

1st Spanish Soft Matter 1 ½ Day

2023, Oct 29 – Oct 31

Centro de Ciencias de Benasque Pedro Pascual

<https://www.benasque.org/2023ssm/>

$$\rho \frac{Du}{Dt} = \rho k - \nabla P + \mu \left(\frac{1}{3} \nabla (\nabla \cdot u) + \nabla^2 u \right)$$

$$\sigma(t) = E\alpha(t) + \eta \frac{d\alpha(t)}{dt}$$



División de Física de
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Organizers:

Juan L Aragonés (IFIMAC-UAM)

Laura R Arriaga (IFIMAC-UAM)

Alberto Fernández-Nieves (UB-ICREA)

Miguel Ruiz-García (UCM)

Schedule	Sunday, October 29 th
15:00	Bus from Barcelona, Universitat de Barcelona, Diagonal 686, Metro: L3 Palau Reial (Note that the bus stops opposite University of Barcelona, Facultat de Física I Química)
15:30	Bus from Barcelona airport 'El Prat', Terminal T2A (on leaving exit, turn left and you will find a police building called 'Mossos d'Escuadra'. Cross the road using the zebra crossing and turn left. The bus will stop there.)

Schedule	Monday, October 30 th
9:00 - 9:45	Opening by Alberto Fernández-Nieves and Invited Talk by Enrique Velasco
9:45-11:05	Session on Active Matter I
11:05-11:30	Coffee
11:30-13:30	APS Sponsored Session on Fluid Dynamics and Granular Matter
13:30-15:00	Break
15:00-15:30	Coffee
15:30-17:30	Session on Networks and Rheology
17:30-19:00	Poster Session
19:00	Reception and Posters

Schedule	Tuesday, October 31 st
9:00 - 9:36	Invited Talk by Eva Noya
9:36-10:36	Session on Active Matter II
10:36-11:30	Coffee
11:30-11:50	Session on Active Matter II
11:50-12:26	Invited Talk by Ignacio Pagonabarraga
12:26	Adjourn
15:30	Bus to BCN



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Schedule	Program on Monday, October 30th
9:00 - 9:45	Opening by Alberto Fernandez-Nieves and Invited Talk by Enrique Velasco Ordering of 2D fluids: Entropy driven clustering and exotic symmetries
9:45-11:05	Session on Active Matter I <ol style="list-style-type: none"> 1. Light management in microalgae: metabolism, motility and communication. I Tuval 2. Deciphering chemically-controlled dynamics in active matter: A study of motile colloids and elastic shells. DA Matoz Fernandez 3. Driven and ratchet transport on self assembled colloidal tracks. F Martinez-Pedrero 4. Transport of active colloids in structured environments. AE Ortiz
11:05-11:30	Coffee
11:30-13:30	APS Sponsored Session on Fluid Dynamics and Granular Matter <ol style="list-style-type: none"> 1. Force on a sphere suspended in flowing granulate. RC Hidalgo 2. Biomicrofluidic analysis of hematological diseases by means of mathematical biomechanical models and statistical analysis. A Hernandez-Machado 3. Past, Present and Future of Clogging in Bottlenecks. I Zuriguel 4. Let the splat out of the bag: The fluid mechanics of splat painting. L Champougny 5. An interfacial dripping faucet. J Rodriguez-Rodriguez 6. Computational fluid dynamics predictions of hierarchical vascular networks. P Padmanaban
13:30-15:00	Break
15:00-15:30	Coffee
15:30-17:30	Session on Networks and Rheology <ol style="list-style-type: none"> 1. Cross-linker mobility governs fracture behavior of catch-bonded networks. J Ruiz-Franco 2. Star-like polymers as tunable soft nano-objects. P Bacova 3. Bio-inspired soft matter at the service of interactive biointerfaces and synthetic cells. C Rodriguez-Emmenegger 4. Rheology of fatty acid Langmuir monolayers during isobaric 2D melting. P Sanchez-Puga 5. Water solvation in bio-nano complex matter. G Franzese 6. Financial markets as soft matter systems. J Clara-Rahola
17:30-19:00	Poster Session <ol style="list-style-type: none"> 1. The uncanny weight of granular columns. R Planet 2. Performing 3DDLs to study the dynamics of dense microgel suspensions. A Arenas-Gullo 3. Statistical properties of the dynamics of a fan air-fluidized chiral particle. F Vega Reyes 4. Swelling of alginate gel. G Briand 5. First order alignment transition in an interfaced active nematic. O Bantysh 6. Motion and control of virtual colloidal particles in confined chiral liquid crystals. J Torres-Andres 7. Aggregation of discoidal particles due to depletion interactions. C Calero 8. Discovering Dynamic laws from observations: The case of self-propelled, interacting colloids. M Barriuso Gutierrez 9. Macroscopic active particles driven by light. S Levay 10. Aqueous two-phase systems within selectively permeable vesicles. B Tinao 11. Rolling backward: Tuning microroller locomotion in an obstacle lattice. G Geva 12. Rolling vesicles: From confined rotational flows to Surface-enabled motion. P Magrinya 13. Collective sensing of E. coli under local flows. R Campusano 14. Self-organized states of solutions of active ring polymers in bulk and under confinement. JP Miranda-Lopez 15. Curvature sorting of rotating proteins into lipid filaments. I. Lopez-Montero 16. Where do virions localize in the residue of a dry sessile respiratory drop? C. de la Torre
19:00	Reception and Posters

Schedule	Program on Tuesday, October 31st
9:00 - 9:36	Invited Talk by Eva Noya A one-component icosahedral quasicrystal formed by particles with directional bonds
9:36-10:36	Session on Active Matter II <ol style="list-style-type: none">1. Active defects in flat and curved surfaces. J Nambisan2. Force measurements in active nematics. I Velez Ceron3. Nematic colloid transport in microchannels. R Herrera
10:36-11:30	Coffee
11:30-11:50	<ol style="list-style-type: none">4. Confinement-induced dynamics of microscopic active-passive mixtures. M Polin
11:50-12:26	Invited Talk by Ignacio Pagonabarraga Active matter and active materials: Emerging behavior in intrinsically out of equilibrium systems
12:26	Adjourn
15:30	Bus to BCN

Plenary Contributions

ORDERING OF 2D FLUIDS: ENTROPY DRIVEN CLUSTERING AND EXOTIC SYMMETRIES

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Two-dimensional (2D) hard particles with polygonal shapes exhibit intriguing ordering properties at fluid densities. Similar to other hard particles, the equilibrium ordering behaviour is solely governed by entropy, which reveals its most subtle aspects as a generator of order. Our focus lies in exploring the fluid phase and, specifically, the liquid-crystal phases that exist between the isotropic fluid and the fully ordered crystal. These phases exhibit positional disorder, while particles are aligned on average along specific *directors*.

While the symmetry of oriented fluid phases can often be inferred from the symmetry of individual particles, this is not always the case due to the clustering tendencies exhibited by certain particle geometries. These clusters can be regarded as *superparticles* with symmetries different from those of the individual particles. Different clusters may compete, which results in nontrivial phases, sometimes with high-index symmetries. A dramatic example of this behaviour is the case of right-angled triangles, which tend to form relatively stable square-shaped tetramers, resulting in fluid phases with 4-fold symmetry. However, these clusters compete with square dimers and other clusters, giving rise to strong fluctuations exhibiting 8-fold symmetry in the system.

In this presentation we show several illustrative examples of the effects that give rise to “exotic” fluid phases characterised by high-index symmetries, which are not immediately apparent from particle shape alone. Since clustering effects are not adequately accounted for by standard density-functional theories, we employ more sophisticated versions to explore and understand these effects. Our investigations are complemented by simulations and experiments on vertically-vibrated granular monolayers of metallic particles. The latter enable us to assess the extra contributions of dissipation to the problem. In addition, they can be used to excite different types of topological defects by using containers with particular shapes (an example is shown in the figure below). In general these defects comply by the rules of topological theory, and contain information on the intrinsic symmetry of the phases.

All of these theoretical and experimental techniques can be used with advantage to explore the role of entropy in the stabilisation of complex phases with high symmetries and, as a bonus, to investigate the connections between 2D fluids in thermal equilibrium and their vibrated-monolayer counterparts, which dissipate energy but exhibit similar properties in the steady-state regime.

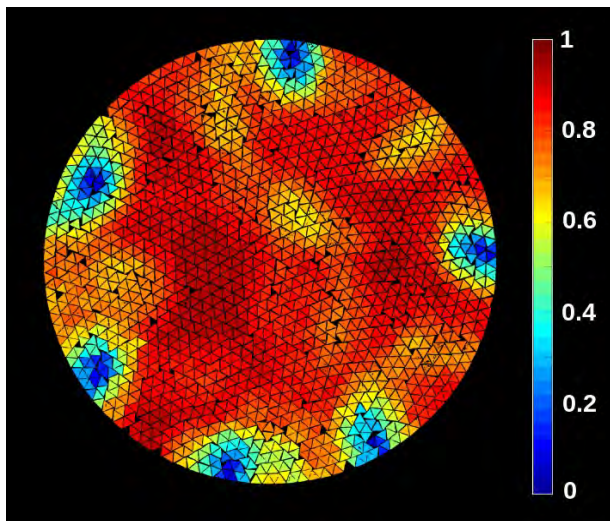


Figure. False-colour map of the Q_6 order parameter, which measures local particle arrangements with six-fold symmetry, in a quasi-two dimensional horizontal cavity of granular equilateral triangles. Particles are vibrated in the vertical direction and organise themselves into a fluid phase with a high value of the order parameter, except for the presence of six regions where the order parameter is depleted. These regions correspond to topological defects with a charge +1. The presence of exactly six defects is dictated by topology in a system with an intrinsic six-fold symmetry when the shape of the container is not commensurate with this symmetry. These defects restore the global symmetry of the system, and can be seen to behave as repulsive “particles” with a force which is transmitted at long distances through the fluid because of the inherent orientational stiffness of the latter.

A one-component icosahedral quasicrystal formed by particles with directional bonds

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Icosahedral aperiodic crystals, or quasicrystals, (IQCs) are materials that are ordered but lack periodicity in any direction of space. The first experimentally observed quasicrystal was obtained by rapid quench of an Al-Mn alloy by Shechtman *et al.* [1]. This first quasicrystal had icosahedral symmetry and, since then, many IQCs have been found in other metallic alloys [2], but, so far, never in non-metallic or one-component systems. On the contrary, axial quasicrystals, which are aperiodic in two dimensions but periodic in the third one, have been also observed in some soft matter systems, in some cases with only one-component [3].

Using computer simulations, we have recently shown that IQCs can be formed from colloidal particles with directional bonds [4], by designing model particles whose geometries mimic the local environments of the target IQCs. This strategy was first validated for IQCs of body-centered (BC) and primitive (P) types, with the simplest models consisting of two particle types. Here, we will show that using the same approach it is possible to design model systems with only one-particle type that robustly assemble into a target face-centered (FC) IQC. We hypothesize that the designed models might be experimentally realizable in light of the impressive recent advances in the design of DNA origamis [5] and proteins [6].

Acknowledgements: E.G.N. acknowledges financial support from Agencia Estatal de Investigación, Grant No PID2020-115722GB-C21.

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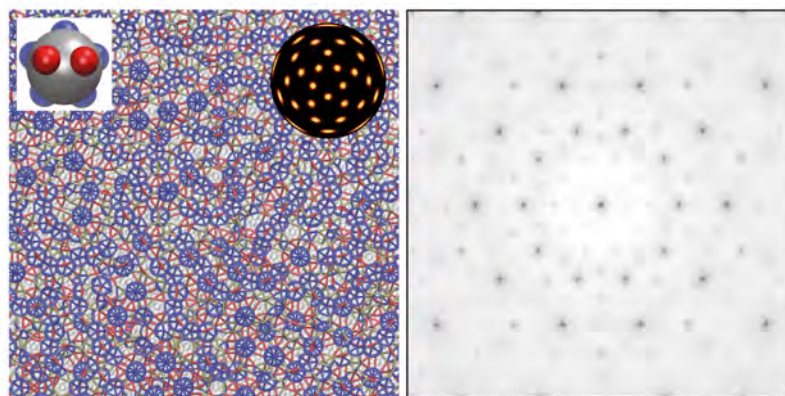


Fig.1: One-component FC IQC structure formed colloidal molecules with seven interaction sites. The diffraction pattern projected along a 5-fold symmetry axis is also shown.

Active matter and active materials: Emerging behavior in intrinsically out of equilibrium systems

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Flocks of birds, schools of fishes, or bacterial colonies constitute examples of living systems that coordinate their motion. In all these systems their constituent elements generate motion due to energy consumption and can exchange information or react sensitively to chemical cues to move together or to react collectively to external signals. Artificial systems, such as nanorobots, exploit the heterogeneous compositions of their surface to displace as a result of the heterogeneous chemical processes that take place in the presence of appropriate chemical substances.

All these systems are intrinsically out of equilibrium in the absence of any external driving, and their collective properties result as a balance between their direct interactions and the indirect coupling to the medium in which they displace. The mechanical balance that determines the states they develop spontaneously make these systems very versatile and have a natural tendency to form large scale aggregates. An understanding on the basic principles underlying the emergence and self-assembly on active systems poses fundamental challenges: How do the relevant entities interact with each other? Can we identify universal, generic principles associated to the main features in the self assembly and emergent behavior of intrinsically out of equilibrium systems? Are there mechanisms that can be shared by living systems and synthetic, active materials?

I will consider simple statistical models to address fundamental aspects of active systems and will analyze the implications that self-propulsion has in the emergence of structures in suspensions of model self-propelled particles. I will discuss the potential of schematic models to address fundamental questions that still remain open, such as the connection of the effective phase diagram and pressure with effective equilibrium concepts. These approaches allow to understand the transformations that characterize these systems as effective phase transitions out of equilibrium.

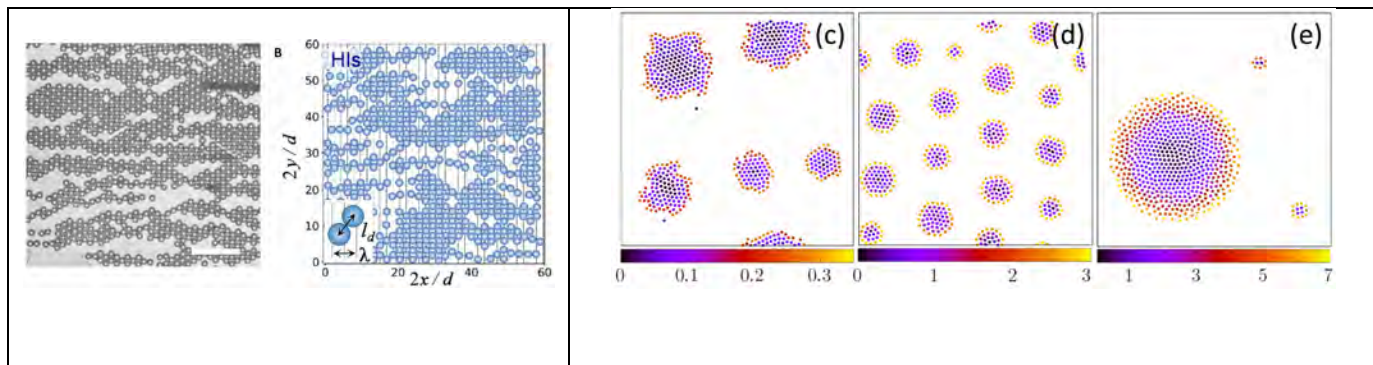


Figure 1 Anisotropic clusters of dipolar colloids propelled by a rotating magnetic field controlled by the hydrodynamic coupling.

Figure 2: Self assembled clusters of rotating colloids. Particles attract and interact hydrodynamically. The relative strength of the attraction with respect to hydrodynamic force controls the characteristic size of the self-organized discoidal clusters.

ORAL Contributions

Session on Active Matter I

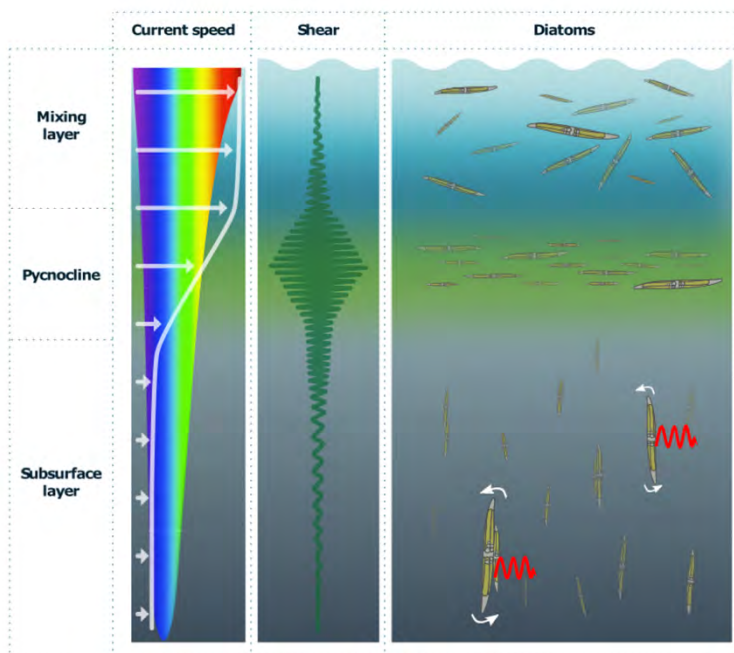
Light management in microalgae: metabolism, motility and communication

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Photosynthetic microorganisms underpin major food webs, contribute half of the global oxygen production, and promise new avenues to produce complex chemicals and biofuels. Their fitness hinges on the ability to sense, elaborate and respond to external stimuli, especially light. Light has several roles for photosynthetic microorganisms: sensed by photoreceptors it provides spatiotemporal information, used e.g., to regulate cell cycle or as means for intercellular communication; absorbed by chloroplast pigments it supplies energy for photosynthesis, crucial for life on Earth.



To thrive, plants and algae evolved the ability to integrate information and energy provided by light, through complex mechanisms currently not well understood. Motile microalgae can do so *via* phototaxis, an active steering response based on light reception (swimming towards/away from light), often with unexpected collective consequences. Non-motile species rely on intracellular photo-responses capable of inducing social patterns. Here I will summarise our current understanding of how microalgae combine these responses into a coherent and effective strategy for light management.

Fig.1 - Diatoms have functional red-light photoreceptors (of the phytochrome superfamily) ideal for sensing and communication at depth.

Deciphering Chemically-Controlled Dynamics in Active Matter: A Study of Motile Colloids and Elastic Shells

D A Matoz Fernandez

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The interdisciplinary domain of active matter, intrinsically non-equilibrium, explores the profound interplay between physical properties and chemical interactions. In this talk, we shed light on the collective behavior of motile colloids and the chemically induced morphological transformations in responsive elastic shells, both steered by chemomechanical processes.

We begin with the exploration of crowding and chemotactic interactions on the collective behavior of motile colloids. Using Brownian dynamics simulations, we examine the effect of packing fraction on the formation of non-equilibrium structures within a monolayer of diffusiophoretic self-propelled colloids. Particular attention will be paid to the emergence of a new phase-separated state, born out of the competition between long-range diffusiophoretic interactions and motility, observable at moderate activities and across an extensive range of packing fractions.

We then shift our focus to responsive elastic shells, illustrating how chemical reactions incite significant morphological changes. We elucidate the coupling of local mechanical response with chemical processes occurring within the shell, leading to swelling and deswelling dynamics that yield diverse morphological adaptations, including periodic oscillations and buckling-unbuckling dynamics. The feedback from the mechanical changes to the chemical reactions further leads to the generation of specific dynamic patterns triggered by an initial deformation.

This talk will offer an in-depth understanding of active matter, highlighting the pivotal role of chemical interactions in controlling and modulating their behavior, from motile colloids to autonomously responsive elastic shells. Such insights hold the promise to inspire new design paradigms for future responsive materials.

References:

Fadda, F., Matoz-Fernandez, D. A., van Roij, R., & Jabbari-Farouji, S. (2023). The interplay between chemo-phoretic interactions and crowding in active colloids. *Soft Matter*, 19(13), 2297-2310.

Li, S., Matoz Fernandez, D., & Olvera de La Cruz, M. (2021). Chemical controlled tangential growth leads to autonomous shell morphology. In *APS March Meeting Abstracts* (Vol. 2021, pp. C02-008).

DRIVEN AND RATCHET TRANSPORT ON SELF ASSEMBLED COLLOIDAL TRACKS

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In this work, we investigate different mechanisms of transport of matter through a liquid suspension at the microscale, where low Reynolds number conditions and thermal noise determine the strategies to be adopted. To this end, we have exploited the microstructured magnetic properties of different magnetic colloidal self-assemblies attached to a solid substrate. When excited by rotating or pulsating magnetic fields, these engineered tracks create travelling or on/off switching potentials that promote pulsed or ratchet transport of nearby non-adsorbed magnetic colloids [1,2]. These approaches serve both to transport matter under different conditions and to provide suitable models for analyzing different aspects of such approaches.

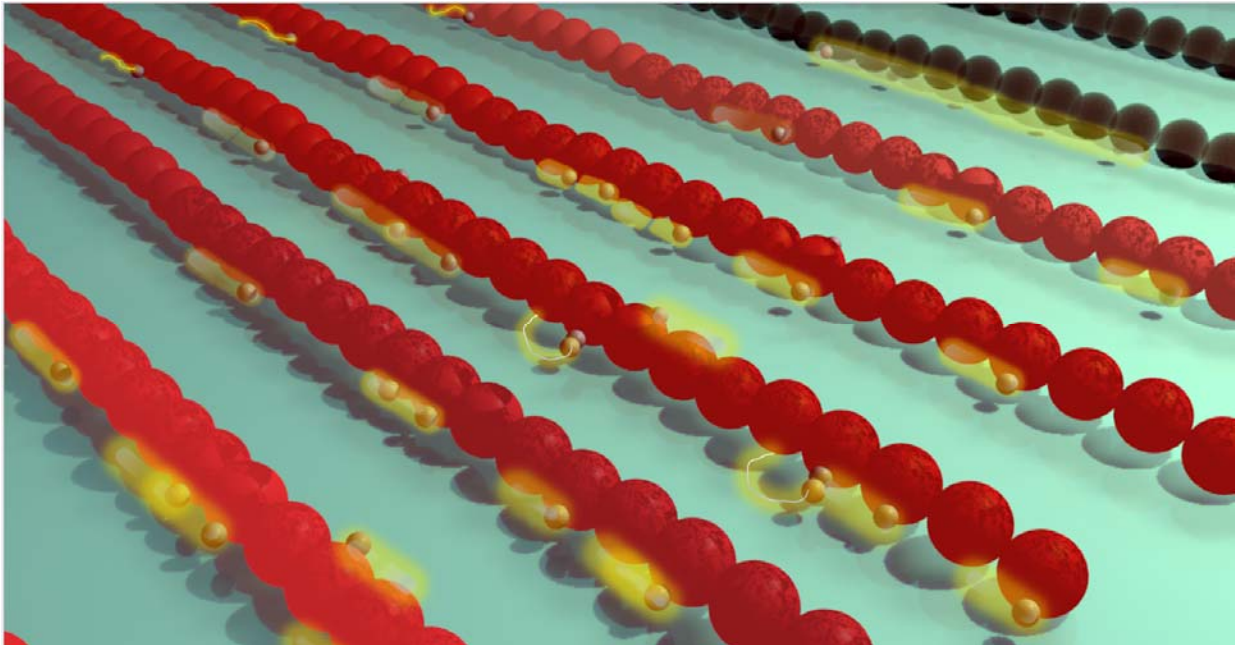


Figure 1 – A swarm of small, non-adsorbed superparamagnetic spheres is driven along parallel tracks of larger magnetic colloids, adsorbed on a solid surface. The non-adsorbed spheres are transported by the action of a magnetic field, rotating parallel to the confining plane.

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TRANSPORT OF ACTIVE COLLOIDS IN STRUCTURED ENVIRONMENTS

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Transport of active or driven particles plays a crucial role in a multitude of processes ranging from biological systems to electrons in solids. In all these systems, transport is controlled by the structure and properties of the environment. Therefore, we are studying the physical principles that control the transport of active particles in structured environments to eventually be able to program their transport depending on their dynamics and environment structure.

Specifically, we study the two-dimensional transport of active rotating particles, or spinners, on a substrate containing arrays of fixed obstacles. In the absence of obstacles, the spinners just rotate in place [1]; however, in the presence of one or more fixed obstacles, the spinner translates due to the hydrodynamic coupling with the obstacles. Contrary to the behavior of passive Brownian-diffusive colloids [2], the transport of spinners is enhanced in the presence of disorder on the positions of the obstacles. The spinner is trapped at two different steady-state trajectories in square and triangular obstacle lattices, but confinement size increases greatly even at small amounts of disorder on the obstacles' lattice positions. If the spinner-obstacle interaction includes attraction, spinner transport can be achieved in disordered obstacle lattices. Thus, we analyze the role of attraction and disorder on the transport properties of spinners on these structured environments.

The disorder-induced transport mechanism here described is robust, and similar physical principles might be relevant to understand non-thermal transport processes in biological systems. Moreover, our model system is the first step in the design of a smart material for controlled transport and separation of colloidal particles based on their physicochemical properties, which will find applications in microfluidics and soft robotics.

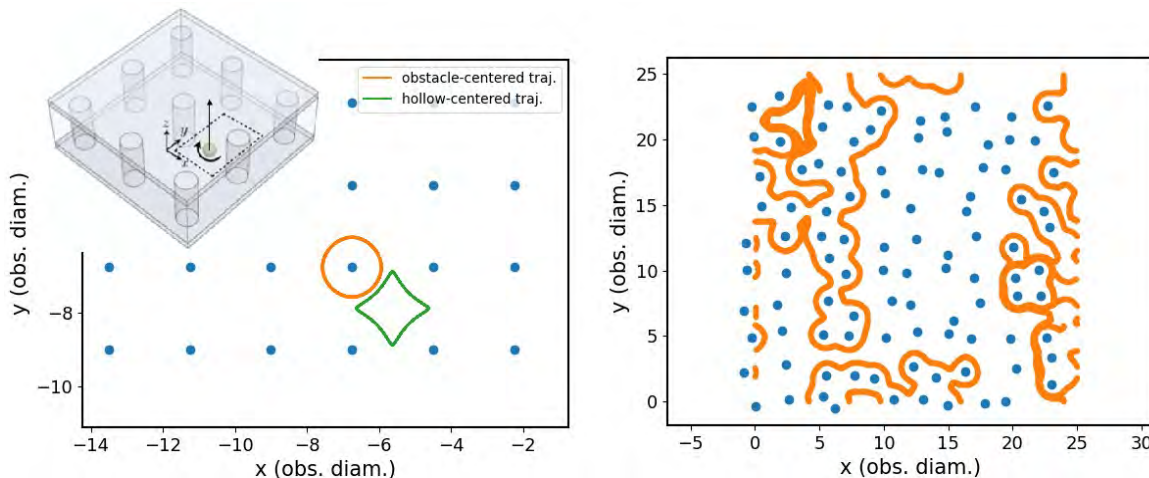


Figure 1 – Left, upper-left corner: a simple diagram of the system. The colloidal particle rotates in place and moves between fixed obstacles in the XY plane. Left: the two possible steady-state trajectories in an ordered square lattice. Right: a trajectory in a square array where obstacles have undergone random Gaussian displacements in their positions, showing that disorder opens up the path for a wider range of spinner behaviours.

- [1] Aragonés, J. L., Steinel, J. P., & Alexander-Katz, A., Nature Communications, 7, 11325 (2016)
[2] Chakraborty, I., & Roichman, Y., Physical Review Research, 2, 022020 (2020)

ORAL Contributions

Session on Active Matter II

ACTIVE DEFECTS IN FLAT AND CURVED SURFACES

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The interaction and dynamics of topological defects have inspired numerous studies across physics over centuries. They manifest as salient features in liquid crystalline materials, as regions where the underlying director field is undefined. Liquid crystals can be intrinsically driven out of equilibrium via an energy input at the level of the constituent particles, thus forming a unique class of non-equilibrium systems, known as active liquid crystals. In this work, we explore the rich phenomenology of topological defects observed in the microtubule-kinesin active nematic system, confined to surfaces of different topology and varying curvature. We image the active nematic via fluorescence confocal microscopy and implement our image analysis algorithms based on a computer vision technique called Coherence Enhanced Diffusion Filtering to extract the underlying director fields [1]. We then identify defect positions and orientations to define order parameters for the set of active defects. In 2D flat space experiments, we observe short-range ferromagnetic alignment of $+1/2$ defects, mediated by $-1/2$ defects in between [2]. This is primarily driven by passive elastic mechanisms, as confirmed via hydrodynamic simulations of active and passive liquid crystals. However, the system does not develop any long-range or quasi-long-range order over time. The qualitative features of defect-defect correlations are found to be independent of defect density [2]. In curved space experiments, we observe a clear preference for the orientation of defects and persistent long-range order detected on highly curved regions of toroidal drops [3]. This is a remarkable confirmation that curvature, and gradients of it, have a major role in intrinsically biasing the alignment of defects. This is in stark contrast to random, isotropic defect orientations found in locally flat regions. We then propose an idealized mechanism of defect alignment subject to curvature gradients, which is currently being inspected via agent-based simulations of an active multi-defect system [3]. The observation of surface curvature as an aligning field is much more fundamental than recent works in similar systems, where patterned substrates and external fields have been used to align defects and create order. Overall, our work explores the rich interplay of activity, topology and curvature in a liquid crystalline system and how topological defects interact to develop correlations and orientational order subject to the governing factors. More generally, our work provides an exciting test bed with associated techniques to study active matter in a controlled experimental setting.

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- [3] Work In Progress (2022-)

FORCE MEASUREMENTS IN ACTIVE NEMATICS

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Active nematic dynamics are governed mainly by means of elastic, active and viscous stresses [1], which reveal the elastic constant (k), activity (α) and viscosity (η) as key parameters of the material. However, the values of these parameters are still unclear. Different approaches have been used to determine them. For example, active nematic viscosity has been studied experimentally [2] and theoretically [3], [4] giving out results with different order of magnitude.

In this work, we present a novel method to determine both the activity and viscosity of active nematic based on force measurements using elastic cantilevers. With a custom DMD-based photolithography technique [5], we are able to build polymeric cantilevers in a microtubule-kinesin based active nematic [6], from the bottom to the surface. Measuring the deflection of the cantilevers the force applied by the active material can be determined, and then, the force is correlated to the director and velocity fields to obtain the values of the activity and the viscosity of active nematics. The results obtained show that the ratio between activity and viscosity is proportional to the mean vorticity as was previously predicted by Giomi [7], and the variation of this ratio with the activity follows the trend that was also predicted [8].

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Nematic Colloid Transport in Microchannels

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Particle transport at the microscale is characterized by the breaking of the fore-aft particle symmetry to achieve propulsion. Chemical or physical changes in half of the particle's surfaces, i.e. Janus particles, is the most common approach to unbalance the forces around the particle, but it involves the use of complex techniques or hazard substances. Directional control of Janus particles is achieved by the application of external fields, such as magnetic fields to navigate them at any point of the space. The use of nematic liquid crystal environments allows to counter back these limitations. The required asymmetry is a consequence of the liquid crystal interaction and organization around the particle surfaces. Moreover, this complex medium offers additional properties such as levitation, locking on direction of transport, and different driving methods, among others. In this work, we highlight the effect of transporting colloids dispersed in a nematic liquid crystal when confined to microchannels of different shapes. Polystyrene pear-shaped particles transported by Liquid Crystal Enabled Electrophoresis (LCEEP) and sedimentation. [1,2] We confined this transport to rectangular channels of variable width (Fig. 1A) and observed an acceleration effect correlated to the change of width (Fig. 1B). Gravitational experiments allowed us to highlight that the phenomenon was independent of the driving mechanism. We emphasize the contribution of the anisotropic medium and provide different interpretations for the acceleration mechanism depending on the driving force.

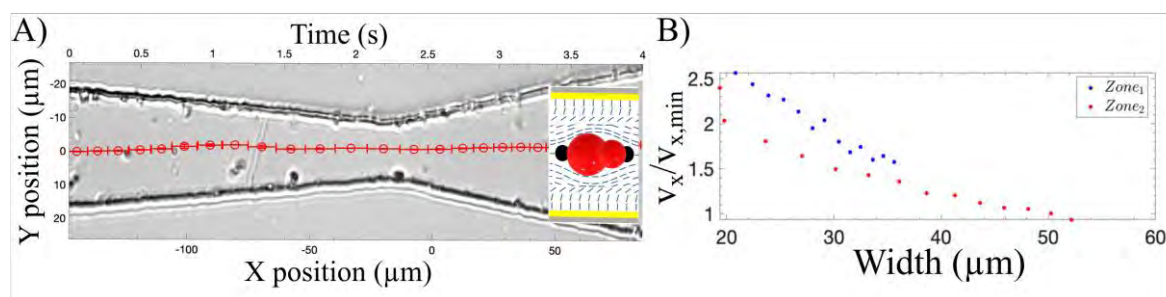


Figure 1. A) Particle tracked path. B) Particle normalized speed as a function of the particle channel width (bottom). Zone 1 and Zone 2 are the regions before and after the smallest width found in the microchannel.

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ORAL Contributions

**APS Sponsored Session on Fluid
Dynamics and Granular Matter**

Confinement-induced dynamics of microscopic active-passive mixtures

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Abstract. Understanding the out-of-equilibrium properties of noisy microscale systems and the extent to which they can be modulated externally, is a crucial scientific and technological challenge. It holds the promise to unlock disruptive new technologies ranging from targeted delivery of chemicals within the body to directed assembly of new materials. Here we focus on how active matter can be harnessed to transport passive microscopic systems in a statistically predictable way. Using a minimal active-passive system of weakly Brownian particles and swimming microalgae, we show that spatial confinement leads to a complex non-monotonic steady-state distribution of colloids, with a pronounced peak at the boundary. The particles' emergent active dynamics is well captured by a space-dependent Poisson process resulting from the space-dependent motion of the algae. The space-dependence of this dynamics and the resulting particle distribution can be modified by changing the interaction of the active elements with the confining walls. Based on our findings, we then realise experimentally the de-mixing of the active-passive suspension, opening the way for manipulating colloidal objects via controlled activity fields [1].

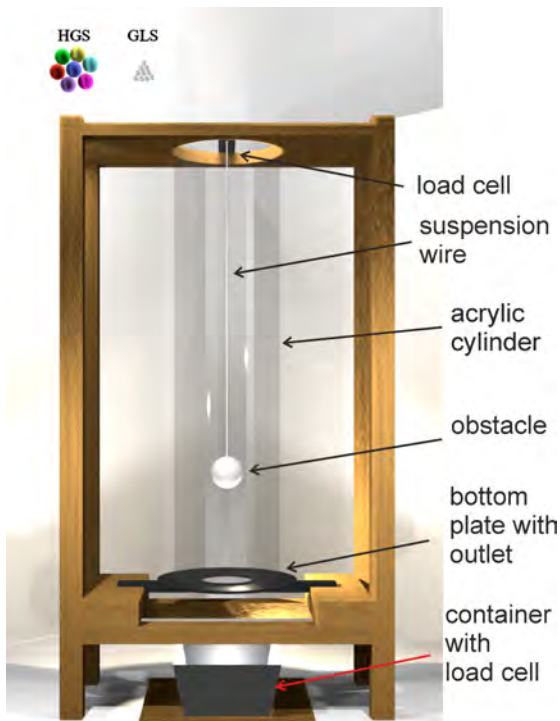
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Force on a sphere suspended in flowing granulate

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We investigate experimentally and numerically the force of flowing granular material on a static obstacle. A sphere suspended in a discharging silo experiences both the weight of the overlaying layers and drag of the surrounding moving grains. In experiments with frictional hard glass beads, the force on the obstacle was practically flow-rate independent. In contrast, flow of nearly frictionless soft hydrogels added drag to the gravitational force. The dependence of the total force on the obstacle diameter result qualitatively different for the two types of material: It grows quadratically with the obstacle diameter in the soft, low friction material, while it grows much weaker, nearly linearly with the obstacle diameter, in the bed of glass spheres. In addition to the drag, the obstacle embedded in flowing low-friction soft particles experiences a total force from the top as if immersed in a hydrostatic pressure profile, but a much lower counterforce acting from below. In contrast, when embedded in frictional, hard particles, a strong pressure gradient forms near the upper obstacle surface.



Figur: Schematic drawing of the experimental setup.

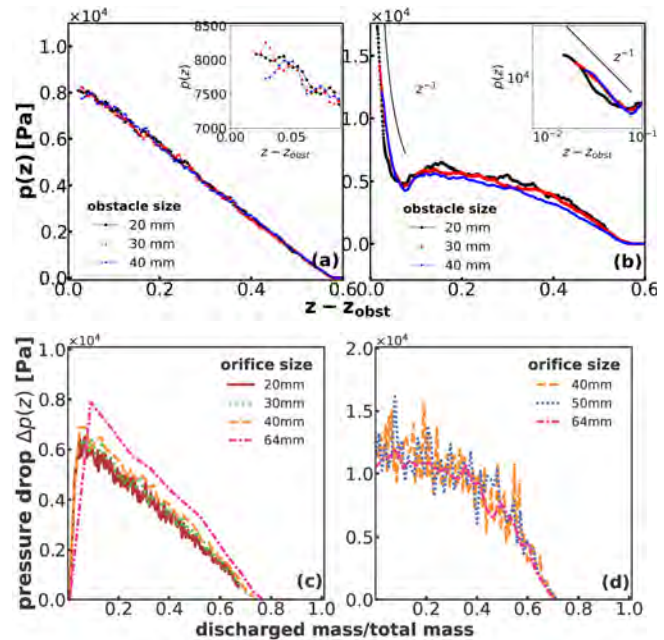


Figure: The pressure profiles $p(z)$ obtained numerically above the intruder for HGS (a) and GLS (b), silo with an orifice size $D = 64$ mm, the insets show zoom of the profiles near the obstacle (log-log in panel (b)). The mean pressure drop (obstacle size $d=40$ mm), depending on the outflow mass in terms of the total mass, for HGS (c) and GLS (d).

Title: Biomicrofluidic analysis of hematological diseases by means of mathematical biomechanical models and statistical analysis

Author: A. Hernandez-Machado

Abstract: We have developed microfluidic devices for precise characterization of hematological diseases. By means of one drop of blood and combining front microfluidics with mathematical models based on biomechanics, we analyze the properties of red blood cells and microrheological properties such as the viscosity of blood. We detect the advancement of microfronts of fluid inside microchannels. By means of statistical analysis we improve the diagnosis of the hematological diseases. We predict if a sample of blood corresponds to healthy blood or to blood with an hematological disease. We have obtained different performance for the different methods, some of them with very good results and an accuracy of 94%.

Past, Present and Future of Clogging in Bottlenecks

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When a group of discrete bodies passes through a narrowing, the flow may be arrested due to the spontaneous formation of a clog (Fig. 1). For inert particles (Fig. 1d), if the clog is stable once the energy of the system is dissipated (an instance that typically occurs in few tenths of a second), it will last forever unless an external input of energy is supplied. In the latter case, the external excitation may break the clog and resume the flow, hence leading to intermittent flow dynamics. In this intermittent scenario, two independent processes are important: i) the formation of clogs (clogging), which determines the time the system is flowing; i.e. the time since the flow restarts until it stops again; ii) the clog destruction (unclogging), which determines the time the flow is temporally interrupted. Interestingly, over the past few years, it has been demonstrated that the statistical features of these two processes are completely different. While the flow intervals display exponential distributions (implying a constant probability of clogging over the whole flowing period), the arrest intervals show heavy tailed distributions (power laws or other). Curiously, this phenomenon, which has been thoroughly studied for externally excited inert grains, it has also been observed for different sorts of active matter (Fig. 1b, Fig. 1c and Fig. 1e) or particle suspensions (Fig. 1a) where the fluid passing through the clogged structure seems to act as a perturbation.

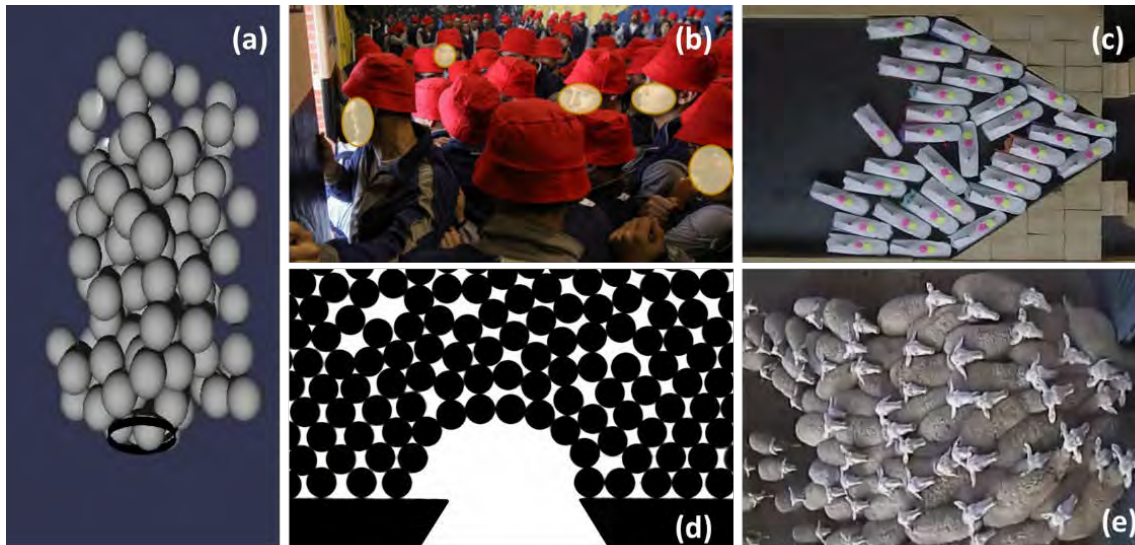


Fig.1. Several examples of bottleneck flow. a) colloidal suspension driven by pressure gradient; b) crowd evacuating a room; c) self-propelled 1 cm-hexbugs; d) inert spheres 1 mm diameter; and e) sheep entering a barn looking for food.

In this presentation I will introduce the basic principles of clogging and talk about the exciting research progress recently achieved in systems as different as colloids, active matter, robotics or pedestrians. Also, I will discuss the substantial knowledge gaps there still are to fully understand the main mechanisms controlling both, clogging and unclogging processes.

LET THE SPLAT OUT OF THE BAG: THE FLUID MECHANICS OF SPLAT PAINTING

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In art, splat painting consists in subjecting a paint-loaded brush to an acceleration (for example by “flicking” the brush or tapping its handle) to detach paint filaments or droplets. These are projected onto the canvas, leaving aesthetic filamentary or spotty patterns. In this technique, perhaps most emblematically used by American painters Jackson Pollock and Sam Francis, the brush never touches the canvas, making the control of the final pattern challenging for the artist. In this study, we develop an experimental setup to produce repeatable tapping on a paint-loaded brush, mimicking the acceleration imposed by the artist’s hand. Using a Newtonian model liquid, we characterize how the amount of paint detached and its final spatial distribution on the substrate depend on control parameters such as paint viscosity and brush acceleration. This allows us to identify different splatting regimes and understand how artists adjust these parameters to tune the final splatter pattern.



Figure 1 – Left panel: Artwork based on splat painting by Caroline Champougny. “Sunday Afternoon” (acrylic paint on paper, 15 x 20.5 cm), 2022, used with permission. Right panel: High-speed snapshots showing ejection of 40 cSt silicone oil from a round brush of base diameter 4.7 mm subjected to an impact on its wooden handle.

J.R.R. acknowledges funding from the Spanish MCIN/AEI/10.13039/501100011033 through Grant No. PID2020-114945RB-C21. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 882429 (L.C.).

AN INTERFACIAL DRIPPING FAUCET

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The dynamics of floating liquid lenses encompasses many interesting and relevant fundamental problems in fluid mechanics, soft matter and material science. Despite this, the generation of liquid lenses has received much less attention than the generation of drops. As a result, there are not many techniques to generate series of them in a controlled manner. Here, we present an unexplored system, analogous to a dripping faucet, where monodisperse lenses of a viscous liquid drip periodically from a rivulet that slides down a water-solid meniscus. To rationalize the dependency of the lenses volume on the flow parameters, we carry out experiments where we inject several liquids at different flow rates, varying the injected liquid viscosity by three orders of magnitude and the flow rate by two. We find that the lens volume, non-dimensionalized with the maximum volume that capillarity can sustain against gravity, depends linearly on a capillary number based on the parameters of the injected liquid. Using this simple scaling we collapse all the experiments on a master curve. Finally, we show that the periodic dripping regime ends when lenses pinch off away from the meniscus at a distance of the order, or larger, than the bath's capillary length. When this happens, the system transitions into regime where a continuous jet feeds a large liquid pool that floats on the bath.

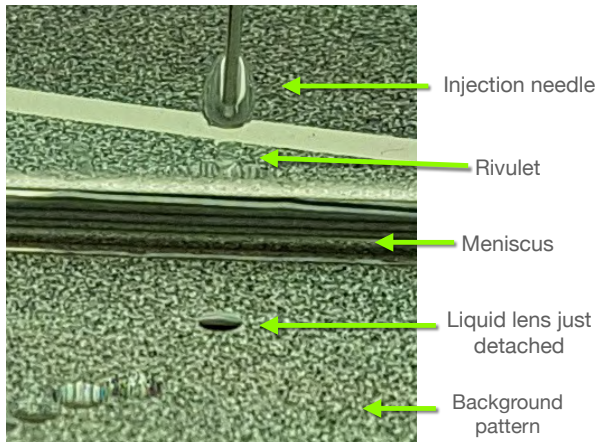


Figure 1 – Picture of a liquid lens just detached from the meniscus.

In figure 1 we show a picture of the configuration when a liquid lens has just detached from the rivulet and slides away from them meniscus. At the bottom left corner of the image we can see a line of previously detached lenses. The granular background shown in the background is used to aid the detection of the liquid lens using digital image processing.

J.R.R. acknowledges funding from the Spanish MCIN/AEI/10.13039/501100011033 through Grant No. PID2020-114945RB-C21. L.C. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 882429.

COMPUTATIONAL FLUID DYNAMICS PREDICTIONS OF HIERARCHICAL VASCULAR NETWORKS

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Vascular networks and blood flow dynamics exhibit remarkable heterogeneity across living systems. Very often they contain varying proportions of small and large blood vessel structures, that undergo continuous changes during development.¹ Reported investigation has demonstrated that biomechanical forces such as interstitial flow and shear stresses play significant roles in vascular development, remodeling, and regression.^{1,2} Nevertheless, the specific range of interstitial flow and shear stresses that govern these mechanisms remain unclear. In this study, we elucidate that interstitial flow and shear stresses within a defined range actively steer vascular development, remodeling, and regression in both native and engineered vascular systems.^{3,4} Computational fluid dynamics (CFD) simulations were employed to perturb the systems by altering pressure and induce diverse flow patterns within multiscale vasculature of varying complexities. This proposed methodology presents a robust predictive approach for understanding the intricate interplay between structure and function in modeling and assessing various vascularization processes across living systems, both in healthy and pathological situations.

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ORAL Contributions

**Session on Networks and
Rheology**

Cross-linker Mobility Governs Fracture Behavior of Catch-Bonded Networks

J. Ruiz-Franco, J. Tauber, and J. van der Gucht

In polymer science, slip bonds represent the most common type of interaction. These bonds weaken due to the increased tensile forces, showing in this way higher rupture kinetics. By contrast, Nature surprises us with the existence of catch bonds which manifest an intriguing behavior. Indeed, whereas they are deactivated at mechanical rest and their half-life is shorter than slip bonds, they stiffen by applying a small tensile force, inducing thus longer-lived [1]. This counter-intuitive behavior is fundamental to understanding the properties of cell adhesion [2]. However, how catch bonds influence the failure of biopolymer materials regarding slip ones is a question that remains open.

In this contribution, we address this problem using athermal simulations of 2D transient networks under uniaxial deformation, where bonds can be immobile or mobile [3]. Thus, whereas immobile bonds always form in the same network location, mobile ones are able to rebind in a new place [4]. We observe that catch bonds can sensibly postpone the fracture. Furthermore, we find that the combination between mobile and catch bonds translates into a remarkable delay in network failure. Then, to decipher how the fracture is developed, we translate the crack nucleation and propagation in the formation and growth of pores under deformation. This approach provides an avenue for understanding that the presence of slip bonds induces a brittle behavior, characterized by a prevalent pore that expands up to percolate. On the other hand, catch bonds cause a ductile behavior clearly marked by the creation of many pores that finally merge, leading to a fracture.

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Star-like polymers as tunable soft nano-objects

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It has been shown recently that the microscopic details related to the local packing play a crucial role in the final performance of polymer-based materials. These details appeared to be particularly important in melts of nanostructured materials composed of polymer-grafted nanoparticles [1].

In this contribution we turn our attention to the homopolymer star-like polymers, which share some features with the well-known hairy nanoparticles but have the advantage of a well-defined molecular structure. Star-like polymers belong to the family of soft nano-objects, whose dynamical behaviour ranges from the linear-like to the colloidal-like. We used atomistic molecular dynamics simulations to address the dependence on the chemistry-specific details characteristic for each polymer type and we quantify the “effective softness” of a wide range of star-shaped structures [2].

Our results together with the recently introduced two-layer model provide a generic classification of the star-shaped polymers in melt according to their degree of penetrability and thanks to our chemistry-specific method, going beyond the generic models, they contribute to the elucidation of the structure-dynamics relation in materials with branch-like architecture, such as those used e.g., in all-polymer nanocomposites.

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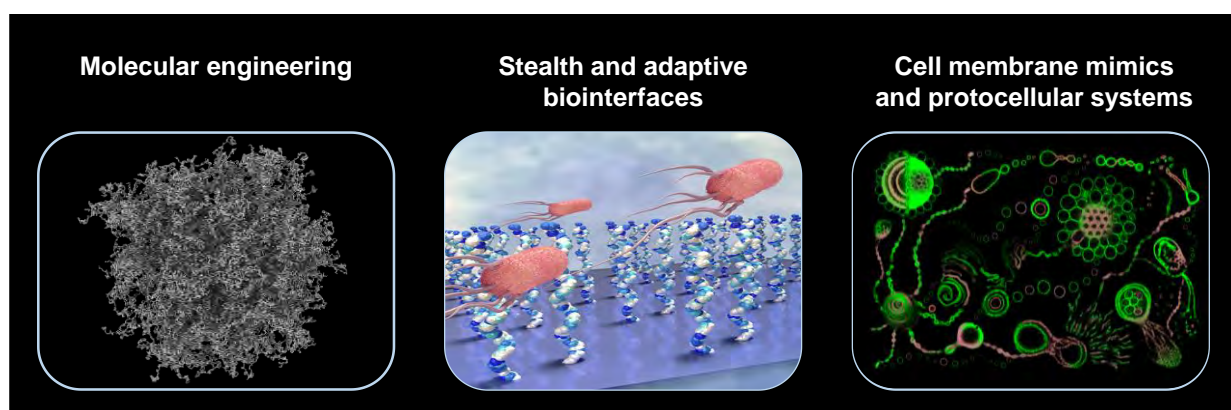
Bio-inspired soft matter at the service of interactive biointerfaces and synthetic cells

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Nature achieves unmatched functionality by the self-assembly of (macro)molecular building blocks in a hierarchical manner. All information necessary for the function is encoded at the molecular level. Unraveling such blueprints serves as a powerful paradigm in the bio-inspired synthesis of materials that can seamlessly interface with living matter or perform non-natural functions. In this talk, I will present a selection of research studies from my lab addressing the overarching task of developing bio-inspired interactive materials and their application in the biomedical field. Three themes will be considered. Firstly, I will present hydrophilic arborescent polymers, a new class of quasi-dendritic macromolecules in which the topology codes for extreme flexibility and enables a myriad of multivalent interactions. Secondly, I will present highlights of the antimicrobial Kill&Repel and Adaptive hemocompatible nanocoatings and our efforts in translating them to medical devices. The last part of the talk will focus on the development of Membrane Machines, tailor-made synthetic vesicles capable of recapitulating some fundamental biological properties and performing specific tasks. We take advantage of these systems to study how biological selectivity can emerge from the lateral organization of ligand in static and dynamic systems such as the bacterial divisome. We are also developing synthetic macrophage-mimetic microrobots capable of endocytosing bacteria and viruses, including SARS-CoV-2.



Research lines of Bioinspired Interactive Materials and Protocellular Systems group.

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Rheology of fatty acid Langmuir monolayers during isobaric 2D melting

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Keywords. *Interfacial Rheology, fatty acids, Langmuir monolayers, phase transitions.*

Abstract. Two-dimensional melting is a topic of great scientific interest and is still object of debate today. The most accepted theoretical framework is the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) scenario [1] in which two continuous transitions occur giving rise to a new intermediate phase called hexatic fluid. However, according to some authors, the hexatic to isotropic fluid transition may be discontinuous depending on the interparticle interactions [2,3]. Experimental confirmations of such scenario based on the characterization of structural properties have been found in several physical systems [4]. Interestingly, the KTHNY framework also contains predictions regarding the mechanical properties. Structural and rheological [5] measurements at untilted phases of fatty acid Langmuir monolayers indicate that the CS phase behaves as a solid and the LS phase behaves as a liquid. Hence, the CS – S and S – LS transitions appear to be a good candidate for testing 2D melting theoretical models. We will report on an experimental study of these transitions in Langmuir monolayers of arachidic (C₂₀H₃₈O₂) and behenic (C₂₂H₃₈O₂) fatty acids at the air/water interface through the measurement of the complex dynamic moduli under isobaric cooling/heating. by means of a magnetic tweezers interfacial shear rheometer [6]. We will show evidence that the CS and the LS phases behave as viscoelastic solid and liquid, respectively. Moreover, we will show that the CS – S transition appears to be continuous for both fatty acids while the S-LS transition appears to be continuous for arachidic acid but discontinuous for behenic acid. A possible explanation will be suggested building on the results of recent Monte Carlo simulations [3].

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Water solvation in bio-nano complex matter

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Water-solvation effects on biological and nanoscopic solutes are of utmost importance in applications but their mechanisms are not fully understood yet. For example, when an aqueous mixture embeds a graphene nanopore (sponge), the concentrations of the mixture components in solution depend on the fine details of the interaction of each component with the pore and on the pore size [1]. Furthermore, hydration water modulates the folding, condensation, aggregation, and adsorption onto nanomaterials of proteins in solutions (Fig.1) [2]. We will discuss these results within a multiscale approach we developed to calculate the water solvation contribution to the free energy of bio-nano complex matter [3-7].

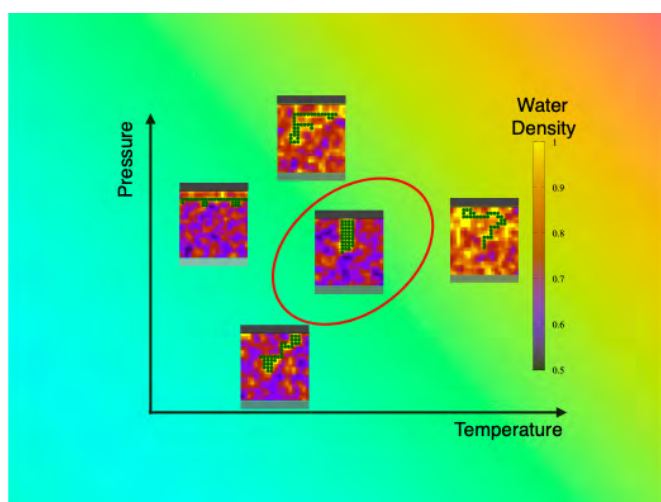


Figure 1: Water solvation of an intrinsically disordered protein absorbing onto a nanointerface reveals an intriguing interplay with its coil-to-globule structural changes, depending on the confining and thermodynamic conditions [2].

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Financial Markets as Soft Matter Systems

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Price fluctuations from the Foreign Currency Exchange Market exhibit a strikingly similar profile than the ones found in supercooled or arrested Soft Matter Systems, such as colloids or granular materials. We resolve such market distributions by considering van Hove fluctuation distribution functions [1]. Such distributions are well known for depicting fluctuations in Soft Matter systems, not only colloid or polymer ones, but also granular materials or Lennard-Jones particles [2, 3]. Within this framework, computed price fluctuation distributions efficiently resolve empirical fat-tailed Foreign Exchange Market ones. More importantly, it must be remarked that our approach resolves any currency pair from the Foreign Exchange Market, where we have studied decades ranging from 2010 to 2020 [4].

Furthermore, once the price fluctuation distributions have been resolved, we study parameters characteristic to market dynamics, by employing the ones from Soft Matter. In symmetry with the particle mean-squared displacement (MSD), we calculate the mean squared price displacement (MSPD), both, to experimental prices and by employing our experimental fluctuation model, finding excellent agreement between them. At long times and when focused on the Euro – US Dollar pair, i.e., for periods of about a year, the MSPD exhibits diffusive behavior. However, when considering hourly time frames in a day, the Euro – US Dollar displays a transition from diffusion at the opening of Wall Street, towards an arrested state, at the closure of this floor. The MSPD transits from a linear profile, towards a MSPD hallmarked by a plateau, which is characteristic to the MSD profile commonly found in colloidal gels and glasses, differentiating microscopic and structural dynamics. Such evolution is reversed in time as when the Tokyo Stock Exchange opens, a gradual shift of the MSPD towards a diffusive profile is observed. Therefore, a daily reentrant phase transition from diffusion towards an arrested state and back is observed in the Euro-US Dollar [5], which strikingly resembles the phase behavior of soft systems that can undergo such transitions, for example in the case of core-shell thermally responsive colloidal particles, Janus particles or globular proteins. It must be emphasized that although we have considered the MSPD, the same behavior is found when studying parameters such as price correlation functions, or the non-Gaussian parameter α_2 .

The previous approach has also proven successful when depicting price fluctuations and their dynamics in stock markets [2,6]. Also, Time Resolved Correlation techniques, usually employed in Light Scattering methods for identifying dynamics in soft systems [7], are excellent resources in understanding real time fluctuations in most markets. The time resolution in the degree of correlation not only depicts the different classes of fluctuations in relation to market events but displays market profiles that are as well characteristic to particles in diffusion, highly correlated systems, gels, or glasses. It is thus suggested that Financial Markets are candidates to be regarded as Soft Matter systems such as colloids or polymers.

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Posters

THE UNCANNY WEIGHT OF GRANULAR COLUMNS

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Granular matter exhibits unusual mechanical properties. For example, when filling a cylindrical column with grains, the weight measured at the bottom of the column does not scale linearly with added mass, but asymptotically saturates towards a constant value. This observation is well-known in the granular matter community; it is referred to as the "Janssen's effect". The weight is partially supported by the lateral walls through frictional interactions with the grains. However, it has been recently observed that the weight measured at the bottom can become larger than the total added mass when the columns are sufficiently small compared to the diameter of the grains [S. Mahajan, et al., *Phys. Rev. Lett.*, 124, 128002 (2020)]. In this poster, we will review this "reverse" Janssen effect using grains with different geometries (spherical, oblate, and prolate particles). We find that all three geometries display the overshoot in weight, and we argue that packing effects are behind the quantitative differences between spherical to non-spherical grains.

Performing 3DDLs to study the dynamics of dense microgel suspensions

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Abstract

The dynamics of a microgel suspension is highly influenced by its particle concentration. Performing light scattering experiments with a system consisting of NIPAM, a crosslinker (pEG-d) and AAc, we find that dilute suspensions exhibit the usual exponential relaxation characteristic of diffusion processes. However, increasing ζ leads to a stretched exponential behavior. The structural relaxation time, τ_α , increases sharply, but quite remarkably, this trend does not persist. Instead, τ_α plateaus at some ζ . To unravel this behavior, we study the dynamic susceptibility, $\chi(\tau_\alpha)$, at different particle concentrations. The goal is to elucidate whether the levelling-off of τ_α is due to shrinking, and the subsequent persistence of the supercooled liquid phase, or rather whether it is aging of a soft-particle glass.

STATISTICAL PROPERTIES OF THE DYNAMICS OF AN AIR-FLUIDIZED CHIRAL PARTICLE

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Diffusion is one of the most fundamental aspects of transport processes in biological systems, including those that are relevant in developmental biology [1]. For this reason, detailed knowledge of the diffusive properties of active particles is crucial. However, interpretation of the diffusive phenomenology in active matter is not straightforward due to its complex dynamics, which is inherently out of equilibrium. Furthermore, detailed balance is not fulfilled in active matter and, as a consequence, many of the fundamentals of equilibrium statistical mechanics do not hold.

Within this context, the analysis of diffusion for the specific case of chiral active particles (active particles with persistent rotations) is specially involved. We know for instance that diffusion in a chiral fluid is not only anomalous but also strongly non-Gaussian [2]. Moreover, even if the chiral fluid is isotropic its diffusion cannot be characterized by a scalar diffusion coefficient [3]. On the contrary, diffusion is mathematically expressed here as a 2nd-rank tensor with two parts; one that is symmetric (whose information is provided by the usual diffusion coefficient) and one that is antisymmetric (that is characterized by the new *odd diffusion* coefficient, which in general can be either positive or negative and even, in some particular cases, zero) [3]. In addition, according to experimental evidence, rotations of chiral particles undergo strong autocorrelation, featuring conspicuous harmonic oscillations [4].

These results indicate that deeper insight on the structure of thermal-like fluctuations of a chiral particle is needed.

For this, we analyze in the present work the case of an air-fluidized chiral particle, in analogy with a previous experiment with a passive macroscopic particle; a ping-pong ball [5] that keeps rolling over an air table. In our case, we dispose on the air table a 3D printed disk instead [2]. The disk is provided with blades and so, upflow causes the bladed disk to persistently rotate; hence its chiral dynamics. Diffusive trajectories of this chiral disk are recorded with a high-speed camera (at 900 fps) and, after particle tracking, the trajectories are obtained. We have observed that the typical trajectory of a chiral disk qualitatively differs much from that of a Brownian particle. We analyze the reasons for this in the present work.

Much like in the case of the passive particle [5], in our experiment there is a dissipative and a fluctuating contribution to the particle dynamics. The latter term comes from the stochastic (turbulent) part of the air upflow and the former comes from drag due to air viscosity. Their properties are analyzed here in detail. However, as we will see, small-scale oscillations in the velocity autocorrelations [4] imply that the memory kernel of the drag for a chiral particle needs to be generalized.

In this way, our work deals with an analysis of the extension of the fluctuation-dissipation theorem to the dynamics of a chiral particle.

Our study aims to cast more light to the understanding of macroscopic response to statistical fluctuations in a chiral particle.

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Finding and exploiting biomaterials for medical applications such as the delivery of bioactive agents and macromolecular pharmaceuticals is very challenging [1]. Alginate-based hydrogels are a promising one.

Alginates are extracted from seaweed and are therefore natural. From a chemical point of view, alginate is a family of unbranched polymers composed of 1,4-linked β -D-mannuronic and α -L-guluronic acid residues. When divalent cations, for example Ca^{2+} , interact with blocks of guluronic acid residues, complex crosslinks made of the cations embedded in a structure generally called an "egg box" [2], form resulting in a polymer gel. Some studies have reported that alginate gels in contact with pure water or under a change in salt concentration and pH swell to eventually dissolve.

Furthermore, it is often suggested that this behavior is due to the hypothetical physical character of the crosslinks.

Our experiments indicate that our alginate gels are stable, and that they swell and deswell as regular ionic gels, questioning conventional wisdom.

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FIRST ORDER ALIGNMENT TRANSITION IN AN INTERFACED ACTIVE NEMATIC

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Liquid crystals (LCs) are a special type of materials that form one or more intermediate phases (mesophases) between the liquid isotropic and the crystalline solid ones. Soft matter mesophases can also be formed by biomolecules, such as lipids [1], concentrated DNA [2], or in vitro reconstructed from microscopic components like cells' filaments and protein motors [3, 4]. The latter form a biomimetic active material, which consumes surrounding energy and generates continuous motion. Such active systems are capable of self-organization at different length and time scales, often exhibiting turbulent flows and the emergence of long-range orientational order, which is characteristic of active nematics.

In the present work we investigate experimentally the dynamic phase transition of a two-dimensional active nematic layer formed by microtubule filaments and recombinant kinesin motors [4] that is interfaced with a passive liquid crystal. Under a temperature ramp that leads to the transition of the passive liquid into a highly anisotropic lamellar smectic-A phase, and in the presence of a magnetic field, the coupled active nematic reorganizes its flow and orientational patterns from the turbulent into a quasi-laminar regime aligned perpendicularly to the field [5]. Remarkably, while the phase transition of the passive fluid is known to be continuous, our observations reveal intermittent dynamics of the order parameter and the coexistence of aligned and turbulent regions in the active nematic, a signature of discontinuous, or first order, phase transitions.

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MOTION AND CONTROL OF VIRTUAL COLLOIDAL PARTICLES IN CONFINED CHIRAL LIQUID CRYSTALS

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Cholesteric phases are liquid crystals in which a helical twist is induced by the presence of a chiral agent [1]. This twist can be frustrated by the application of confinement comparable to the spatial extension of the twist. Under those conditions, skyrmions can be formed if the material undergoes an instability [2]. Skyrmions are topologically protected solitonic-like structures, formed by the spatial discordance in the orientation of the molecules of the liquid crystal, forming a torus in which the principal axis of the molecules turns 180° . Skyrmions behave as quasi-particles and can be driven by the action of a modulated AC electric field [2]-[4]. However, the directionality of the movement has, so far, only been *in-situ* controlled using complex optical systems [5]. In our work, we study the propulsion of skyrmions under modulated AC electric fields of different amplitude, carrier, and modulation frequencies. Moreover, we also study the collective behaviour of skyrmions, showing different self-assembly regimes in high areal density configurations. We also demonstrate the capability of an external fixed magnetic field to steer driven skyrmions, which can be inserted and controlled within microfluidic channels (figure 1 (a)). Preliminary experiments suggest an acceleration when skyrmions are introduced in microchannels with a width comparable to the size of the soliton. We also show that skyrmions can act as micro-cargo transporters, with a slight modification of their velocity of displacement when loaded (figure 1 (b)).

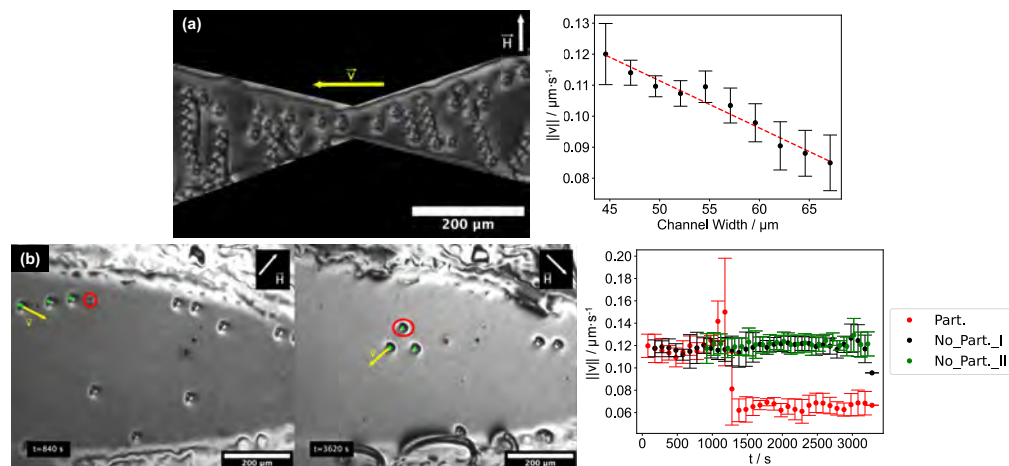


Figure 1 – (a) Modulated AC electric field-driven skyrmions inside a microchannel whose width is comparable to the size of the quasi-particle. The steering of the solitons is controlled through the application of a fixed magnetic field. (b) Micro-cargo transport capacity of skyrmions. The red circle indicates the location of the particle to be transported, and the yellow arrow refers to the direction of motion of skyrmions.

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AGGREGATION OF DISCOIDAL PARTICLES DUE TO DEPLETION INTERACTION

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Depletion forces are effective interactions of entropic origin ubiquitous in a large variety of colloidal systems [1]. They are of special relevance in biological systems, where the medium is often crowded with different types of polymers. Indeed, depletion interactions might play a crucial role in the formation of columnar aggregates of erythrocytes in blood, which largely determines its rheological properties [2]. In this contribution we propose a simple thermodynamic model to understand the equilibrium aggregation properties of a solution of disc-shaped colloids due to depletion interactions [3]. Built upon simple arguments borrowed from the theory of self-assembly of micelles, the model is analytically solvable, providing simple expressions to predict the equilibrium distribution of aggregates in terms of the relevant parameters of the problem (concentrations of discs and polymers, size of the discs and length of polymers). To validate the model, we also report the results of molecular dynamics simulations of a system of discs and polymers in contact with a thermal bath interacting solely via steric repulsive interactions; the agreement between both approaches is excellent. Additionally, we consider the possibility of an energetic affinity of the depleant polymers to the discoids, which results in a reentrant aggregation dependence with temperature.

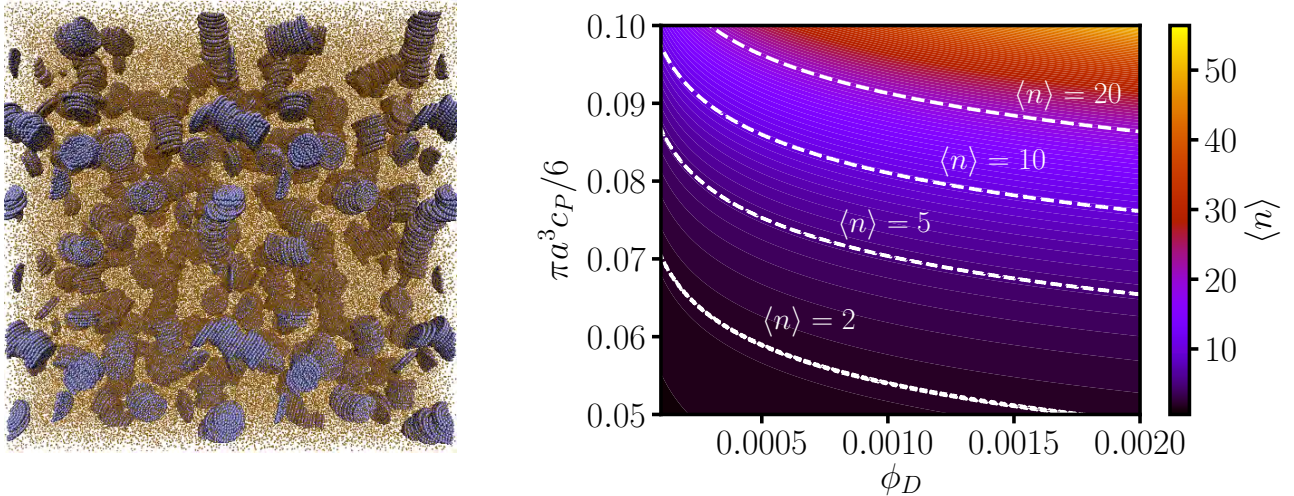


Figure 1 - Left: snapshot of simulated system, with discs and depletant particles. Right: diagram of aggregation of columns of average length $\langle n \rangle$ as a function of polymer concentration c_P and disc volume fraction ϕ_D .

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DISCOVERING DYNAMIC LAWS FROM OBSERVATIONS: THE CASE OF SELF-PROPELLED, INTERACTING COLLOIDS

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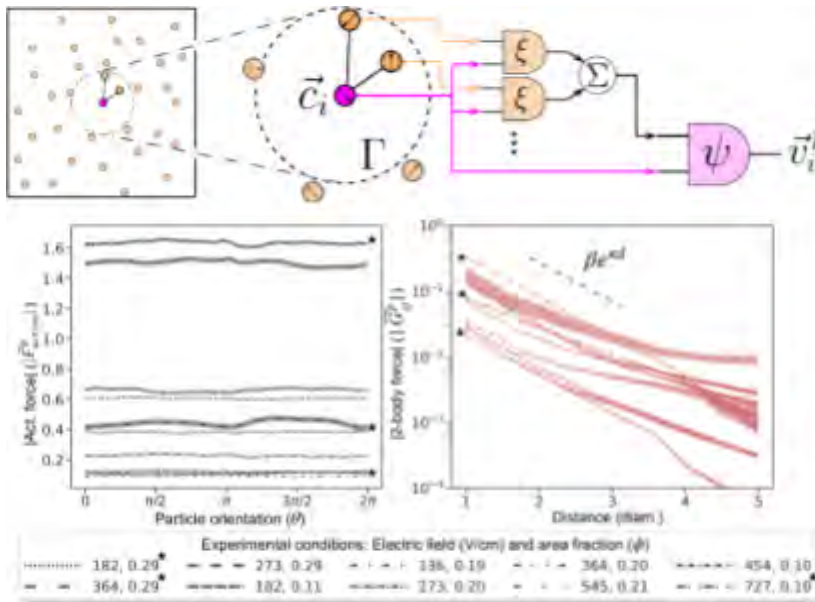
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Active matter spans a wide range of time and length scales, from groups of cells and synthetic self-propelled colloids to schools of fish and flocks of birds. The theoretical framework describing these systems has shown tremendous success in finding universal phenomenology. However, further progress is often burdened by the difficulty of determining the forces controlling the dynamics of individual elements within each system. For systems of many active particles, it can be very challenging to estimate the forces governing the dynamics of each particle. Are individuals attracting or repelling each other? At which length scale? Are they self-propelling? Our work builds on the concepts and formalism introduced by Cranmer *et al.* [1] and focuses on extracting the interacting and active forces directly from experimental trajectories of electrophoretic Janus particles [2], testing the stability of the method within an ensemble approach, and validating the method with data from simulations of overdamped and underdamped active particles with a wide range of interparticle potentials, estimating its robustness against the available amount of input data with different levels of noise. The main goal is to propose a ready-to-use tool that can be of use to unravel the dynamical features of experimental realizations of active particles' systems.



ActiveNet is composed of a node function ψ (in pink) and an edge function ξ (in orange). Function ξ takes the coordinates of two particles and, after training, it outputs a linear transformation of the two-body force acting between them. Function ψ takes the coordinates each particle and the sum of the outputs of ξ for all the edges of the particles in neighborhood Γ . During the learning process the internal parameters of ξ and ψ are optimized so that all the predicted velocities approach the real velocities. After training, the output of ψ is the predicted velocity (or acceleration) of each particle. Then the active and 2-body forces are extracted from ψ and ξ yielding the two bottom graphs for different experimental conditions.

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MACROSCOPIC ACTIVE PARTICLES DRIVEN BY LIGHT

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Systems consisting of a large number of interacting self-propelled agents are commonly known as active matter. In those systems, each agent consumes and converts energy into mechanical motion, representing a nice example of out-of-equilibrium system. The study of such ensembles of self-propelling particles is getting increased interest due to the broad range of its applications in physics, biology, chemistry, and robotics. Examples are the self-organization of bird flocks, the formation of human stampedes, the motion of molecular motors, and the collective cell migration, just to mention a few. It has been observed that, regardless of the type of particles in question, active systems share certain properties at the group level. Accordingly, several models have been developed to describe the emergence of collective behavior [1, 2].

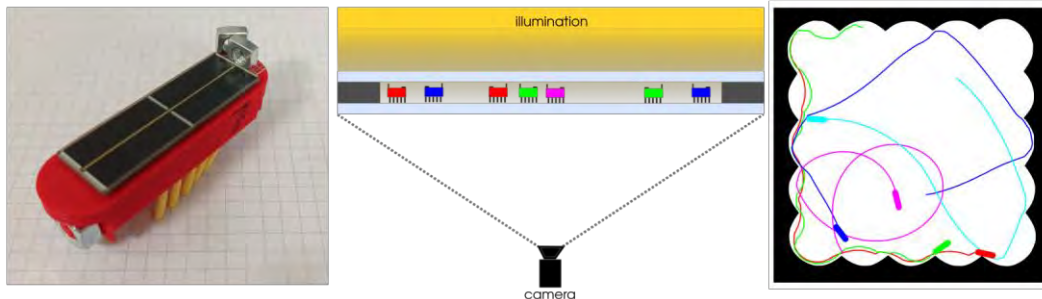


Figure 1 – Left: HEXBUG Nano with a 3D printed cover holding the photovoltaic cell. Middle: sketch of the experimental setup. Right: sample particle trajectories recorded with homogeneous illumination.

Among all the different types of active matter, here we work with active granular matter; i.e. macroscopic active particles that only interact through physical contact. These are of particular interest because they allow more freedom of fine-tuning, as opposed to the difficulty of controlling the experimental parameters in real active systems. Another reason is that lab experiments can be repeated, as many times as necessary under the same conditions, a scenario that cannot be always warranted in biological active systems. As said, in active granular media the interactions take place exclusively by contacts, as there is no interstitial fluid or social interaction among the agents. This makes systems of macroscopic active particles a genuine limit case of other, more sophisticated systems and allows us to isolate the contribution of some physical variables regarding the collective behavior.

In general, in active granular matter, some kind of energy is converted into directed mechanical motion. Indeed, the energy can come from the particle itself (e.g. bird flocks), or from an external source, acting locally or at the boundary (e.g. moving or shaking boundaries in the case of granular systems). In our work, we focus on the response to a stimulus, called taxis. We present novel, macroscopic self-propelled agents excited by light. The agents are small robots called HEXBUG Nano [3], with photovoltaic cells mounted on their top (see Fig. 1, left). Using this configuration the behavior of the agents can be influenced by changing the light intensity. Thus, in our system, the activity of the internally excited agents can be externally controlled. This is a concept common in microscopic systems, but pioneering in experiments with macroscopic active matter. The middle part of Fig. 1 shows the sketch of the experimental setup, while the right-hand side represents example trajectories of five particles obtained with homogeneous illumination. As our system has a fully controllable illumination panel (LED panel with ~ 80 lines), we are able to change the illumination intensity spatially and temporally. In this way, we can impose both spatial and temporal gradients and analyze the system response by analyzing the diffusion, mixing, and clustering of the particles. In this work, we present the first results about the collective behavior of these macroscopic, photosensitive agents.

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Aqueous Two-Phase Systems within Selectively Permeable Vesicles.

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Keywords: Microfluidics • Vesicles • Membranes • Mixtures

An aqueous two-phase system (ATPS) inside a vesicle organizes the vesicle core in two distinct phases, sorting the encapsulated solutes within. Using microfluidic technologies, we produce vesicles that efficiently encapsulate mixtures of two polymers, offering a versatile platform to study the phase behavior of ATPSs. We further use these compartmentalized vesicles to investigate the impact of membrane permeability on the dynamics of the encapsulated ATPS. By creating a membrane that selectively allows the permeation of one of the components of the ATPS, we demonstrate that out-of-equilibrium phase separated vesicles formed by a fast water outflow can be spontaneously reversed by a more gradual outflow of the permeating solute across the membrane. Such dynamics could be beneficially exploited by cells to regulate metabolic and signaling pathways within their nucleoplasm or cytoplasm based on external factors.[1]

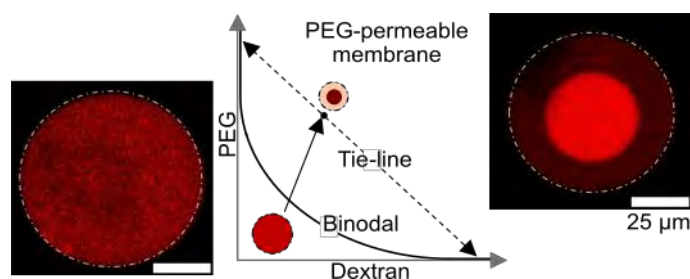


Figure 1. Confocal fluorescence microscopy images showing a vesicle encapsulating a non-phase separated (left) and a phase separated (right) mixture of PEG and Dextran fluorescently labeled in red.

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Rolling backward: Tuning Microroller Locomotion in an Obstacle Lattice.

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Abstract: The ability to control transport at the micro-scale presents unique challenges due to the dominance of viscous over inertial forces and the influence of thermal fluctuations. At this inertialess regime, motion requires the breaking of flow field symmetry. One example is microrollers, particles driven into rolling motion near a solid boundary by an external field and then propelled due to the breaking of the generated rotational flow field symmetry.

In this work, we examine the motion of microrollers in a square lattice of obstacles. Specifically, we focus on quantifying the relation between the microroller velocity and two governing parameters: the lattice parameter l_p and the roller diameter d . We identify distinct dynamical regimes governed by the ratio between the two parameters. We find that for lattice parameters larger than the roller diameter, $1 \leq \frac{l_p}{d} \leq 2$, the roller travels through the lattice in the direction opposite to its rolling motion. At $l_p/d \approx 2$, the roller is essentially confined within a unit cell of the square obstacle lattice, oscillating back and forth within it. For $l_p/d > 2$, the roller translates through the lattice in the same direction as its rolling motion.

Our results provide new insights that could be useful for numerous applications, including bacterial flow management to mitigate infection risks and the targeted deployment of micro-robots in vascular systems for surgical and drug delivery purposes.

Rolling vesicles: From confined rotational flows to surface-enabled motion

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In wet environments, surfaces in relative motion are controlled by lubrication forces. Lubrication holds the key to advances in dynamic microscopic systems and has a crucial role in various biological processes. In this study, motile vesicles that harness lubrication forces to facilitate rolling on substrates are developed. These active vesicles are composed of a polymeric membrane that encapsulates in its core an externally-driven magnetic particle. When this encapsulated particle rotates clockwise, it follows a clockwise motion near the inner vesicle membrane, resulting in a circular trajectory within the vesicle's equatorial plane, perpendicular to the axis of rotation. This clockwise rolling behavior arises due to the curvature of the enclosing membrane, which generates a flow field capable of reversing the direction of lubrication forces compared to what is typically observed on a flat substrate. These confined fluid flows turn inert vesicles to active ones by inducing vesicle rotation, thereby enabling the vesicles to roll on a substrate. Our findings shed light on the fundamental principles of lubricated friction in confined spaces. These insights could potentially have implication for force transduction in biological systems and provide a valuable guidance for the development of motile vesicles that exploits frictional forces to precisely target specific locations.

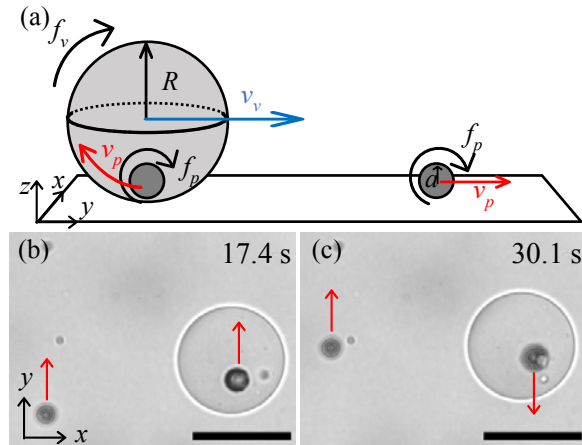


Figure 1: Schematic illustration of our experimental system (a) with a time sequence (b-c) of bright field image of a polymeric vesicle with an encapsulated ferromagnetic particle together with a free rotating particle.

COLLECTIVE SENSING OF *E. COLI* UNDER LOCAL FLOWS

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Active matter systems consume to generate self-generated motion, which brings these systems out-of-equilibrium. [1-2] One of the most paradigmatic active matter system is a suspension of bacteria. In this study, we investigate the collective behaviours of *E. coli* in the presence of magnetic microparticles that spin under the actuation of an external homogeneous rotating magnetic field. Like Sokolov and Aranson's study, [3] these spinning microparticles generate local rotational flows around them, as schematically shown in figure 1. At low densities of *E. coli*, bacteria adjust their route to avoid the microparticle without making significant changes in their collective dynamics. However, high *E. coli* densities induce an alignment of neighbouring bacteria as shown in figure 2. Therefore, we conclude that *E. coli* responds to local flows, thus demonstrating a bacteria "collective sensing" of its environment.

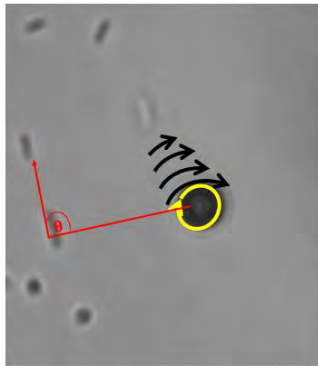


Figure 1: Vortex due to particle rotation

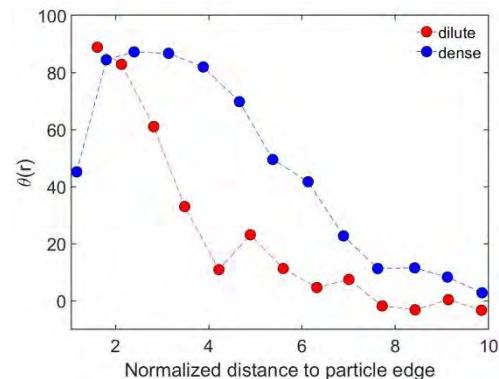


Figure 2: Collective response of bacteria for a dilute concentration and for a dense one

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SELF-ORGANIZED STATES OF SOLUTIONS OF ACTIVE RING POLYMERS IN BULK AND UNDER CONFINEMENT

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In the presented work we study, by means of numerical simulations, the behaviour of a suspension of active ring polymers in the bulk and under lateral confinement. When changing the separation between the confining planes and the polymers' density, we detect the emergence of a self-organised dynamical state, characterised by the coexistence of slowly diffusing clusters of rotating disks and faster rings moving in between them. This system represents a peculiar case at the crossing point between polymer, liquid crystals and active matter physics, where the interplay between activity, topology and confinement leads to a spontaneous segregation of a one component solution.

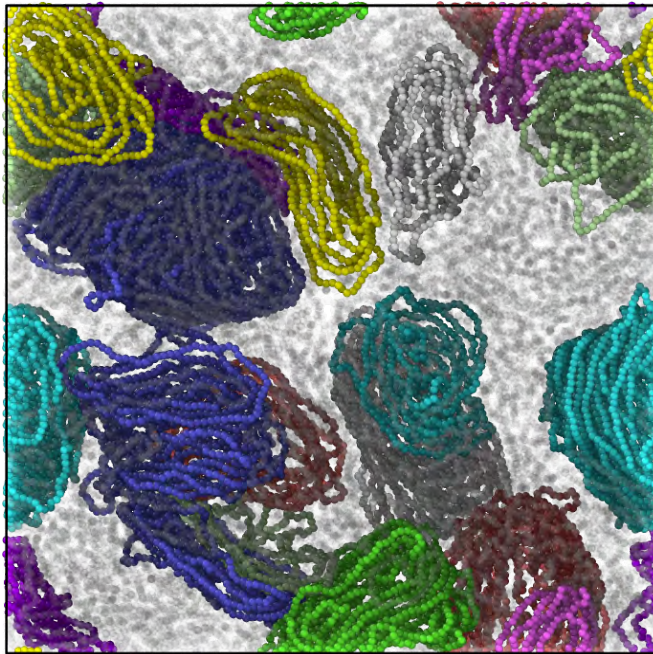


Figure 1 – Snapshot from above of the active ring suspension, where the polymers clusters are shown in different colors and the other population is colored transparent

Curvature sorting of rotating proteins into lipid filaments

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ATP synthases are proteins that catalyse the formation of ATP through the rotatory movement of their membrane-spanning subunit. In mitochondria, ATP synthases are found to arrange as dimers at the high-curved edges of *crisetae*. Here, a direct link is explored between the rotatory movement of ATP synthases and their preference for curved membranes. An active curvature sorting of ATP synthases in lipid nanotubes pulled from giant vesicles is found. Coarse-grained simulations confirm the curvature-seeking behaviour of rotating ATP synthases, promoting reversible and frequent protein-protein contacts. The formation of transient protein dimers relies on the membrane-mediated attractive interaction of the order of $1.5 k_B T$ produced by a hydrophobic mismatch upon protein rotation. Transient dimers are sustained by a conic-like arrangement characterized by a wedge angle of $\theta \approx 50^\circ$, producing a dynamic coupling between protein shape and membrane curvature. The results suggest a new role of the rotational movement of ATP synthases for their dynamic self-assembly in biological membranes.

WHERE DO VIRIONS LOCALIZE IN THE RESIDUE OF A DRY SESSILE RESPIRATORY DROP?

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Respiratory viruses are expelled inside water-based droplets composed of salts, proteins, and surfactants. These components segregate during the evaporation process, making the dry residue highly heterogeneous. The spatial distribution of virions inside this residue, which remains unknown, is crucial to understand the mechanisms that allow them to remain infective for so long after the drop has lost its water content.

We propose a modelling and experimental approach to shed light on the fluid dynamics of virus-laden, sessile respiratory droplets. An analytical capillary flow is found to dominate sessile droplets composed of water, leading to the coffee-ring effect. In droplets containing a minimal concentration of NaCl, as is the case of respiratory-like droplets, a Marangoni flow is obtained by means of Finite Element Method in COMSOL. This effect competes with the previous capillary velocity field, leading to higher concentrations of NaCl near the contact line of the droplet. The analytical velocity field is then used to develop a model to track the location of virions, treated as Brownian particles transported by the fluid flow inside the droplet. Results show a preferential accumulation of virions near the contact line region. Virus inactivation rate is observed to increase as NaCl concentration increases throughout evaporation, yielding a decrease in viable virions.

Simulation and analytical results are quantitatively validated with experimental evaporation of respiratory-like droplets composed of Transmissible gastroenteritis coronavirus and TNE buffer solution. Image analysis from evaporation dynamics yields a good agreement with the analytical results. TEM and FIB-SEM observation of the evaporated deposits confirms the coffee-ring effect, as higher crystallized salt concentration is found near the contact line. Virions are also qualitatively observed in higher concentrations near the contact line, thus confirming the localization modelling results. We also find that virions arrange into monolayer aggregates inside the dry residue. These aggregates are predominantly localized close to the contact line, as suggested by other authors. However, we also find these aggregates everywhere else in the residue far away from the edges. Interesting, the aggregates are located in protein-rich regions. The virion organization into aggregates suggests that they agglomerate at the drop interface while water is still present and then these agglomerates are gently deposited on the dry residue as the water evaporates. This mechanism is responsible for the formation of similar aggregates of colloidal particles in salty water solutions. Our observations explain how virions stay away from salt-rich regions as the drop water content decreases, revealing the crucial role that the protein plays in shrouding the virions from the chemically hostile environment found in the drop during evaporation.

This work addresses a critical knowledge gap in our understanding of the airborne transmission of respiratory infectious diseases via virus-laden fluid particles, which could have potential applications in the development of effective engineering control methods for infectious viruses.

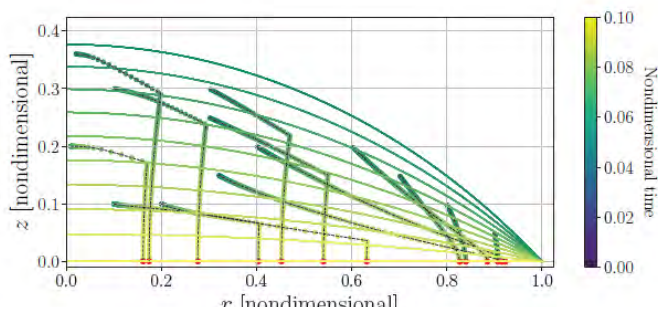


Figure 1 – Particle tracking of multiple virions

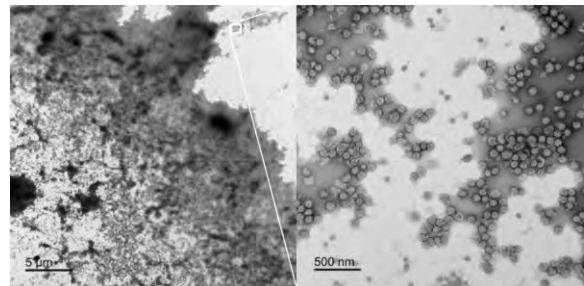


Figure 2 – TEM images of a virus-laden evaporated droplet (9 μL of TGEV + 21 μL of TNE) at a relative humidity of 30%