Bidirectional sorting of flocking particles in the presence of asymmetric barriers

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We numerically demonstrate bidirectional sorting of flocking particles interacting with an array of asymmetric barriers. Each particle aligns with the average swimming direction of its neighbors according to the Vicsek model and experiences additional steric interactions as well as repulsion from the fixed barriers. We show that particles preferentially localize to one side of the barrier array over time, and that the direction of this rectification can be reversed by adjusting the particle-particle exclusion radius or the noise term in the equations of motion. These results provide a conceptual basis for isolation and sorting of single- and multi-cellular organisms which move collectively according to flocking-type interaction rules.

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I. INTRODUCTION

The ensemble dynamics of self-driven particles can differ significantly from those of Brownian random walkers. For example, in experiments on microfabricated habitats connected by funnel-shaped channels, self-propelled E. coli bacteria preferentially migrated to the chamber towards which the funnels pointed even though Brownian particles would have remained equally distributed in both chambers. A simple simulation model showed that the rectification arises due to the modification of the run-and-tumble swimming dynamics of the bacteria by the walls of the microenvironment. When a running bacterium encounters a wall, it does not reflect away from the wall or immediately tumble, but swims in the direction of the wall while preserving as much as possible its prior direction of motion. Refs. and found rectification under this interaction rule for independent swimmers that did not interact with each other. The rectification in the bacteria system resembles a ratchet effect in which a net dc motion occurs in the absence of a dc drive due to the application of an external ac drive or flashing substrate.

For self-driven particles, however, no external driving is necessary. In addition to demonstrations of directed bacterial motion achieved through a ratchet mechanism, it has also been shown that baths of swimming bacteria can induce directed rotational motion of asymmetric flywheels.

Interactions between self-propelled particles can lead to distinctive dynamical behaviors that are more complex than those of independently moving particles. Simple models such as that of Vicsek et al. capture many features of the dynamics of species with strongly collective motion, in which individuals preferentially align with their neighbors and form moving groups. These models qualitatively reproduce the motion of both macro-scale groups, such as fish schools and bird flocks, and micro-scale groups, such as bacterial swarms and cancerous tumors. The original Vicsek model includes only a term for preferential velocity alignment with all neighbors within a fixed flocking radius, yet it exhibits a phase transition to unidirectional motion as a function of particle density and noise amplitude. Although numerous modifications of the Vicsek model have been proposed, such as the addition steric interactions and/or cohesion, only a very limited amount of work has been done on the interaction of flocking particles with walls or barriers. Walls can impose a directional symmetry breaking, induce the formation of a vortex state or flashing substrate, or simply serve as aggregation focal points.

In this work we simulate a modified version of the Vicsek flocking algorithm that includes both steric repulsion between particles and confinement within a two-dimensional microenvironment with strategically placed gates similar to those of Ref. Here we consider strictly repulsive particle-wall interactions, so that the particles do not follow the walls when swimming independently. As the particle density increases, we find rectification effects once the density is high enough to permit collective motion to occur. By varying the interparticle exclusion radius, the flocking radius, or the noise, we can reverse the direction of the rectification. This result has implications for the potential sorting of self-propelled particles that move according to these types of interaction rules.

Simulation—We consider a two-dimensional L × L system of N self-driven particles at number density ρ0 = N/L2 with fixed, repulsive boundaries on all sides. The overdamped equation of motion for a single particle i is

\[ dx_i = v_i(t) dt \]

All quantities are rescaled to dimensionless units. The time step \( dt = 0.002 \) and we take \( L = 66 \). The velocity consensus force \( f^i_{vc} \) also called the alignment force, is determined by the velocities of all M particles, including particle i, within a flocking radius \( r_f \) of particle i:

\[ f^i_{vc} = \frac{A_f}{r_f} (\cos(\Phi^i_{vc}(t))\hat{x} + \sin(\Phi^i_{vc}(t))\hat{y}) \]

(2)
Equations of motion are then integrated for gates bisect the system into top and bottom chambers, after a sufficient amount of time elapses, the particles concentrate in one of the two chambers, reaching a steady state or flocking state. In Fig. 1(b), after $7 \times 10^5$ simulation time steps the particle density is clearly higher in the top chamber.

We find that we can vary whether the rectification moves the particles into the top ($\rho_{\text{top}} > \rho_0$) or bottom ($\rho_{\text{top}} < \rho_0$) chamber by altering $r_f$, $r_e$, or $\eta$, as shown in Fig. 2(a-c) where we plot $\rho_{\text{top}}$ after $3 \times 10^6$ simulation time steps. For small values of $r_e$ and $\eta$, particles are rectified into the top chamber, but a rectification reversal occurs at $r_e = 0.12$ and drops to zero for $r_e \geq 0.3$. b) $\rho_{\text{top}}$ vs $\eta$ for $r_e = 0.12$ and $r_f = 1.0$. The rectification reverses at $\eta \sim 1.0$ and drops to zero for $\eta \geq \pi$. c) $\rho_{\text{top}}$ vs $r_f$ for $r_e = 0.12$ and $\eta = 1.5$. For $r_f < r_e$ only steric particle interactions occur and rectification is negligible. There is a rectification reversal at $r_f \approx 1.2$, and for large $r_f$ when all the particles tend to align into a giant flock, the particles accumulate in the top chamber. d) Rectification phase diagram for $r_e$ vs $\eta$. Lower contours (red) indicate rectification into the top chamber and upper contours (blue) indicate rectification to the bottom chamber.

Figure 1: Simulation images. Lines: barriers and walls; dots: particle positions. a) Initial state of sample with $r_f = 1.0$ and $r_e = 0.07$ at $\rho_0 = 0.4$. b) The same sample after $7 \times 10^5$ simulation time steps shows rectification of particles into the top chamber.

Figure 2: (a-c) $\rho_{\text{top}}$, the density in the top chamber, after $3 \times 10^6$ simulation time steps for a sample with initial density $\rho_0 = 0.4$, indicated by the dashed line. (a) $\rho_{\text{top}}$ vs $r_e$ for $\eta = 1.5$ and $r_f = 1.0$. The rectification reverses at $r_e = 0.12$ and drops to zero for $r_e \geq 0.3$. b) $\rho_{\text{top}}$ vs $\eta$ for $r_e = 0.12$ and $r_f = 1.0$. The rectification reverses at $\eta \sim 1.0$ and drops to zero for $\eta \geq \pi$. c) $\rho_{\text{top}}$ vs $r_f$ for $r_e = 0.12$ and $\eta = 1.5$. For $r_f < r_e$ only steric particle interactions occur and rectification is negligible.
no flocking interaction, and the repulsive barrier walls produce no rectification in the absence of flocking. For $r_e < r_f < 1.2$, we find a reversed rectification into the lower chamber, while for all $r_f \geq 1.2$, the particles rectify into the top chamber. For $r_f > 2.0$, the value of $\rho_{top}$ saturates at $\rho_{top} = 0.8 = 2\rho_0$, indicating that nearly all of the particles are located in the top chamber.

The rectification reversal occurs due to a change in the nature of the microscopic interaction between the flocks and the funnel channels. For example, as the exclusion radius $r_e$ increases, the particles are less able to form tight and cohesive flocks. At low values of $r_e$, particles are rectified into the top chamber when flocks, incident on the gates from the bottom, rearrange into oblong shapes and pass efficiently through the funnel aperture, as illustrated in Fig. 3. For higher values of $r_e$, the steric interparticle repulsion prevents the flocks from condensing and makes it impossible for more than one particle at a time to pass through the funnel aperture. As a result, the particles clog inside the funnel rather than passing through, as illustrated in Fig. 3(a). The flock reverses direction due to the repulsion from the barrier walls, and at most one or two particles occasionally manage to escape the flock and enter the top chamber, as shown in Fig. 3(b). In contrast, a flock that approaches the gates from the upper chamber is fragmented by the gates into two smaller flocks; when this occurs, particles that are directly incident on the aperture between gates can escape from both flocks and pass in a single file into the lower chamber, as illustrated in Fig. 3(c,d,e). Since the average number of particles escaping the flock and crossing the barrier is larger when the flocks are approaching from above than when they are approaching from below, a net rectification into the lower chamber occurs over time. We note that the reversed rectification into the lower chamber (Fig. 3) is a much slower process than the forward rectification into the higher chamber (Fig. 4), although we are able to reach a steady state within our simulation time for either process. In spite of this, we find that the maximum possible amount of rectification that can be achieved in steady state as the parameters are varied is the same for both directions of rectification, as shown in Fig. 2(a).

Reversed rectification into the lower chamber also occurs whenever the flocks become fragile or prone to breakup. This occurs both when the noise parameter $\eta$ is increased and when the flocking radius $r_f$ is reduced. Under these conditions, the flocks are not cohesive enough to flow as a unit through the funnel aperture in the manner illustrated in Fig. 3 at the same time, the probability that a flock will fragment and lose some of its members to the lower chamber when approaching the gates from above, as in Fig. 3(c-e), is increased. In Fig. 5(a), we plot the average flock size $N_c$ as a function of $r_f$, $r_e$, and $\eta$ for the systems in Fig. 2. We separate the particles into clusters iteratively by identifying particles that are within the flocking radius $r_f$ of each other; $N_c$ is then the average number of particles per cluster. The value of $N_c$ is higher in regimes where the particles are rectified to the top of the container, and lower in the reversed rectification regime.

One of the unique aspects of the rectification behavior
Figure 5: Mean flock size $N_c$, in number of particles, vs $r_f$ (blue circles), $r_e$ (red squares), and $\eta$ (green diamonds). Error bars indicate standard deviation.

Figure 6: Dependence of rectification on initial particle density $\rho_0$ for a system with $r_f = 1.0$ and $\eta = 1.1$. (a) $\rho_{\text{top}}/\rho_0$ after $3 \times 10^6$ simulation time steps vs $r_e$ for different values of $\rho_0$. From blue to red, $\rho_0 = 0.004$ (⋄), 0.01 (□), 0.03 (x), 0.05 (△), 0.08 (▽), 0.1 (○), 0.12 (+). A rectification reversal emerges as $\rho_0$ increases. b) $\rho_{\text{top}}/\rho_0$ after $3 \times 10^6$ time steps vs $\rho_0$ for $r_e = 0.05$ (upper red curve) and $r_e = 0.23$ (lower blue curve).

Conclusion– We have implemented a simple model of flocking particles in the presence of fixed, repulsive barriers, and find that such particles will concentrate on one side of a set of asymmetric V-shaped gates. The direction of the rectification can be reversed by modulating any of three parameters: the flocking radius $r_f$, the exclusion radius $r_e$, or the noise parameter $\eta$. The existence of the rectification and its direction are determined by the ability of the particles to form flocks and the robustness of the flocks against breakage; in the low density limit, when no flocks appear, we find no rectification due to the purely repulsive interactions of the particles with the barrier walls. Thus, the rectification we observe arises strictly due to collective effects. The bi-directional rectification behavior we describe could be used to sort particles which tend to concentrate on different sides of the barriers. This effect is similar to the sorting phenomenon observed by Mahmud et al. for cancer cells. We expect sorting devices based on these principles to have broad potential applications with regard to both biomedical diagnostics and therapeutics.

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Figure 7: Supplemental Figure. Demonstration of two-species sorting. Simulation of system containing 871 "A" particles with $r_e = 0.22$ (green) and 871 "B" particles with $r_e = 0.055$ (pink). $r_f = 1.0$ and $\eta = 1.1$ in both cases. Particles of different species repel via steric repulsion but only experience alignment forces with particles of the same species. Simulation shown (a) at time $t = 0$ and (b) after $4 \times 10^9$ simulation time steps when many of the "A" particles have rectified into the bottom chamber and most of the "B" particles have rectified into the top chamber. The bidisperse system requires longer times to reach a steady state compared to the monodisperse system.

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