Flocking of Active Particles in a Turbulent Flow

Anupam Gupta,¹ Amal Roy,² Arnab Saha,³ and Samridhhi Sankar Ray⁴

¹John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138
²Department of Computer Science and Automation, Indian Institute of Science, Bangalore 560012, India
³Department of Physics, Savitribai Phule Pune University, Pune 411007, India
⁴International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bangalore 560089, India

(Dated: December 27, 2018)

We investigate the effect of cooperative interactions in an ensemble of microorganisms, modelled as self-propelled disk-like and rod-like particles, in a three-dimensional turbulent flow to show flocking as an emergent phenomenon. Building on the work by Choudhary, et al. [Europhys. Lett. 112, 24005 (2015)] for two-dimensional systems, and combining ideas from active matter and turbulent transport, we show that non-trivial correlations between the flow and individual dynamics are essential for the microorganisms to flock in, for example, a turbulent three-dimensional, marine environment. Our results may have implications especially in the modelling of artificial microswimmers in a hostile environment.

PACS numbers: 47.63.-b 92.20.Jt 47.27.-i

The understanding of collective, cooperative motion of organisms is one of the most important problems in areas spanning physical biology, soft matter, and statistical physics. This is largely due to its ubiquity in the natural world spanning a range of scales from macroscopic (birds and fish) to microscopic (bacteria and plankton) organisms. Therefore it is reasonable to expect that insights to this phenomenon is critically related to understanding self-organised behaviour as well as ecological and evolutionary strategies. Such insights, drawn from a variety of models, show that combining long-range attraction, short-range repulsion and alignment rules between self-propelling individuals of model active systems lead to self-organised collective dynamics of the individuals. It thus allows us qualitative as well as quantitative understanding of the dynamics of real active systems such as cells, autophoretic colloids, macroscopic, yet small, organisms or droplets, synchronised oscillators and bacterial lattices.

Developing an understanding of flocking has been largely confined to the problem of directed motion where the effects of the ambient medium, air or water—typically noisy, random and spatio-temporally complex—and the shapes and sizes of the individuals, are ignored. Such an assumption for the natural world, where the environment can be non-trivial and even turbulent (such as for marine life), is an over-simplification. Indeed, the few studies which have tried to answer this question use either model flows with mass-less, point-sized organisms or the relatively more realistic and instructive, but still academic, case of two-dimensional turbulent flows with finite-sized spherical particles and, more recently, flocking colloids in a randomly and artificially disordered environment. These studies, however, strongly suggest the need to study whether collective motion can exist in the most general, even if simplified, setting. Therefore in this paper, we now show how and why flocking emerges—surprisingly—for microorganisms in a turbulent environment by combining ideas from turbulent transport and active matter and elucidate the critical role of the non-trivial correlations between the flow and individual dynamics. Our work shows that the principles of fluid mechanics leave little choice for organisms but to flock based on their sizes and shapes. Thus the inevitable ubiquity of this phenomenon.

For several reasons, the collective behaviour of self-propelled (active) individuals depends on their ambient medium. Firstly, self-propulsion of active particles—which is key to their self-organisation—arises from the fact that each individual is able to convert the available free energy into directed motion and elucidate the critical role of the non-trivial correlations between the flow and individual dynamics. Our work shows that the principles of fluid mechanics leave little choice for organisms but to flock based on their sizes and shapes. Thus the inevitable ubiquity of this phenomenon.

For organisms which move and flock in air or water, a naive guess would be that the flocks ought to break up in the presence of such strong perturbations. However, observations show that a wide class of organisms are able to overcome such strong perturbations and show evidence of collective behaviour. Therefore it is important to investigate if the active nature of microorganisms and their strategy to self-organise can overcome their Stokesian drag and turbulent mixing, to show or-
organised, flocking behaviour in a three-dimensional (turbulent) fluid environment? And, if so, are there preferred sizes and shapes which lead to flocking as a spontaneously emergent phenomenon in a collection of self-propelled particles in a turbulent flow?

We therefore perform detailed numerical simulations of the motion of a suspension of self-propelled active particles, of different shapes and sizes, in three-dimensional turbulence. We use a standard pseudo-spectral method to obtain turbulent solutions of the driven, incompressible Navier-Stokes equation and choose parameters to ensure a Taylor-scale Reynolds number $Re_{\lambda} = 130$ which is consistent with typical marine settings \[38\]. These microorganisms, modelled as spheroids, have both rotational and translational degrees of freedom and their dynamics is governed by (a) the drag due to the carrier flow which depends on their individual sizes and shapes, (b) their self-propelled velocity, and (c) their short-ranged alignment interactions with other individuals within a neighbourhood. We ensure that the particle sizes are smaller than the characteristic Kolmogorov length scales of the fluid. The dynamics of such particles are characterised by their (unit) orientation vector $\hat{p}_i$ following \[39\]

$$
\frac{d\hat{p}_i}{dt} = \Omega \times \hat{p}_i + \frac{\alpha^2 - 1}{\alpha^2 + 1} [S \hat{p}_i - (\hat{p}_i \cdot S \hat{p}_i) \hat{p}_i]
$$

(1)

and their translational velocity vector, determined from the linear Stokes drag model (valid for small particles) for non-spherical particles \[20, 21, 40\]

$$
\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i; \quad \frac{d\mathbf{v}_i}{dt} = -\frac{A^T K A \left[\mathbf{v}_i - \mathbf{u}(\mathbf{r}_i, t)\right]}{6\pi \alpha \lambda},
$$

(2)

where $i$ is the particle index. Not surprisingly the instantaneous orientation is determined by the local geometry of the advecting flow $\mathbf{u}$, namely the symmetric $S$ (strain rate) and antisymmetric $\Omega$ (vorticity) tensors of the fluid-velocity-gradients at the particle positions and inertial effects in the rotational dynamics are negligible as shown in previous studies \[41, 42\]. Inertial effects are however important in the translational degrees of freedom (Eq. (2)) where the effective drag on the individual depends on the instantaneous orientation in the flow as well as its shape $\alpha$, the ratio of the semi-major and minor axes of the particles \[43, 44\]: $\alpha = 1$ is a spherical; $\alpha < 1$ is disk-like (oblate) and $\alpha > 1$ is rod-like (prolate). Thus, the resistance tensor $K$ and the orthogonal transformation matrix $A$ are necessary to take into account the shape of the microorganism \[43, 45\] and this leads to a time-dependent drag coefficient, in contrast with the constant drag associated with a spherical particle. However, for convenience we define the average Stokes number $St = \tau_p/\tau_\eta$ \[41, 45\] to quantify our results as well as compare microorganisms of different shapes; $\tau_\eta$ is the characteristic small-scale Kolmogorov time-scale of the ambient fluid. Our particles are of course active with a self-propelled velocity along the orientation vector $v_0\hat{p}_i$. Coupling this with translational equations of motion, the instantaneous velocity vector of the $i$-th individual is a superposition of these two competing effects, namely $\mathbf{v}_i = \mathbf{v}_i + v_0\hat{p}_i$.

Let us finally introduce interactions in a collection of such active microorganisms. We use Vicsek-like interactions \[23\] to ensure that at discrete time intervals $\Delta T$ each individual $i$ orients itself along the average direction $\hat{n}_i^\text{avg}$ of all individuals $N_{\text{int}}$ (with the same shape and size) within a radius of interaction $r_{\text{int}}$ of it. This radius of interaction is a way to ensure, as is the case in actual living organisms, that an individual is not able to see others in the population who are physically far away. Of course this assessment of the average orientation cannot be perfect. To account for this imperfection we introduce an additive small random noise in the calculation of $\hat{n}_i^\text{avg}$ for each individual. This implies

$$
\mathbf{v}_i(t) = |\mathbf{v}_i(t)|\hat{n}_i^\text{avg},
$$

(3)

where $t = m\Delta T$ ($m$ is an integer). A similar strategy is used for the re-orientation at discrete time intervals for the vector $\hat{p}_i$. Between successive reorientations, particles evolve through the linear, Stokes drag model and its self-propelled velocity as described. We report results from 3 different values of $r_{\text{int}}$, namely, 0.03$\pi$, 0.2$\pi$, and 0.4$\pi$. (This strategy is also found to be useful for many other purpose such as collective foraging \[50\].) We also
use three different values of the self-propelled velocity: \(v_0 = 0\) (the passive case), \(v_0 = 0.2u_\eta\), and \(v_0 = 1.7u_\eta\), where \(u_\eta\) is the characteristic small-scale (Kolmogorov) fluid velocity. Furthermore we use several values of \(\alpha\) and \(St\) (which corresponds to particles, or microorganisms with sizes which vary between 1\(\mu m\) to 50\(\mu m\)) and perform simulations with \(N_p = 50,000\) particles for every \(\alpha, St, r_{\text{int}},\) and \(v_0\).

It is useful to begin with an intuitive picture of whether there is any evidence of collective motion in our model. This is best seen online in videos [46] of the time evolution of a collection of such microorganisms with different shapes, sizes, activity \((v_0)\) and ranges of interaction \((r_{\text{int}})\) with random initial positions. These simulations show convincingly how flocking emerges only when conditions are right in terms of not only shapes and sizes but also \(v_0\) and \(r_{\text{int}}\). Indeed, for the cases where they do flock, a snapshot of the velocity vectors of the individuals (Fig. 1) clearly reflect the level of ordering in our model. For clarity, in Fig. 1 we only show a randomly chosen subset of the total \(N_p\) rod-like \((\alpha = 2.0)\) and inertial \((St = 2.0)\) microorganisms in the flow.

With this picture in mind, and visual evidence of flocking (depending on the type of microorganism), we cannot refrain anymore from making our study quantitative. A convenient way to quantify the degree of flocking, is to measure the global order parameter \(\Phi_v\)

\[
\Phi_v = \left\langle \frac{1}{N_p} \sum_{j=1}^{N_p} \hat{v}_j \right\rangle
\]

where the angular brackets denote a time-average (after the initial transients in their motion have died down) and \(\hat{v}_j\) is the unit velocity vector of the \(j\)-th individual. This order parameter ought to vary from species to species of different shapes and sizes as well as depend on the level of activity and radius of interaction. Should organisms flock, then all velocity vectors must point in the same direction yielding \(\Phi_v = 1.0\). On the other hand, if there is no ordering, then the velocity vectors ought to point in different directions for different individuals leading to \(\Phi_v = 0.0\). Hence, since by definition \(0.0 \leq \Phi_v \leq 1.0\), such a global order parameter quantifies the degree of flocking in a species unambiguously.

Figure 2 shows representative pseudo-color plots of \(\Phi_v\) as a function of \(\alpha\) and \(St\) (on a log scale) for different \(r_{\text{int}}\) and \(v_0\) (see figure caption). These results are intriguing for several reasons. For individuals which are not active, i.e., \(v_0 = 0\), microorganisms flock only when they are sufficiently large, rod-like and with a very large radius of interaction. This clearly shows that in the absence of activity, it is extremely hard for microorganisms which are small, slender or disk-shaped, to overcome turbulent mixing and drag to self-organise. In this parameter space, even if an individual aligns with its neighbour, eventually that direction gets randomised due to the turbulent medium and therefore it cannot continue with the direction over time which is necessary for the flocking to emerge.

However as soon as we turn on activity, i.e., \(v_0 \neq 0\) but still small (Fig. 2b), we obtain non-zero values of the order parameter for all species only for large sizes \((St > 1)\). For smaller-sized microorganisms for a given radius of interaction, the shape plays a crucial role: Rods are more likely to show collective behaviour than disks because, as has been known, correlation time-scales for rods are considerably longer than disks [45]. Understandably, as the \(r_{\text{int}}\) and \(v_0\) increase (e.g., Fig. 2c), the degree of flocking enhances for all species. Nevertheless, it is clear from our results that both size and shape matter—in a non-monotonically and complicated way—decisively in determining the ability of a species to overcome turbulent mixing and drag to swarm. Indeed for a significant range of values of \(\alpha, St, v_0,\) and \(r_{\text{int}}\), we do find evidence of near perfect flocking \((\Phi_v \to 1.0)\).

This is the first clear evidence of how collective behaviour can emerge in a collection of microorganism in a complex, random turbulent medium. Before we provide a theoretical explanation of this emergent phenomenon,
P bility of finding two particles within a distance $r_{\text{int}} = 0.2 \pi$. We show results for both active ($v_0 = 0.2u_\eta$) as well as (inset) passive ($v_0 = 0$) microorganisms.

it is useful to characterise one additional aspect, namely the nematic order [47], of these flocks. This is done most conveniently through the tensorial order parameter

$$Q = \langle \hat{v}_i \otimes \hat{v}_j - \frac{1}{3} \mathbf{1} \rangle;$$

whence we can calculate the scalar order parameter, associated with the nematic order, $S_\alpha(x) = n_\alpha^i n_\beta^j Q_{\alpha\beta}$, where $n^i(x)$ are the local symmetry directions of the fields.

Since we are interested in the global behaviour of this system, we calculate the global nematic order $\Theta_n = \int d\mathbf{x} S_n$. In Fig. 3 we show a representative plot of $\Theta_n$, for a given radius of interaction and self-propelled velocity as well as, in the inset, the same $r_{\text{int}}$ but for $v_0 = 0$, as a function of the Stokes number and for different shapes $\alpha$. Although we have not obtained perfect nematic ordering, we do see that a certain level of order emerges only for Stokes numbers larger than 1. From the inset, it is clear there is no ordering when particles are essentially passive but still allowed to interact over the same length scale. This is of course consistent with the picture that emerged when we looked at the global order parameter $\Phi_v$. (A similar definition is possible for the orientation vector $\mathbf{p}$; we have checked that the fluctuations are far stronger for the orientation vector as discussed at the end of this paper.)

We know that finite-sized, passive, inertial particles tend to preferentially concentrate for a range of Stokes numbers. A convenient quantification of this inhomogeneous distribution of particles in a flow is through the correlation dimension $D_2$ which is measured via the probability of finding two particles within a distance $r$, namely, $P^< (r) \sim r^{D_2}$. For tracers ($St = 0$), which are space filling, $D_2 = 3$ (in 3 dimensional flows). However for non-tracers ($St \neq 0$), it decreases from $D_2 = 3$ with increasing $St$ and reaches a minima for $St = O(1)$, before increasing again to saturate at $D_2 = 3$ for $St \gg 1$ [21]. It is this non-monotonic (as a function of the Stokes number) nature of preferential concentration of heavy, inertial particles which we show is central to flocking of our active particles. Hence, the particle dynamics ensure that for certain values of $\alpha$ and $St$ more organisms are forced, mechanically, to be close to each other and hence an enhancement in the degree of flocking. Therefore if the microorganisms are active, such preferential concentration plays a dominant role in the emergence of flocking. In the absence of preferential concentration, the chances of a large fraction of microorganisms clustered close enough for their mutual alignment-interactions to become effective would be minimal.

Our findings could be of importance for fabrication and design of artificial micro-swimmers. But are they equally relevant for observations in nature? Typical marine environments are known to be turbulent with a Reynolds number comparable to the ones we use in our simulations and a Kolmogorov scale $\eta$ of the order of a few mm [36 48]. In such an environment, microorganisms—not necessarily spherical—such as zooplankton often show collective behaviour [48]. Recent measurements suggest that this class of organisms have a variety of sizes which could range from $1 \mu\text{m}$ to $10 \mu\text{m}$, and, hence, less than $\eta$ [30 48]. This scale separation ensures that our modeling of microorganisms through a combination of the linear Stokes drag model [20–22], for the translational degrees of freedom and the Jeffery equation [39–41] [49–50], for the rotational degrees of freedom, is valid. Additionally, the associated response time scale, the Stokes time, $1 \mu\text{s} \leq \tau_p \leq 1 \text{s}$, of such microorganisms when compared to the Kolmogorov time scale $\tau_\eta$ of the ocean environment leads to Stokes numbers of the same order as we have used in our study [48].

These arguments suggest that our theoretical framework, even with its limitations (see below), is a relevant model for small organisms in a marine environment. Our results show that collective, ordered motion in active systems is an emergent phenomenon which can spontaneously occur even in a hostile environment where the range of interactions (here, quantified by $r_{\text{int}}$) for a collection of individuals is restricted. These results show that purely mechanical principles related to the dynamics of finite-sized particles in turbulence are critical in forcing certain organisms to flock: Given the right size and shape, microorganisms are brought in much closer proximity to each other allowing them to behave cooperatively and flock. Indeed recent studies of passive, non-interacting, non-spherical particles shed light on the correlation between particle trajectories and flow directions [45 49 50]; as particles become interacting and self-propelled the competing effects between the pas-
sive and active cases lead to our very interesting—and surprising—discovery that shape and size both matters for stabilising model flocks in turbulent flows. Without these underlying principles of fluid mechanics a random, chaotic environment would have pushed individuals far apart leading to a break up of flocks. Hence, by bringing together basic principles of turbulent transport and active matter, we have, for the first time, shown how model flocks can form in a collection of self-propelled individuals moving in a turbulent flow. Such cooperative behaviour has recently been reported for dry, granular systems \[51\] but not for the complex system that we report here. More pertinently, Durham, \textit{et al.} \[82\], considered modelled active tracers to understand the observed \textit{patchiness} of microorganisms such as phytoplankton: However, the idea of collective motion and the role played by inertia as well as the translational and rotational degrees of freedom was largely ignored in this and other studies.

Before we conclude, it is essential to understand some of the limitations of our model. Our model cannot capture the more dramatic instances of flocking in nature which involve macroscopically large organisms such as birds. This class of phenomena should be studied with a similar fluid mechanics approach in future by resolving boundaries and developing ideas for large structure-fluid interactions. Furthermore, the role of hydrodynamic interactions in flock stability ought to be investigated systematically within the present model. Finally, a more systematic study of finite (population) size effects and the effect of intrinsic noise as well as the level of activity is left for future work.

We hope that this novel—yet simple—mechanical approach, bringing together already well-established concepts in different areas, is an important ingredient in explaining why flocking is ubiquitous, and is as much a strategy as it is \textit{forced}. Such an approach could also lead to new ideas beyond the present study such as developing more realistic predator-prey models in complex environment.

SSR acknowledges the support of the DAE, Indo-French Center for Applied Mathematics (IFCAM) and the Airbus Group Corporate Foundation Chair in Mathematics of Complex Systems established in ICTS. AR and SSR acknowledges the support of the DST (India) project ECR/2015/000361. The simulations were performed on the cluster \textit{Mowgli} and workstations \textit{Goopy} and \textit{Bagha} at the ICTS-TIFR. AS acknowledges start-up grant (No.4-5 (206-FRP)/2015(BSR)) from UGC.
References:

[33] P. Mazur, Physica 110A, 128 (1982).
[34] P. Mazur and W. Van Saarloos, Physica, 115, 21 (1982).
[35] E. M. Purcell, Am. J. Phys. 45, 3 (1977).
[36] R. Stocker, Science 338, 628 (2012); H. Marcos, H. C. Fu, T. R. Powers, R. Stocker, Proc. Natl. Acad. Sci. U.S.A. 109, 4780 (2012).
[37] W. M. Durham, E. Climent, M. Barry, F. De Lillo, G. Boffetta, M. Cencini, and R. Stocker, Nat. Comm. 4, 2148 (2013).
[38] J. Jiménez, Sci. Mar., 61 47 (1997).
[39] G. B. Jeffery, Proc. R. Soc. A 102, 161 (1922).
[40] M. R. Maxey and J. J. Riley, Physics of Fluids 26, 883 (1983).
[41] L. Zhao, N. R. Challabotla, H. I. Andersson, and E. A. Variano, Phys. Rev. Lett. 115, 244501 (2015).
[42] C. Marchioli, L. Zhao, and H. I. Andersson, Phys. Fluids 28, 013301 (2016).
[43] P. H. Mortensen, H. I. Andersson, J. J. J. Gillissen, and B. J. Boersma, Phys. Fluids 20, 093302 (2008).
[44] N. R. Challabotla, L. Zhao, and H. I. Andersson, J. Fluid Mech. 766, R2 (2015).
[45] A. Roy, A. Gupta, and S. S. Ray, Phys. Rev. E, 98, 021101(R) (2018).
[46] Online videos from our simulations:

1. [https://youtu.be/yPNb6SKRNV] [Disk-like Microorganisms showing Collective Behaviour]
2. [https://youtu.be/VR9HqAC-kzk] [Disk-like Microorganisms not showing Collective Behaviour]
3. [https://youtu.be/s7lh-s2NTZk] [Rod-like Microorganisms showing Collective Behaviour]
4. [https://youtu.be/6z0ky_Z29s] [Rod-like Microorganisms not showing Collective Behaviour].

[47] F. Ginelli, F. Peruani, M Bár, and H. Chaté, Phys. Rev. Lett. 104, 184502 (2010).
[48] J. Yen and E. A. Bundock, Aggregate behavior in zooplankton: Phototactic swarming in four developmental stages of Coullana canadensis (Copepoda, Harpacticoidea), in Animal Groups in Three Dimensions, ed. J. K. Parrish and W. M. Hamner (Cambridge University Press) pp. 143-162 (1997); J. W. Ambler, Hydrobiologia, 480 155164 (2002).
[49] A. Pumir and M. Wilkinson, New J. Phys. 13 093030 (2011); A. Gupta, D. Vincenzi and R. Pandit, Phys. Rev. E 89 021001(R) (2014).
[50] S. Parsa, E. Calzavarini, F. Toschi, and G. A. Voth Phys. Rev. Lett. 109, 134501 (2012).
[51] N. Kumar, H. Soni, S. Ramaswamy, and A. K. Sood, Nat. Comm. 5, 4688 (2014).