**Project Title: Transport properties of self-propelled micro-swimmers**

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## 1. Background and purpose of the project, relationship of the project with other projects

Brownian motion in convective laminar flows is a topic of interdisciplinary research for its applications to transport phenomena at large and small scales. For instance, under quite general conditions, advection has been proven, both analytically and experimentally , to enhance the diffusion of passive colloidal particles along a linear array of convection rolls. This is a combined effect of thermal noise and advection. Indeed, a noiseless particle would keep circulatig inside the convection roll where it had been injected.

Active particles in a linear convection array behave differently. An active particle is modeled as a particle propelling itself with tunable constant speed and direction changing because of collisions with obstacles [1-6] and other particles, or the torque associated with the convective flow, or fluctuations (either of the suspension fluid or the self-propulsion mechanism) . A slow active particle ends up trapped in a convection roll as long as the fluctuations affecting its dynamics are negligible, whereas a fast active particle tends to sojourn against the array walls, in the stagnation areas separating the convection rolls. In the latter regime, the particle diffusion along the array is dominated by the self-propulsion mechanism[7-9].

So far, all studies on the advection-diffusion of colloidal suspension in convection arrays were conducted in the low-density regime, namely, they focused on the diffusion of a single particle. Of course, the dynamics of a of Brownian particles is in itself a well established topic due to its applications in colloids and aerosols science. Weakly attracting colloidal particles are known to cluster into a variety of continuously time-evolving structures, ranging from dimers to crystals. Most remarkably, in the context of soft matter, clustering of overdamped active particles in a stationary suspension fluid can occur even in the absence of particle attraction, because the particles on the cluster surface point mostly inwards. Under the same conditions, steric interactions do not suffice to make passive particles cluster; their distribution would remain uniform at all times.

However, despite the wide literature on colloidal suspensions, the impact of collisions on particle transport in a convection array has been addressed only recently [9]. Extensive numerical simulations showed, for instance, that particle-particle collisions allow convection cell crossings by noiseless particles (active and passive, alike) and, therefore, athermal diffusion in convection arrays and turbulent flows at large.

We investigate the collisional effects in a binary mixture made of colloidal particles of the same size, one species active and the other one passive. As mentioned above, single active and passive particles advected in a linear convection array exhibit different diffusion properties. On the other hand, steric collisions, due to the particle finite size, allow the two mixture fractions to interact, so that the question arises about the advection-diffusion of a binary mixture. mixture. To avoid unnecessary numerical complications, we restrict our study to planar convective flows and particles are modeled by hard disks. Our numerical simulations reveal a number of interesting new features, like the strong stirring action exerted on a passive colloidal fluid by a small fraction of slow active particles, or the separation of the mixture into two distinct colloidal fluids for strong self-propulsion of the active fraction, the passive fluid circulating inside the convection rolls and the active one accumulating in stagnation areas along the array walls.

**2. Specific usage status of the system and calculation method** -- This fiscal year we used Hokusai supercomputer mainly for simulation of active-passive binary mixture in a linear array of convection rolls. Specifically, we explore phase behavior and diffusion properties of the binary mixture. Detailed results presented in the next section. Our primary observations on interesting mixing and de-mixing phenomenon demands detailed quantitative description of phase separation and segregation processes considering more general 2D convection roll arrays. Further, important extension of this study is to consider chiral mixture. To address these issues more simulation work is needed.

**Theoretical and simulation method**

***Model*** - We model a 2D linear convection array as a stationary laminar flow with stream function

$$\psi(x,y)=\frac{U_0 L}{2\pi}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right) \quad \text{- - (1)}$$

confined between two parallel edges, y = 0 and y = L/2, which act as dynamical reflecting boundaries. The unit cell of the array consists of two counter-rotating convection rolls.

We simulated a colloidal suspension consisting of a mixture of N hard disks per unit cell, including a fraction η of active disks. All disks, active and passive alike, repel each other with a potential function modeled by the truncated-shifted Lennard-Jones function,

$$\begin{aligned} V_{ij} &= 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \text{ if } r_{ij}\le r_m \\ &= 0 \text{ otherwise,} \end{aligned}$$

with $r_m = 2^{1/6}\sigma$ and σ representing the particle "diameter".

As we are interested in colloidal mixtures at very low Reynolds numbers, the dynamics of the i-th disk will be modeled by an overdamped (massless) active Brownian particle (ABP) governed by two translational and one rotational Langevin equation (LE) [7-11],

$$\begin{aligned} \dot{\mathbf{r}}_i &= \mathbf{v}_{LJ,i}+\mathbf{v}_{\psi,i}+\mathbf{v}_{0,i}+\sqrt{D_0}\,\boldsymbol{\xi}_i(t) \\ \dot{\theta}_i &= (\alpha/2)\,\nabla\times\mathbf{v}_{\psi,i}+\sqrt{D_\theta}\,\xi_{\theta,i}(t), \end{aligned} \quad \text{- - - - (2)}$$

where $\mathbf{r}_i$ = ($x_i$, $y_i$), $\mathbf{v}_{\psi,i}$ is the corresponding advection velocity introduced above, and $\mathbf{v}_{LJ,i}$ is the collisional term due to pair repulsion. In the case of an active particle, its self-propulsion vector, $\mathbf{v}_{0,i} = v_0(\cos\theta_i,\sin\theta_i)$, has constant modulus, $v_0$, and is oriented at an angle $\theta_i$ with respect to the array axis.

The translational (thermal) noises in the x- and y-directions, $\xi_{x,i}(t)$, $\xi_{y,i}(t)$ and the rotational noise, $\xi_{\theta,i}(t)$, are stationary, independent, delta-correlated Gaussian noises,

$$\begin{aligned} \left\langle \xi_i^q(t)\right\rangle &= 0 \\ \left\langle \xi_i^q(t)\xi_j^{q'}(0)\right\rangle &= 2\delta_{ij}\delta_{qq'}\delta(t) \end{aligned}$$

Where q or q' = {$x, y, \theta$}. $D_0$ and $D_\theta$ are the respective noise strengths, which for generality we assume to be unrelated. The reciprocal of $D_\theta$ coincides with the angular persistence (or correlation) time. The flow shear exerts a torque on the particle proportional to the local fluid vorticity. For simplicity, we adopt second law, which, for an ideal no-stick spherical particle, yields $\alpha$=1.

***Simulation method*** **-** The stochastic differential equation (2) for $D_0 > 0$ and/or $D_\theta > 0$, were numerically integrated by means of a standard Milstein scheme to obtain particles position as a function of time. Then, we estimated diffusivity of the particles in the mixture. The numerical integration was carried out using a very small time step, $10^{-3}$ -$10^{-4}$ to ensure numerical stability. We assume initially the particles were uniformly distributed in cell of convection roll with random orientation of the self-propulsion velocities. The results reported in the figures shown here are obtained by averaging over $10^4$ trajectories. Based on the time evolution of phase points, we analyze clustering, mixing, de-mixing processes in the advected binary mixture under different conditions. Diffusion constant defined as,

$$D = \lim_{t\to\infty} \frac{\langle [x(t)-x(0)]^2 \rangle}{2t}.$$

In the noiseless regime particular caution was exerted, because transients can grow exceedingly long, thus affecting the computation of both the long-time spatial distribution of the mixture in the array and the diffusion constants.

### 3. Results

Binary mixtures made of different active species have been the subject of extensive numerical and analytical investigations for at least a decade now. The attention of most researchers focused on the phenomenon known as motility induced phase separation (MIPS), whereby the mixture components tends to separate as an effect of their motility difference. Phase separation can occur on either local or global scales, with the formation of one-species clusters of various size. Clustering is initiated by the confining action exerted by the active particles.

In the following we study phase aggregation and segregation of an active-passive binary mixture advected in a linear convection array.

(i) **Stirring** -- Consider a suspension of noiseless passive particles in the convection array of equation (1). Earlier investigation show that for not too small packing fractions the particles tend to aggregate in regular patterns rotating around the center of the convection rolls. Assume now to add a small amount of slow active particles with the same

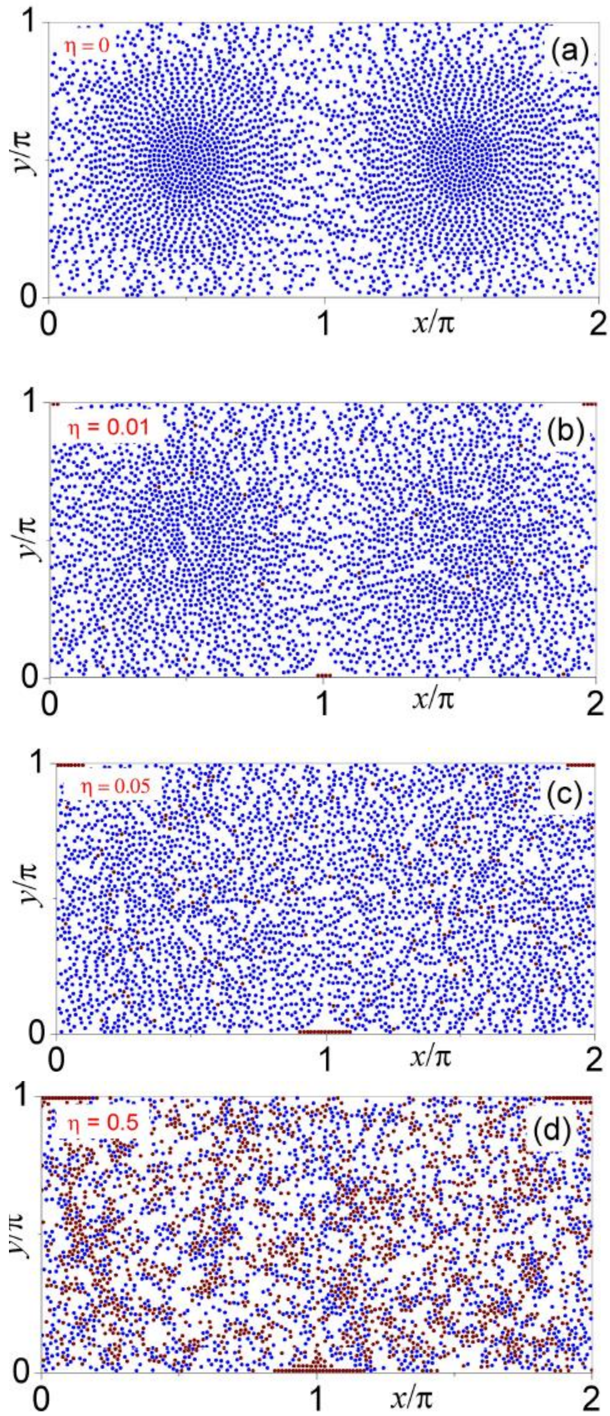


Figure 1: Binary mixture of active (brown) and passive disks (blue) with $D_0 = 0$, $D_\theta = 0.01$ and $v_0 = 0.1$ at $t = 10^5$. $N = 3420$ is the total number of disks, and $\eta$ (see legends) the active fraction. At t=0 all N disks were randomly distributed in the unit cell. Other parameters are: $\sigma= 0.05$, $v_\varepsilon = 1$, $L = 2\pi$ and $U_0 =1$.

geometry, and ask ourselves what is their impact on the dynamics of the passive fluid. We simulated numerically this situation for a mixture of N = 3420 disks in Fig. 1, were the self-propelling disks have speed $v_0 = U_0/10$. An active fraction as small as $\eta = 0.01$, panel (b), suffices to destroy the clustering pattern of the pure passive suspension, panel (a). As a result, for $\eta = 0.05$ the passive particles circulate inside the convection rolls with almost uniform spatial distribution. Mixture stirring by active swimmers is a well-known mechanism; here, it can be invoked to mimic the effects of a tunable translational noise.

On further increasing the active fraction, η, the distributions of both phases undergo micro-clustering. For η=0.5, panel (d), both species aggregate in small, short-lived clusters. This effect is clearly due to the behavior of the active component of the mixture.

**Demixing** - On increasing the speed, $v_0$, of the active disks, the scenario changes dramatically, as illustrated in Figure 2. The micro-clustering phenomenon disappears for $v_0/U_0 = 0.3$. Similarly to the pure active suspension, for $v_0 > U_0$ self-propulsion wins over advection, and the active disk pile up in the stagnation areas at the base of the ascending (descending) flows against the lower (upper) array walls. As a result, the passive disks, separated from the active ones, toward the center of the convection rolls, regrouping in dynamical patterns. Phase demixing grows more effective with increasing $v_0$, its onset being retarded at large |. A large packing fraction of active disks is harder to be contain in the stagnation areas separating the convection rolls.

**Diffusion** - The pair collisions in a colloidal fluid of appropriate density suffice to make an individual particle cross the convection roll separatrices even in the absence of thermal noise and self-propulsion. As reported in Ref. [9], the particles of a noiseless passive suspension may thus diffuse along a linear convection array as an effect of steric collision alone (athermal diffusion). On the other hand, advection hinders the phenomenon of athermal clustering that takes place in dense active suspensions under no-flow conditions. Not surprisingly, in a binary mixture the interplay between active and passive phases affects the diffusion of both species.

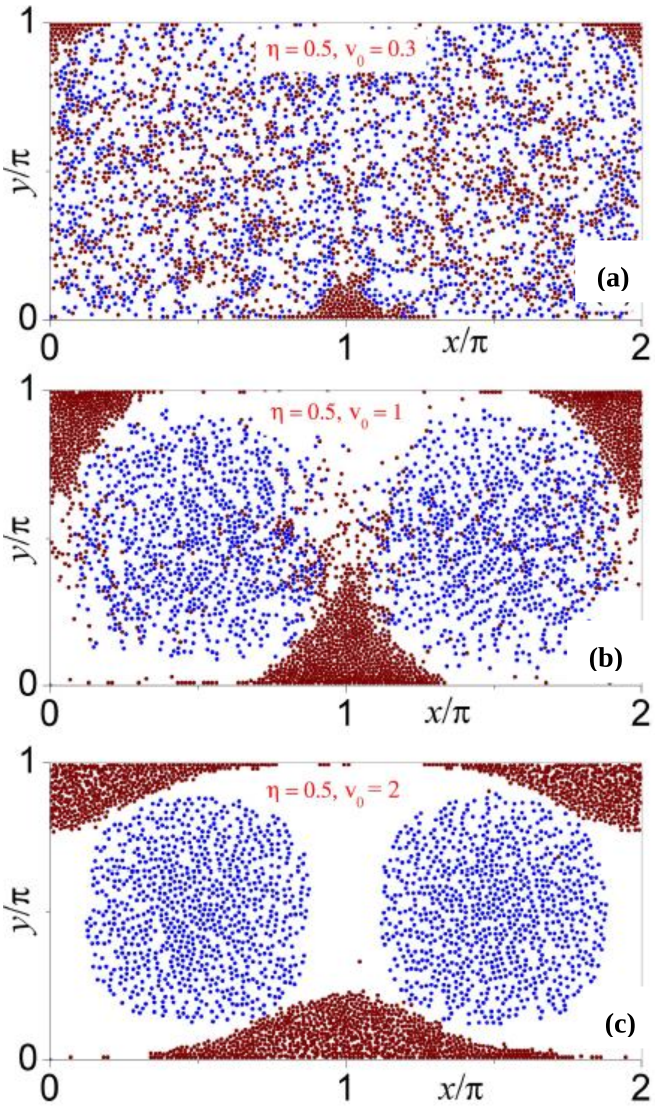


Fig.2: Binary mixture of N=3420 active (brown) and passive disks (blue) with $D_0$=0, $D_\theta$=0.01 and $v_0$=0.3,1.0 and 2.0 (from top to bottom) and η=0.5. At t=0 all N disks were randomly distributed in the unit cell ; all snapshots were taken at $t=10^5$. All other simulation parameters are as in Fig. 1.

For $v_0$=0, the mixture is a passive fluid with $\eta = 0$ and its diffusion is purely athermal.[9] In the opposite limit, $v_0 >> U_0$, the active phase accumulates against the array walls, leaving the passive one largely undisturbed. The passive particles then form regular patterns that rotate around the center of the convection rolls; the area accessible to them is restricted to the sinusoidal effective channel delimited by the lateral aggregates of active particles. This suppresses the diffusion of the passive mixture fraction almost completely, as apparent in Fig3 (a,b) for $v_0 > U_0$. Such an effect grows more prominent on increasing the active fraction|.

Adding slow active disks to a passive suspension favours its diffusivity. Accordingly, the curves of passive particle diffusivity ($D_p$) versus $v_0$, $D_p(v_0)$ exhibit two maxima, a smaller one for $v_0/U_0$ =0.03 and a higher one for $v_0/U_0$ = 0.2. We attribute such optimal diffusive regimes to two distinct mechanisms; (i) the first $D_p$ peak is a signature of the stirring effect introduced in sub-section stirring, whereby the motility of the active disks destroys the dynamical clusters of the passive disks localized at the center of the convection rolls, thus favoring their diffusion along the array; (ii) the higher peak is related to the formation of micro-clusters, with active and passive disks clumping together into

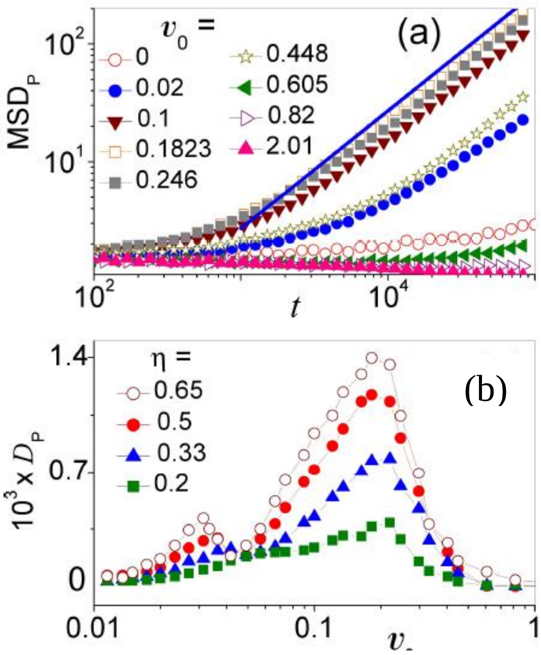


Figure 3: (a) Mean-square displacement of passive particles MSDp as a function of t for different v0. (b) Passive particle diffusivity as a function of self-propulsion velocity for different h. Model parameters are: $D_0 = 0$, $D_\theta = 0.01$, $\sigma = 0.05$, $v_\varepsilon = 1$, $L = 2\pi$ and $U_0 = 1$.

short-lived small-scale structures. The higher motility of the active phase is thus transferred to the passive one, whose diffusivity is thus enhanced.

In the Fig.4 we presented diffusivity of active component ($D_a$) in the mixture as a function of $v_0$ and η. For $v_0 \lesssim 0.2$, $D_a$ is quite insensitive to the density of the active disks, panel (a), and grows linearly with $v_0$ panel (b). The depinning of the active

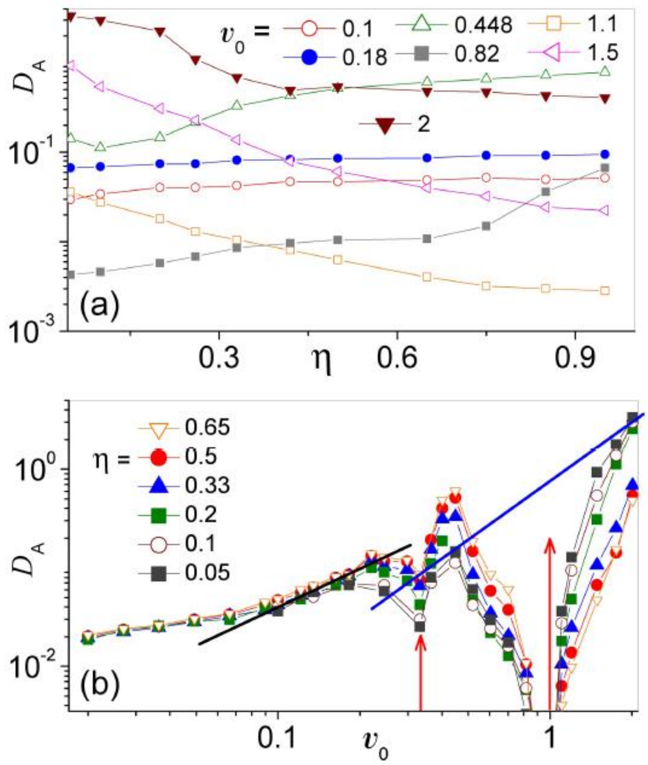


Figure 4: (a) Diffusivity of the active component ($D_a$) vs h for different self-propulsion velocity. (b) $D_a$ vs v0 for different η. The vertical arrows in (b) correspond to the higher maxima of the curves $D_p(v_0)$ in Fig. 3(b) (left) and the single-particle depinning condition from the wall advective flow, $v_0 = U_0$ (right). Straight lines are linear and quadratic reference power laws. Model parameters are: $D_0 = 0$, $D_\theta = 0.01$, $\sigma = 0.05$, $v_\varepsilon = 1$, $L = 2\pi$ and $U_0 = 1$.

disks from the convection rolls, signaled by an increase of $D_a$, and then their aggregation in the appropriate stagnation areas along the channels walls, with a consequent drop of Da. The growth of the diffusion constant of a single active particle in a convection array is known to turn from linear to quadratic,[19] as suggested in Fig. 4(b). In the presence of steric interactions, however two dips appear in the $D_a(v_0)$ curves: (i) one in correspondence with the higher maximum of $D_p(v_0)$, which can be attributed to the “diffusivity transfer” [6] between the active and passive mixture components; (ii) a deeper one for v0 ’ $U_0$, which marks the aggregation of the fast active disks at the bases of the ascending (descending) flows along the lower (upper) array walls. The active disks resume their typical motility with $D_a \sim v_0^2$ only for much larger self-propulsion speeds, when the advection effects grows negligible. For details about diffusion in the active-passive binary mixture we refer [8].

**4. Conclusion**

We have investigated the diffusion properties of a mixture of active and passive colloidal particles of finite size advected in a linear convection array. The combination of advection and steric collisions results in peculiar mixing and demixing mechanisms, which depend on the motility and density of the active fraction. Besides its fundamental interest in the field of soft and biological matter, this problem has practical implications, for instance, in medical sciences. Let us consider a convection flow along a narrow channel, say, the vessel of a biological organism. The particles advected by the flow can be either passive drug complexes or active swimmers (synthetic or biological, alike), or a mixture thereof. Based on the outcome of the present study, a small fraction of active nano-particles can help control drug delivery by preventing the passive suspension from clustering in the convection rolls. Vice versa, an excess of more motile active swimmers tends to sediment in stagnation areas against the channel walls, thus causing solid occlusions that may hinder transport in the channel. As the focus of this report was on the interplay of advective and collisional dynamics, two important ingredients were ignored, namely, inertia and hydrodynamical interactions. While this assumption may be justified at low Reynolds numbers, appreciable inertial and hydrodynamical effects are expected in the case of large and massive advected particles, irrespective of their motility. This question will be addressed in a forthcoming publication.

**5. Schedule and prospect for the future**

In the next fiscal year, we plan to explore the following issues, some of which arose during the research work of the current fiscal year.

(i) Our simulation results prove that active and passive phases are segregated in convection roll arrays Active particles pile up in the stagnation areas and passive ones get separated forming a dynamical pattern about the centre of the convection rolls. It is apparent from snapshots phase point distribution that the structure of two phases largely depends on the self-propelled parameters and thermal fluctuations. To explore structural details of these two phases, we plan to calculate the relevant radial distribution functions, g(r). Here, g(r)dr is defined as the number of particles within a spherical shell with inner and outer radius, r and r+dr, respectively. Once we obtain a radial distribution function, we can calculate other associated quantities, like, structure factor and virial pressure of the system.

(ii) Further to better examine the structure of the mixture in the convection roll when two phases are not clearly separated, we plan to calculate the demixing order parameter [10] defined as,

$$\langle \chi \rangle = \frac{1}{A_a} \left\langle \eta_a \left[ \sum_{i=1}^{N_a} (n_i^a - n_i^p) / 6N_a - 2\eta_a + 1 \right] \right\rangle.$$

$$+ \frac{1}{A_p} \left\langle (1 - \eta_a) \left[ \sum_{i=1}^{N_p} (n_i^p - n_i^a) / 6N_p + 2\eta_a - 1 \right] \right\rangle.$$

Here, $n_i^{a/p}$ denote the numbers of active/passive particles among the 6 nearest neighbour of the i-th particles, $N_{a/p}$ the total numbers of active/passive particles in the mixture. Moreover, $A_{a/p}$ are appropriate normalization factors to secure that the order parameter is one (zero) for full demixing (mixing) condition.

We will consider binary system of active-passive particles, chiral-achiral swimmers, and levo-detrogyre active particles both in 2D and 1D arrays of convection rolls. Further, the impact of external biases will be examined in case of linear arrays of convection roll.

To address the above-mentioned issues, we will use numerically method described in the section 2. Currently, we have a "Quick Use" user account, and we would like to get our access to the computation facilities extended to the next usage term (up to 31st March 2024) under the same user category.

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**Fiscal Year 2022 List of Publications Resulting from the Use of the supercomputer**

Pulak K. Ghosh, Yuxin Zhou, Yunyun Li, Fabio Marchesoni, and Franco Nori; Binary Mixtures in Linear Convection Arrays, ChemPhysChem, volume - 24, issue 1, pages/article no e202200471, 3rd January 2023.

**[Paper accepted by a journal]**

None

**[Conference Proceedings]**

None

**[Oral presentation]**

None

**[Poster presentation]**

None

**[Others (Book, Press release, etc.)]**

None