamics of our model closely resembles the experimental observations. As a matter of fact, the region of parameter space

\[\text{Fig. 3. Statistical properties of defect cores. Experimental data extracted from the experiment at drug level 45μg/mL that gives a correlation length } L_c = 39.7 \mu m \text{ and a mean flow speed } v = 50 \mu m/s \text{ used in most of the text (blue curves), and from simulations of our model at parameter values optimized for that experiment (red curves), corresponding to 6th column of SI Appendix, Table S1. (A-C): Two-point pair correlation functions } g(r) \text{ for the positions of defect cores (respectively } (+\frac{1}{2}, +\frac{1}{2}), (-\frac{1}{2}, -\frac{1}{2}), \text{ and } (+\frac{1}{2}, -\frac{1}{2}) \text{ pairs). (D-G): probability distribution functions of various defect speeds (respectively speed of } +\frac{1}{2} \text{ and } -\frac{1}{2} \text{ defects in lab frame, and speed of } +\frac{1}{2} \text{ and } -\frac{1}{2} \text{ defects in fluid frame). (H,K): probability distribution functions of angle between defect orientations } \hat{x} \text{ and fluid velocity at their core } \hat{v}_{\text{track}}. (JK): same as (HJ), but for the defect core velocities in the lab frame } \hat{v}_{\text{track}}.\]
where spatiotemporally chaotic active nematics behavior occurs is rather large. To go beyond such qualitative agreement, we have systematically investigated the effects of parameters. We now show that for each experimental dataset, there exists a unique set of parameter values at which the model optimally matches the experiment, in the sense that all quantities studied in the previous section are in quantitative agreement.

**Data-driven parameter optimization.** We proceed in two steps. First, simultaneous measurements of velocity and orientation fields allow us to pinpoint the parameters in Eq. (1) without resorting to the "microscopic" part of the model, i.e. Eqs. [2,3].

Dividing both sides of Eq. (1) by $\alpha$, we are left with two independent parameters, $\mu/\alpha$ and $f_0/\alpha$. Therefore for any given pair of parameters $\mu/\alpha$ and $f_0/\alpha$, and a particular experimentally-measured orientation field $\hat{u}$, we can compute the velocity field $v_*$ solution of Eq. (1). We then compare $v_*$ with $v$, the velocity field measured at the same time as $\hat{u}$. Scanning the whole $(\mu/\alpha, f_0/\alpha)$ parameter plane, we find that there is an optimal point where the difference between $v_*$ and $v$ is minimal on average. Specifically, we measure the quality function $Q_v(\mu/\alpha, f_0/\alpha) = \langle |v_*(r, t) - v(r, t)|^2/|v(r, t)|^2 \rangle_{r,t}$, where the average is carried out over both space and time. A typical result for an experiment with 45 µg/mL drug concentration is in Fig. 6A, where $Q_v$ shows a minimum for $Q_v = 0.23$ at $f_0/\alpha = 6174 \mu m^2/s$ and $\sqrt{\mu/\alpha} = 36 \mu m$. Typical instantaneous velocity fields $v_*$ produced at these parameters compare very well to the corresponding $v$ fields (Fig. 6B,C, movie S3).

After fluid parameters are fixed, we proceed to the second step and match the full model with experiments. Eqs. (2-3) contain six parameters. We first evaluate their influence by varying them individually around a reference point (see SI Appendix, Fig. S4 for details). We find that angular noise level $C_h$ and repulsion strength $C_r$ are not sensitive parameters provided local order is not destroyed by strong noise and particles do not crystallize for too-strong repulsion. We therefore fix $C_h = 1.0$ and $C_r = 0.5$. Nematic alignment parameters $C_s$ and $R_s$ play a major, but similar role, so we decide to fix $C_s = 0.4s^{-1}$ and vary $R_s$, mimicking the change of cell length in experiments. This leaves us with only three parameters to vary, $R_s$, $C_s$, and $C_\alpha$, when looking for an optimal match between model and experiment.

We performed a systematic scan of this restricted parameter space, running the model for many sets of parameter values, and extracting from each of these runs the quantities of interest, i.e. those measured also in the experiment. To quantify the match between model and experiment, we found that using 3 independent quality functions is sufficient. Here we
use $Q_1 \equiv L_n^+ - L_n^-$, the difference in nematic correlation length, $Q_2 \equiv S^+_n - S^+$ and $Q_3 \equiv S^-_n - S^-$ the differences in defect speed ($S^\pm \equiv \langle v^\pm \rangle$), respectively for the $+\frac{1}{2}$ and $-\frac{1}{2}$ defects. (As before, the * subscript denotes quantities measured on the model.) Computed quality functions in the three-dimensional parameter space {$R_n$, $C_v$, $C_s$} are shown in Fig. 6D. Perfect matching ($Q_{1(+,-)} = 0$) occurs for each function on a surface. These three surfaces approximately cross at a single point, as shown in the last row of Fig. 6D. For the particular experiment considered, we find $R_n = 13.8 \mu m$, $C_v = 0.5$, and $C_s = 0.5$, which thus defines our optimal set of model parameters. By construction, these parameter values optimize the match between model and experiment for what concerns the quantities involved in the quality functions used. Remarkedly, we observe that all other quantities not used in these functions are also quantitatively matched. This is in particular the case for all correlation functions in Fig. 2, all distributions of defect speed and orientation, and spatial distributions of defects in Fig. 3, all averaged angular profiles of isolated defects in Fig. 4, defect size and speed in Fig. 5 (see also simulations of the model at optimal parameters in Movie S4).

Fig. 5. Dependence of defects properties on experimental conditions. (A-D): variation with nematic correlation length $L_n$ of defect core size $R^\pm$ (A), mean inter-defect lengthscale $L_d$ (B), mean of $+\frac{1}{2}$ and $-\frac{1}{2}$ defect speed $S^\pm$ divided by local flow speed $\langle v^\pm \rangle$ (C,D). Experiment and simulation results are shown by open squares and solid stars, color-coded by the mean speed $v$, following Fig. 2E. All experiments and simulations collapse onto single straight lines, indicating that $v$ does not influence the quantities represented. (E-L) angular profiles as in Fig. 4 calculated along the circle of radius $0.6R^+$ for 3 experimental datasets obtained at different drug levels (blue: 30 µg/mL, 1st column in SI Appendix, Table S1, green: 45 µg/mL, 6th column in SI Appendix, Table S1, red: 60 µg/mL, 12th column in SI Appendix, Table S1). Corresponding simulation results are shown using dashed lines.

Finally, we performed two ‘consistency checks’. We verified that choosing a different value of $C_s$ yields a different optimal value of $R_n$ but that all other optimal parameter values then approximately remain the same (SI Appendix, Fig. S6). In short, $R_n$ and $C_s$ are fully redundant. Next, taking our optimal parameter set, but now “freeing” the fluid parameters $\mu/\alpha$ and $f_0/\alpha$ from the values determined during our first step, we find that these initial values remain optimal (SI Appendix, Fig. S7). This confirms that our procedure, for a given experiment, yields a unique set of model parameters at which model dynamics optimally matches spatiotemporal data.

Variation of model parameters. We have successfully applied our matching procedure to a large set of experiments with drug concentration above 15 µg/mL, the level below which cells are too short to give rise to a clear local nematic orientation that can be reliably measured. For each experiment, the quality of the matching between experiments and simulations remains excellent. Corresponding orientation and velocity fields from simulations at these optimal parameters are shown in Movie S4. We thus obtained the variation of the optimal model parameter values with the two experimental effective control parameters, the correlation length (proxy for cell size) and the mean flow speed $v$ (see Fig. 7 and SI Appendix, Table S1). This provides us with a wealth of information about our experimental system.

We first discuss the effect of the mean speed $v$ at fixed correlation length. Choosing a subset of experiments yielding approximately the same correlation length, we observe that $v$ almost exclusively influences $f_0$, and does so linearly (Fig. 7A). The other parameters remain constant with the exception of the interaction range $R_n$, which grows slightly with $v$ (Fig. 7B-E). The clear linear growth of $f_0$ confirms that, via $v$, one
We show that the two scalings above are verified for all our data points in (A-E) and full (D) model matching. Optimal parameters are marked by a red dot. (A): quality function $Q_{v}$ in the $(\sqrt{\mu/\alpha}, \sqrt{f_0/\alpha})$ plane. (B): a typical instantaneous experimental velocity field. (C): velocity field reconstructed from the orientation field measured at the same time as (B) at the optimal parameters indicated in (A). The first three rows of (D) contain quality functions of characteristic length ($Q_{l}$), 1/2 defect speed ($Q_{+}$) and -1/2 defect speed ($Q_{-}$). Each panel represent a scan in the $C_v$-$R_a$ plane and panels in the same column use the same $C_v$ value. Black contour lines mark regions of acceptable deviations. Panels in the last row contain acceptable regions of parameters extracted from quality functions: red from $Q_{l}$, green from $Q_{+}$ and blue from $Q_{-}$; they show that $C_v = 0.5$ yields largest overlap area for acceptable regions of parameters and a red dot in the middle panels marks the optimal choice for parameters $C_v$ and $R_a$.

Fig. 6. Quality functions and results from hydrodynamic (A-C) and full (D) model matching.

Fig. 7. Variation of optimal model parameters with mean flow speed $v$ (A-E) and velocity correlation length $L_v$. Data points in (A-E) have $L_v \approx 40 \mu$m and data points in (F-J) have $v \approx 42 \mu$m/s. The numerical values of all these parameters are listed in SI Appendix, Table S1. Dashed lines in A to J are linear fits (see text); dashed line in J is a fit of $R_a \sim \sqrt{L_v}$ with a $R^2 = 0.925$.

Several dipoles stand for a cell, they react individually to the local strain, and thus their response must be weaker than that of a cell, and the longer the cell, the weaker the response. Finally, the range of nematic alignment increases linearly with the area where nematic alignment takes place, i.e. the number of aligning neighbors, in our model.

Discussion

To summarize, we presented a systematic study of collective motion and defect properties in a dense, wet active nematic system composed of filamentous bacteria, and introduced a physical understanding of the factors contributing to the correlation length, and in particular of how it is connected to the fluid effective parameters. The vorticity coupling parameter $C_v$ is approximately a constant, $C_v \approx 0.5$ (Fig. 7H). This is in agreement with Jeffery’s theory, which shows that $C_v = \frac{1}{2}$ for almost any axisymmetric shape from needles to ellipsoids to disks. Nearly constant $C_v$ is also consistent with observations that defect shape changes little in different experiments (Fig. 5E-L) and that $C_v$ is closely connected to defect shape in our model (SI Appendix, Fig. S5). On the other hand, the strain coupling parameter $C_s$ decreases with $L_v$ (Fig. 7I), at odds with Jeffery’s results, which show that longer objects have higher $C_s$. This can be understood by noticing that in the model particles do not represent cells. Rather, over the interaction range $R_a$, several dipoles stand for a cell. They react individually to the local strain, and thus their response must be weaker than that of a cell, and the longer the cell, the weaker the response. Finally, the range of nematic alignment $R_a \sim \sqrt{L_v}$ (Fig. 7J), which shows that the correlation length increases linearly with the area where nematic alignment takes place, i.e. the number of aligning neighbors, in our model.
minimal microscopic model to account for our experiments. We have shown that using both orientation and velocity measurements enables to determine a unique, optimal set of parameter values at which our Vicsek-style model for active suspensions accounts quantitatively for many if not all quantities that one can extract from experimental data. Because the collective dynamics of our bacterial active nematics is always chaotic, we have used topological defects to estimate these optimal parameter values. As a matter of fact, it is sufficient to use a small subset of the various quantities we measured to determine all optimal parameter values, after which the remaining subset is “automatically” matched too. The existence of a unique optimum at which matching is nearly perfect constitutes, in retrospect, evidence of the quality of our model.

Thanks to quantitative match at a remarkable level of detail, the interplay between experiments and model provides new information and a deeper understanding of our system. This is in particular the case for the dynamics and structure of topological defects. Fig. 5C demonstrates that $+\frac{1}{2}$ defects move approximately twice as fast as the background flow. This acceleration can be explained by the local flow field (Fig. 4C), which shows two vortices above and below the strong jet advecting the defects. The shape of defects is essentially governed by the vorticity coupling constant $C_v$ (the orientation field around $+\frac{1}{2}$ defects changes from from arrow-like to mushroom-like shape when increasing $C_v$ (61, 73)). This cannot be seen in our experiments, in which $C_v$ is essentially constant (Fig. 7C,H) but is shown by simulations of our quantitatively faithful model (SI Appendix, Fig. S5). Thus, the vortices can destabilize orientational order ahead of the core, causing the defect to move faster than the background flow. The accelerating effect weakens when particles are less sensitive to flow vorticity or when nematic interaction becomes stronger, as shown in simulation (SI Appendix, Fig. S4C) and experiments (Fig. 5CD).

The averaged orientation and velocity fields around $-\frac{1}{2}$ defects (Fig. 4B,D) show an approximate 3-fold rotational symmetry, which is consistent with the conventional, equilibrium picture: this symmetry implies that active and elastic stresses are balanced around the defect core, and that $-\frac{1}{2}$ defects are passive particles advected by the background flow. However, our experiments and simulations indicate that $-\frac{1}{2}$ defects possess a small but significant velocity in the fluid frame $\Delta v$ (Fig. 3E,I,G,K,5D). Moreover, instantaneous fields around $-\frac{1}{2}$ defects often deviate significantly from 3-fold symmetry, see SI Appendix, Fig. S9. Such deviations break stress balance around the core and give $-\frac{1}{2}$ defects their velocity over the background flow. Our data (SI Appendix, Fig. S9 and S10) indeed show that the degree of deviation from 3-fold symmetry correlates with this velocity.

Our work also explains the multiple effects of cell length (under the influence of Cephalexin). Cell length directly, and not surprisingly, governs all length scales in our system, and does so nearly identically (Figs. 2E, 5AB, 7F-J). More surprising is the observation that the relative speed of defects decreases with cell length (Fig. 5CD) and that the strain coupling constant $C_s$ decreases for long cells (Fig. 7I).

These findings are just a subset of all those illustrating how, thanks to the quantitative modeling, one can not only determine key effective parameters (such as the strength of flagella or the effective viscosity of our suspension) but also “read” important physical mechanisms from observing how model parameters change in experiments or are changed in simulations.

Our data-driven quantitative matching was made possible thanks to the relative simplicity of our Vicsek-style model: even though it deals with wet active suspensions, it possesses a relatively small number of parameters, and is numerically efficient. Treating near-field interactions only effectively, it is also versatile, and we believe the same approach can be applied to other active suspensions and extended to include other effects, such as external field and polar order.

The simplicity of our model should also allow to derive continuous, hydrodynamic equations. Works on hydrodynamic theories of wet active nematoids abound, but they typically lack a direct connection to microscopic mechanisms. Thus deriving a faithful hydrodynamic theory from our quantitatively-valid model is a very promising step. That would in particular allow to estimate how far our active nematoids deviates from elastic theory predictions, something hinted by the structure of defects (Fig. 4EF). This is the topic of ongoing work at the end of which, we hope, we will be able to build a fully quantitative link between experiments and hydrodynamic theory.

Materials and Methods

Bacteria strain and Colony Growth. We use wild type S. marcescens strain ATCC 274 labeled with green fluorescent protein p15A-eGFP. Bacteria colonies are grown on soft (0.5%) Difco agar plate containing 2.5% Luria Broth (Sigma). We mix Cephalexin with molten agar at 70°C. We then pour 40 milliliters of molten agar into a 15-cm-diameter Petri dish, which is then dried with a lid on for 16 hours (25°C and 50% humidity). About 10 µL of overnight bacteria culture is then inoculated on the agar. The inoculated plates are dried for another 15 min without a lid, then stored in an incubator at 30°C and 90% humidity.

Imaging procedure. After a growth time of 8 – 9 hours, collective motion is observed for as long as 2 hours near the expanding edge of a colony, in an active region about 1 mm wide. The colony expansion speed is approximately 2µm/s, i.e. much smaller than the measured bacteria flow speed. Thus its influence on bacteria velocity measurement can be neglected. We capture bacteria motion in the central part (277 × 277µm²) of this active region through a 40×objective (Nikon S plan Fluor). S. marcescens colonies quickly change from mono-layer to 3 layer within 100µm from the swarming edge, thus the thickness of swarming cells are constant in the observation region. A Nikon MBS45510 filter cube (excitation 470/40nm, emission 525/50nm) is used for fluorescent imaging. Images are acquired by a high-speed camera (Basler acA2040-180km) at 100 frame/s for 30s, during which bacteria motility remains unchanged. Bacteria form an immobile film in the central part of the colony. We take videos far enough from this immobile region.

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