Response Letter

Dear Editors,

Thank you for reviewing and handling our submission 'Collective dynamics of densely confined active polar disks with self- and mutual alignment' (manuscript ID: scipost_202501_00037v1).

We are resubmitting a revised version, following the suggestions by the reviewers. We have highlighted our changes to the manuscript in red, and our responses below in blue.

We believe that our manuscript has greatly improved as a result of the reviewers' feedback. All comments, questions, and criticisms have been addressed below. We thus respectfully request that our manuscript be accepted for publication in Scipost.

On behalf of all the authors,

With regards, Pawel Romanczuk and Cristián Huepe

Reply to Report by Referee 2

Comments to the Author:

Strengths

The article presents a confined system of active disks characterized not only by self-alignment but also by mutual alignment with their neighbors. The combined effect leads to a rich state diagram with polarized and milling states. The presented model could be relevant for real systems of drone swarms active solids or wheeled robots.

Weaknesses

The clarity of the manuscript could strongly improved if the authors could plot state diagrams reporting the different emergent states. All suggested changes are reported below.

Report

The manuscript is clearly written and meets the criteria of an article published in SciePost. I would be very happy to support its publication in the journal once the authors have addressed all requested changes.

Response: We thank the reviewer for this positive evaluation and constructive feedback. We have revised the manuscript to include detailed state diagrams in Fig. 9, which clearly illustrate the different emergent states as a function of the parameters. We believe that this and other changes detailed below have significantly enhanced the presentation of our work.

Requested changes:

1. The authors present a numerical model that could mimic the behaviour of realistic systems characterized by self and mutual interactions. At the end of the introduction they state "We expect experimental systems to display both types of self-organised dynamics in realistic setups..." Could the authors better speculate which realistic setups they have in mind?

Response: We thank the reviewer for this request, as we now see that our statement at the end the Introduction was unclear. We have thus modified the last paragraph of the Introduction to specify that some degree of mutual alignment and self-alignment can be expected to naturally occur in any group of self-propelled agents without perfectly axisymmetric interactions with their neighbors and with the substrate. A specific example of such systems could be

given by the experiments presented in reference [24], if carried out at higher densities and with agents with softer elastic interactions. Additionally, even much more complex biological systems (such as dense cellular arrangements) could display some of the robust features of both types of self-organizing dynamics, since some degree of mutual alignment and of self-alignment can also be expected in these more complex setups, given that their interactions will also have nonaxisymmetric components.

- 2. The system presented by the authors presents several emergent states. I think the manuscript would gain clarity if the authors could add figures reporting state diagrams with the different collective states indicated by the polarization and milling order parameter. For a fixed packing fraction, the authors could report two state diagrams, one for the smooth and another one for the rough boundaries, when varying the damping coefficient and the value of R.
- Response: In order to clarify our results and address issues raised by both referees, we have now included in Fig. 9 of Appendix **B** four state diagrams showing P and M as a function of R and D_{θ} for all combinations of isotropic or anisotropic agent-substrate damping, and of a smooth or rough boundary. We also added a new Fig. 10 that plots P and M as a function of R. We did not include figures showing the effect of varying the damping coefficient, however, since this parameter and the preferred speed v_0 , the rotational damping β , and the repulsive strength k tend to change the speed of the dynamics but not its emergent states. A systematic exploration of all these additional parameters would be beyond the scope of this work and we therefore focused on those that appear to have the most significant qualitative effect.
- **3.** The authors simulate the active agents as soft disks. How important is the fact that the interactions are soft? Could the authors have considered harder interactions between disks?

Response: In preliminary analyses, we considered the effect of changing the strength of the linear repulsion force and found that this does not qualitatively alter the collective states observed in our simulations, although it produces quantitative differences. In the limit of perfectly hard disks, however, this situation could change, as it was found in [Phys. Rev. Lett. 132, 238303 - DOI: https://doi.org/10.1103/PhysRevLett.132.238303]. In this paper, the authors showed that there can be significant differences between a lattice formation of active self-aligning disks with elastic interactions when compared to an equivalent setup with rigid interactions. Despite these interesting observations, we believe that discussing and describing this limit of fully rigid interactions would be beyond the scope of this paper.

4. The authors should define all variables used in the equations. For instance,

 D_{θ} in equation (2).

Response: We thank the reviewer for pointing out this issue. We have now properly defined D_{θ} after Eq.(2).

5. At page 5 the authors refer to figure 6 right after referring to figure 1. I would suggest the authors to display the figures in a subsequent order. When referring to figures in the Supporting Material, could the authors explicitly state the figures are in the Supporting?

Response: We agree with the reviewer that it was confusing to refer to Fig. 6 at such an early stage. Given that this reference is not necessary at this point of the paper, we have now removed it from this section of the text.

6. The authors compute global order parameters, such as the polarization and the degree of milling defined in equations 3 and 4, respectively. The authors should explicitly indicate the minimum and maximum value they expect for P and M in each emergent state. To understand the degree of polarization or milling.

Response: We have addressed this issue by adding the following sentence after Eq.(4), where the milling order parameter is defined: "The order parameters P and M range from 0 to 1, where a disordered state will display low values for both, a flocking state will have high P and low M, and a milling state will have low P and high M." We note that polarization and milling are continuous quantities where there is no clear threshold that defines a "polarized" or a "milling" state as such. Yet, the closer the value of either is to 1, the more the system approaches perfectly aligned or milling motion, respectively.

7. Would it be possible to better understand how the different collective states emerges? Could they consider local instead of global order parameters? Such as a polarization computed on each particle, summing over first neighbors. Or the degree of milling computed on each particle, summing over first neighbors. These local order parameters might help understanding the nucleation of the different emergent states.

Response: We agree with the reviewer that it would be interesting to better understand how the different collective states emerge by tracking the local formation and disappearance of vortices. However, we found in our preliminary analyses that the specific features of these dynamics can be very complicated and depend not only on all the model parameters but also on system size. Presenting a clear picture of the nucleation of the different emergent states would thus require significant additional parameter exploration and is beyond the scope of this work. Despite this, we know for topological reasons that vortices should either appear in plus-minus pairs or change the total vorticity at the boundary of the system. We also observe that in the rough boundary case

most vortices appear at the boundary and move into the arena, and that the vortex dynamics become increasingly chaotic for larger system sizes. In order to include these comments and provide more insights into the vortex dynamics in the different phases, we have edited and added a sentence to the last paragraph of Appendix E.

8. Concerning the behavior observed in Figure 3, that reports the orientation autocorrelation functions, could the authors state whether there is a different behavior between particles at the boundary with respect to those at the center of the system (away from the boundary)? Could the authors compute one autocorrelation function for particles at the boundary and another one for particles away from the boundary?

Response: We have followed the Reviewer's suggestion and addressed these questions by computing the autocorrelation function separately for disks in the inner and outer regions of the arena. Figure 1 below shows how we divide the system into two groups: an inner group (the inner half of the arena, away from the boundary) and an outer group (in the outer half, close to the boundary). We then compute separately the autocorrelation functions of the inner group (Fig. 2 below) and the outer group (Fig. 3 below), and their Fourier transforms (Figs. 4 and 5 below). We find that the Fourier components of the orientation autocorrelation of both regions are very similar, showing that the rotational dynamics is essentially homogeneous throughout the system. The only difference is that the inner-circle group displays stronger high-frequency oscillations than that of the outer group, but with the same frequency values. This is consistent with our description of the localized rotation dynamics, which we expect to develop more perfect oscillations without the interference from the boundary. Next to the boundary the dynamics is either more disordered (for rough boundaries) or displays only milling (for smooth boundaries). Despite this, there is no significant difference between the rotational dynamics of the disks unless they are very close to the boundary. We have included this observation in the main paper by adding a sentence at the end of Section 3.2, where Fig.3 is described.

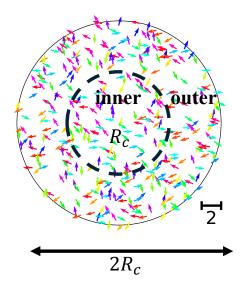


Figure 1: Group stratification diagram: inner (away from the boundary) vs. outer (close to the boundary). The black dashed line partitions the space into an interior and an exterior region.

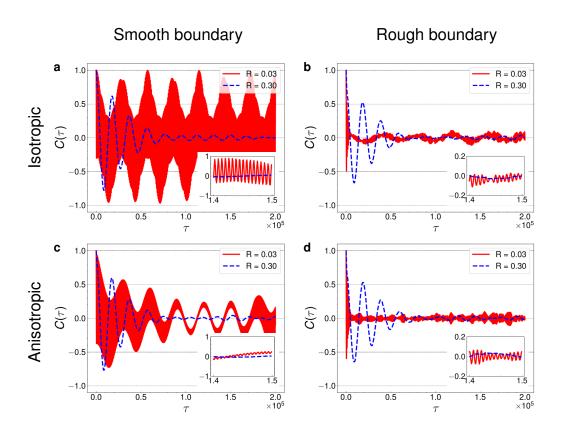


Figure 2: Orientation autocorrelation functions in the inner zone for different boundary and damping conditions. The orientation autocorrelation functions of particles in the inner zone are displayed, for smooth or rough arena boundaries and isotropic or anisotropic mobility. The blue dashed curves correspond to disks with large off-centered rotation distance R=0.3, whereas the red solid curves correspond to the small R=0.03 case. The insets zoom into a short temporal interval to visualize high-frequency oscillations in the correlation functions, which only appear in the small R case. Other simulation parameters are set to: $l_0=1.0$, $v_0=0.002$, $D_\theta=0$, and N=400.

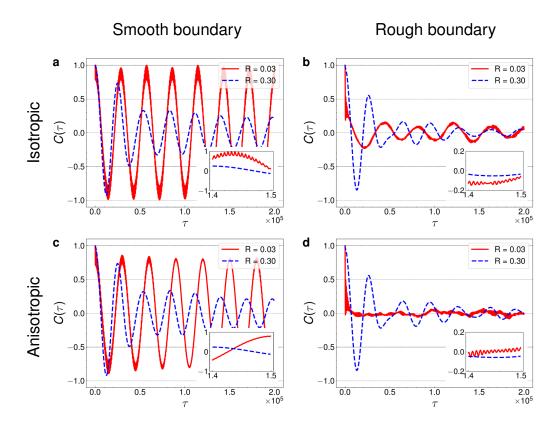


Figure 3: Orientation autocorrelation functions in the outer zone for different boundary and damping conditions. The orientation autocorrelation functions of particles in the outer zone are displayed, for smooth or rough arena boundaries and isotropic or anisotropic mobility. The blue dashed curves correspond to disks with large off-centered rotation distance R=0.3, whereas the red solid curves correspond to the small R=0.03 case. The insets zoom into a short temporal interval to visualize high-frequency oscillations in the correlation functions, which only appear in the small R case. Other simulation parameters are set to: $l_0=1.0$, $v_0=0.002$, $D_\theta=0$, and N=400.

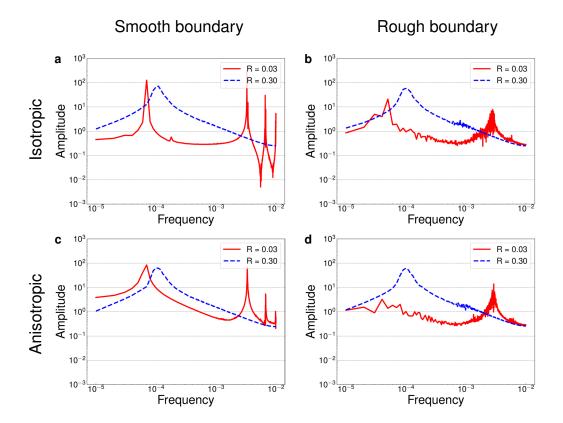


Figure 4: Orientation autocorrelation in Fourier space in inner zone for different boundary and damping conditions. The orientation autocorrelation in Fourier space of inner zone are displayed, for smooth or rough arena boundaries and isotropic or anisotropic mobility. The blue dashed curves represent large off-centered rotation distance R=0.3; the red solid curves correspond to small R=0.03. Low frequency milling can be found to different degrees in all cases, but high-frequency circular oscillations of different intensities, with or without resonances, only appear in the small R=0.03 case. Other simulation parameters are set to: $l_0=1.0$, $v_0=0.002$, $D_\theta=0$, and N=400.

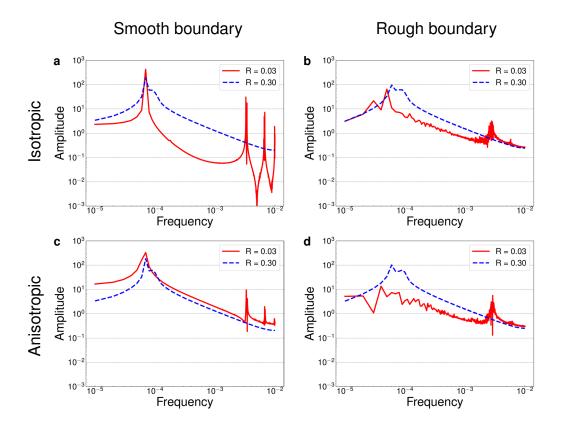


Figure 5: Orientation autocorrelation in Fourier space in the outer zone for different boundary and damping conditions. The orientation autocorrelation in Fourier space of the outer regions are displayed, for smooth or rough arena boundaries and isotropic or anisotropic mobility. The blue dashed curves represent large off-centered rotation distance R=0.3; the red solid curves correspond to small R=0.03. Low frequency milling can be found to different degrees in all cases, but high-frequency circular oscillations of different intensities, with or without resonances, only appear in the small R=0.03 case. Other simulation parameters are set to: $l_0=1.0$, $v_0=0.002$, $D_\theta=0$, and N=400.

9. Could the authors better study the mechanism of appearance and disappearance of a vortex?

Response: We have described some of the vortex dynamics in our response to the reviewer's point 7, above, and added in this context an additional paragraph at the end of Appendix E. In that reply we described our phenomenological understanding of the vortex dynamics and pointed out that, for topological reasons, the vortices should either appear (or disappear) in plus-minus pairs, or do so by changing the total vorticity at the boundary of the system. However, a more detailed study of the appearance and disappearance mechanisms would require understanding better the vortex-vortex and vortex-boundary interactions, which could only be done through multiple simulations in larger arenas. We thus believe that a more detailed study of the specific vortex nucleation and disappearance processes would be beyond the scope of this paper

10. In Section 3.4 the authors study state transitions between rotational states as a function of R. Also in this case, state diagrams would help to clarify the phenomena hereby reported. The same holds for the study of the state

transition as a function of density, reported in section 3.5: state diagrams would help to clarify the phenomena hereby reported.

Response: We thank the reviewer for these insightful suggestions. To address the first point, we have included new phase diagrams in Fig. 9, and plotted the polarization and milling order parameter as a function of R in Fig. 10 of Appendix B in the revised manuscript, both of which clearly delineate the rotational state transitions as a function of R. Regarding the second point, we note that the density dependence observed is qualitatively similar across other parameter values and only produces a transition between solid and fluid states. It is thus much less rich than the R dependence. We therefore considered that constructing a full phase diagram as a function of density would be beyond the scope of this paper and would not contribute significantly to the currently presented results.

11. Concerning localized rotations (at page 12), is it possible to study whether localized rotations are present, and eventually merge, for higher values of R?

Response: We believe that the answer to this question is already in our results. Indeed, given that localized rotation occurs at a higher frequency than the milling rotation, the lack of high-frequency components in the dashed blue R = 0.3 curves in Figs. 5 and 6 appears to show that there are no localized rotations present for higher values of R. The disappearance of localized rotations also seems to occur smoothly as R is increased, as implied by the smooth polarized-to-milling transitions displayed in Fig. 10.

12. Have the authors considered the possibility of changing the shape of the confining walls? How much the emergent states are affected by the confinement's geometry?

Response: We agree with the reviewer that considering different confinement geometries could be very interesting, as they will certainly affect most of our results. Although we have not carried out a systematic study of the effects of changing this geometry, our preliminary analyses show that they can significantly influence the emergent collective behavior, especially the milling regime. In a rectangular arena, for example, the milling dynamics only tend to form in an approximately circular region contained within the rectangle, while the active disks remain jammed in the regions close to the corners. The dynamics can thus become much more complex, as regions with different behaviors can emerge. It is because of this that we focus on a circular arena in this paper, to fully describe as a first step a geometry that equally favors milling dynamics that are not obstructed by the walls, leaving the study of other arena shapes for future work.

13. In the conclusions, the sentence starting with "The implementations details..." is repeated twice.

Response: We thank the reviewer for noticing this typo. We have removed the repeated sentence in the new version of the manuscript.