S11 Frontiers in Soft Condensed Matter
Fronteras en Materia Blanda Condensada (DFMC-GEFES)

13/07 Wednesday afternoon, Aula 1.3

15:30-16:00 Pietro Tierno
Topological Boundary Constraints in Artificial Colloidal Ice

16:00-16:15 Alejandro Cuetos Menéndez
Estudio mediante simulación de propiedades emergentes en colonias celulares

16:15-16:30 Alvaro Domínguez Alvarez
Beyond classic phoresis: new insights into self-phoresis

16:30-16:45 Alexis de la Cotte
Orientational correlations of active defects in flat and curved space

16:45-17:00 Pablo Maynar Blanco
Understanding an instability in vibrated granular monolayers

17:00-17:12 Flash talks of the posters

17:12-18:00 **Posters and Coffee**

18:00-18:15 Ramon Planet Latorre
The uncanny weight of granular columns

18:15-18:30 Carlos Miguel Barriuso Gutiérrez
Discovering dynamic laws from observations: the case of self-propelled, interacting colloids

18:30-18:45 Miguel Ángel Ramos Ruiz
Ultrastable glasses: going very deep into the energy landscape of glasses

18:45-19:00 José Manuel Romero Enrique
Casimir contribution to the interfacial Hamiltonian for 3D wetting

19:00-19:15 José Martín Roca
Magnetic colloids adsorbed at fluid interfaces acting as interfacial swimmers and colloid adsorption probes

Posters:

23 Juan Pablo Miranda López
Collective behaviour of energy depot repulsive particles

24 María Isabel García de Soria Lucena
Dynamics of hard particles confined by an isotropic harmonic potential

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Simulating active agents with Dissipative Particle (hydro)Dynamics

S11 Frontiers in Soft Condensed Matter
Fronteras en Materia Blanda Condensada (DFMC-GEFES)

14/07 Thursday afternoon, Aula 1.3

15:30-16:00 Chantal Valeriani
Trapping active particles up to the limiting case: bacteria enclosed in a biofilm

16:00-16:15 Caleb Anderson
MIPS and Activity Cycles in Fire Ants

16:15-16:30 Raúl Rica Alarcón
Collapse of magnetite-decorated pNIPAM microgels trapped with optical tweezers

16:30-16:45 Alessandro Patti
Phase behaviour and dynamics of colloidal cuboids: paving the path to biaxial nematic liquid crystals

16:45-17:00 Javier Rojo González
Nematics in 3-tori: Doubly twisted structures and defect-populated configurations

17:00-18:00 **Coffee Break**

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Topological Boundary Constraints in Artificial Colloidal Ice

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The effect of boundaries and how these can be used to influence the bulk behavior in geometrically frustrated systems are both long-standing puzzles, often relegated to a secondary role. In this talk, I will investigate boundary effects in a geometrically frustrated system, namely an artificial colloidal ice (ACI). The ACI recently emerge as a microscale soft matter analog of a frustrated nanoscale spin ice system. The artificial colloidal ice is realized by confining interacting paramagnetic colloids to a lattice of gravitational double wells [2]. With this system, both via numerical simulations and "proof of concept" experiments, I will demonstrate that boundaries can be engineered to control the bulk behavior in a colloidal artificial ice [3]. I will also show that an antiferromagnetic frontier forces the system to rapidly reach the ground state (GS), as opposed to the commonly implemented open or periodic boundary conditions. Further, strategically placing defects at the corners may be used to generate novel bistable states, or topological strings, which result from competing GS regions in the bulk. The presented results could be generalized to other frustrated micro- and nanostructures where boundary conditions may be engineered with lithographic techniques.

[1] A. Ortiz-Ambriz and P. Tierno, *Nature Comm.* **7**, 10575 (2016).
[2] Ortiz-Ambriz, C. Nisoli, C. Reichhardt, C. J. O. Reichhardt, and P. Tierno, *Rev. Mod. Phys.* **91**, 041003 (2019).
[3] Carolina Rodríguez-Gallo, Antonio Ortiz-Ambriz, and Pietro Tierno, *Phys. Rev. Lett.* **126**, 188001 (2021).

Acknowledgements: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement no. 811234). P. T. acknowledge support the Generalitat de Catalunya under Program ÏCREA Acadèmia".

Estudio mediante simulación de propiedades emergentes en colonias celulares

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Las colonias celulares (biofilms en el caso de procariotas, pero también órganos o tumores en el caso de eucariotas) son agregados de células que presentan muchas similitudes con fluidos coloidales. Como diferencia fundamental, las colonias celulares son sistemas activos que de forma intrínseca suelen encontrarse fuera del equilibrio. Así, es habitual que las células tengan mecanismos propios (flagelos, cilios, etc ...) que provocan un movimiento autónomo por parte de las células. En otros casos, el carácter de sistema activo y la situación de fuera del equilibrio surge del propio proceso de alargamiento y reproducción celular, que en bacterias suele venir dado por el mecanismo conocido como fisión binaria.

Centrándonos en la situación en que las células no tienen capacidad de movimiento autónomo, pero crecen y se dividen por fisión binaria, las colonias celulares son agregados compactos, pudiendo ser en función del número de células bi o tridimensionales. En función de las características de las células y de las condiciones ambientales pueden presentar distintos niveles de orden parcial, asemejándose a tactoides nemáticos, y una variedad de propiedades mecánicas y estructurales.

En los últimos años se han comenzado a utilizar para el estudio de estas comunidades celulares técnicas de simulación ampliamente utilizadas en la ciencia coloidal. Presentamos en este trabajo algunos ejemplos del uso de estas técnicas, explorando las propiedades físicas que se pueden deducir de estos estudios, presentando resultados experimentales que al menos cualitativamente confirman los resultados obtenidos por simulación. De esta forma, en primer lugar se presentará el modelo que se ha desarrollado para la realización de estos estudios. Nuestro modelo se basa en la descripción de grano grueso de propiedades de las células individuales, como son forma, tamaño, velocidad de crecimiento y coeficiente de difusión, obteniendo con él propiedades emergentes colectivas de toda la colonia. Con este modelo se ha explorado como condiciona la competición entre difusión pasiva de las células y el proceso de elongación/división a las propiedades estructurales globales de la colonia celular [1].

También hemos estudiado el crecimiento de una colonia bacteriana en un entorno rico en polímeros. En este caso hemos comprobado la existencia de distintos escenarios. En estos escenarios, que dependen del tamaño y concentración de partículas poliméricas, las propiedades de la colonia celular pueden venir condicionadas bien por un aumento efectivo de la viscosidad del medio, o bien por la actuación de fuerzas de depleción [2].

Finalmente, mostraremos resultados sobre las propiedades micromecánicas de las colonias celulares. Aquí mostraremos como el crecimiento de la colonia provoca un aumento continuo de las tensiones mecánicas en el interior de la colonia, sugiriendo la existencia de mecanismos biológicos para limitar este aumento de las tensiones internas.

[1] R. D. Acemel, F. Govantes y A. Cuetos, *Scientific Reports* **8**, 5340 (2018).
[2] F. J. Lobo-Cabrera, A. Patti, F. Govantes, and A. Cuetos, *Phys. Rev. E* **103**, 052407 (2021).

Beyond classic phoresis: new insights into self-phoresis

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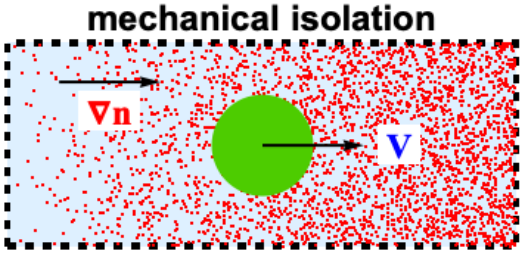
The notion of chemophoresis describes the displacement of a particle in an ambient fluid due to an externally imposed gradient in chemical composition, *and in the absence of a net external force and torque*: therefore, the particle's momentum is balanced by the momentum of the ambient flow, and the particle is not dragged, but instead it *swims*. The phenomenon of classic phoresis can be understood in the context of linear–response theory: the phoretic velocity $\mathbf{V}$ of the particle in a fluid solution can be obtained as

$$\mathbf{V} = \mathcal{L}_{\rm lin}\ (\nabla n)_{\rm ext}\,,$$

for a sufficiently small gradient $(\nabla n)_{\rm ext}$ in solute concentration over the scale of the particle size, in terms of the phoretic coefficient $\mathcal{L}_{\rm lin}$ given by a Green–Kubo expression.



A closely related phenomenology is observed for self-phoretic particles, which have attracted much attention in the last years as a physical realization of artificial swimmers. In this case, the particle's surface is catalytically active, so that it induces a composition gradient $(\nabla n)_{\rm act}$. The experimental observations involving self-phoretic particles are then customarily addressed as another instance of classic phoresis but in a self-generated gradient,

$$\mathbf{V} = \mathcal{L}_{\rm lin}\ (\nabla n)_{\rm act}\,.$$

However, an additional role of the particle's chemical activity has been recently identified [1,2], namely, as responsible for a specific *activity–induced response*, so that one has to write

$$\mathbf{V} = (\mathcal{L}_{\rm lin} + \mathcal{L}_{\rm act})\ [(\nabla n)_{\rm ext} + (\nabla n)_{\rm act}]\,,$$

in the more general scenario, where $\mathcal{L}_{\rm act}$ is the activity–induced contribution to the phoretic coefficient. We will describe the theoretical framework behind this result and possible observational consequences. In particular, we argue that the piece $\mathcal{L}_{\rm act}$ of the response could actually be as large as $\mathcal{L}_{\rm lin}$ in realistic configurations: this would mean a change in paradigm as it disproves the claim that "self-phoresis is phoresis in a self-induced gradient".

[1] A. Domínguez, M. Popescu, C. Rohwer, S. Dietrich, *Physical Review Letters*, **125**, 268002 (2020).
[2] A. Domínguez, M. Popescu, *Current Opinion in Colloid & Interface Science*, submitted (2022).

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Orientational correlations of active defects in flat and curved space

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Topological defects are salient signatures of active nematics, which are partially-ordered systems intrinsically out of equilibrium. We experimentally study the dynamics of microtubule-kinesin active nematics constrained to both flat space and toroidal 2D space and inquire whether the defects develop any form of order. In flat space, +1/2 defects develop short range ferromagnetic order (mediated by -1/2 defects) and antiferromagnetic order at length scales comparable to the mean defect spacing. Both these effects and the corresponding correlations are seen to persist independent of the total defect density, and without any global orientational order [1]. In contrast, on curved space, we find that defect orientations strongly couple to the surface they live in, resulting in both +1/2 and -1/2 defects developing orientational order in regions of non-zero Gaussian curvature.

[1] D. Pearce *et al.*, *Phys. Rev. Lett.* **127**, 197801 (2021).

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Understanding an instability in vibrated granular monolayers

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We investigate the dynamics of an ensemble of smooth inelastic hard spheres confined between two horizontal plates separated a distance smaller than twice the diameter of the particles, in such a way that the system is quasi-two-dimensional. The bottom wall is vibrating and, therefore, it injects energy into the system in the vertical direction and a stationary state is reached. It is found that, if the size of the plates is small enough, the stationary state is homogeneous. Otherwise, a cluster of particles is developed. The instability is understood by using some effective hydrodynamic equations in the horizontal plane. Moreover, the theoretical prediction for the size of the system above which it becomes unstable agrees very well with Molecular Dynamics simulation results without any fitting parameter [1].

[1] P. Maynar, M. I. García de Soria, and J. J. Brey, *Phys. Rev. E* **99**, 032903 (2019).

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 [1]. In this talk, we will review this "reverse" Janssen effect, and present new results using grains with different geometry. We find that columns filled with non-spherical particles also display the overshoot in weight observed with spherical grains, but now the compressive forces responsible for the reverse Janssen behavior are restricted to a narrower range in depth; we argue that packing effects are behind the quantitative differences between spherical to non-spherical grains.

[1] S. Mahajan, M. Tennenbaum, S.N. Pathak, D. Baxter, X. Fan, P. Padilla, C. Anderson, A. Fernandez-Nieves, and M.P. Ciamarra *Phys. Rev. Lett.* **124**, 128002 (2020).

Discovering dynamic laws from observations: the case of self-propelled, interacting colloids

Miguel Ruiz-Garcia[1], **C. Miguel Barriuso Gutierrez**[2,*], Lachlan C. Alexander[3], Dirk G. A. L. Aarts[3], Luca Ghiringhelli[4], Chantal Valeriani[2]

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Active matter spans a wide range of time and length scales, from groups of cells and synthetic self-propelled particles to schools of fish, flocks of birds, or even human crowds. The theoretical framework describing these systems has shown tremendous success at finding universal phenomenology. However, further progress is often burdened by the difficulty of determining the forces that control the dynamics of the individual elements within each system. Accessing this local information is key to understanding the physics dominating the system and to create the models that can explain the observed collective phenomena. In this work, we present a machine-learning model, a graph neural network based on [1], that uses the collective movement of the system to learn the active and two-body forces controlling the individual dynamics of the particles. We verify our approach using numerical simulations of active brownian particles, considering different interaction potentials and levels of activity. Finally, we apply our model to experiments of electrophoretic Janus particles, extracting the active and two-body forces that control the dynamics of the colloids. Due to this, we can uncover the physics dominating the behavior of the system. We extract an active force that depends on the electric field and also area fraction. We also discover a dependence of the two-body interaction with the electric field that leads us to propose that the dominant force between these colloids is a screened electrostatic interaction with a constant length scale. We expect that this methodology can open a new avenue for the study and modeling of experimental systems of active particles.

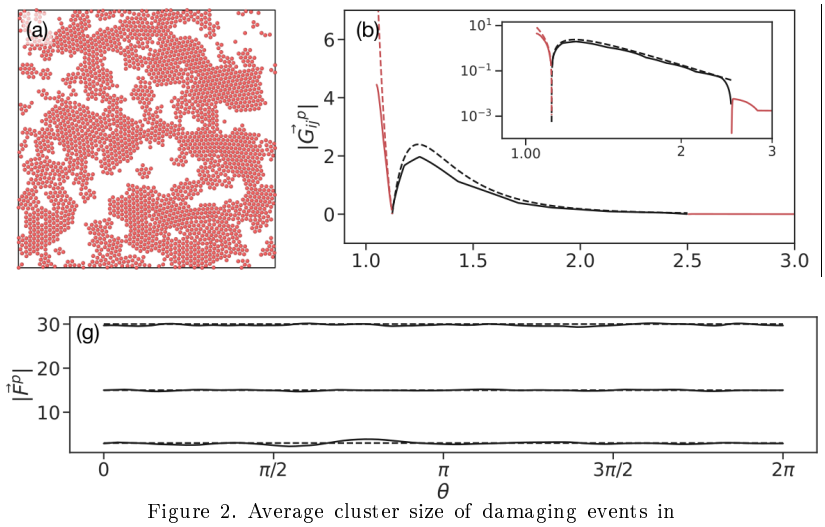

Figure 2. Average cluster size of damaging events in liquid water as a function of the distance from the ion track for different values of the carbon-ion energy.

[1] M. Cranmer, A. Sanchez Gonzalez, P. Battaglia, R. Xu, K. Cranmer, D. Spergel, and S. Ho, *Advances in Neural Information Processing Systems* **33**, 17429 (2020).

Ultrastable glasses: going very deep into the energy landscape of glasses

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Already in 1948 Kauzmann pointed out [1] that the configurational entropy of many supercooled liquids, obtained from their specific heat, extrapolated to negative values below a critical "Kauzmann temperature" T_K. This entropy crisis or "Kauzmann paradox" has led many authors to speculate on the possible existence of an "ideal glass" which should correspond to the best and most stable glass achievable, associated with the lowest relative minimum within the potential energy landscape of the substance (see Fig. 1). This ideal glass would have zero configurational entropy, equal to that of crystals, and has been associated to the possible existence of an underlying thermodynamic glass transition occurring at T_K.

In the last years, the existence of glasses with very high thermodynamic and kinetic stability has been realized experimentally. So-called *ultrastable glasses*, usually prepared through physical vapor deposition (PVD) under optimized deposition rates and temperatures, represent a unique class of materials with low enthalpies and high kinetic stabilities [2]. These glasses show remarkable physico-chemical properties, such as high thermal stability or improved mechanical and thermodynamic behavior, offering unprecedented opportunities for practical applications, as well as to understand many aspects of the glassy state.

Specifically, it is well known that glasses exhibit thermal, vibrational and acoustic properties at low temperatures anomalously different from those found in crystalline solids, and with a striking degree of universality. The question has naturally arisen as whether these peculiar low-temperature "glassy anomalies" persist or vanish in these highly-stable glasses. Interestingly, our earlier low-temperature specific-heat measurements on (highly anisotropic) ultrastable glasses of indomethacin [3] prepared by PVD showed the suppression of the ubiquitous linear term below 1–2 K traditionally ascribed to the existence of tunneling two-level systems (TLS) in glasses. This finding apparently challenged the opposite behaviour found in hyperaged glasses of geological amber [4]. To shed more light on this controversial issue, we will present very recent, unpublished results of low-temperature specific heat on a different ultrastable glass, TPD, whose degrees of anisotropy and stability can be controlled.

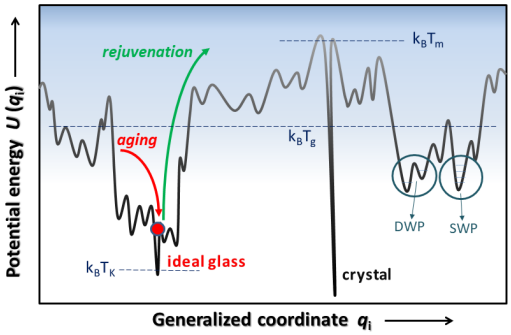

Figure 1. Schematic projection of the potential energy landscape of a substance, ranging from the supercooled liquid state below the melting temperature T_m, through the glass transition temperature T_g, down to the solid states at lower temperatures. Possible aging or rejuvenation processes are depicted. DWP and SWP refer to expected double or single well potentials, respectively, which are relevant for the low-temperature properties of glasses.

[1] W. Kauzmann, *Chem. Rev.* **43**, 219 (1948).
[2] C. Rodríguez-Tinoco, M. González-Silveira, M. A. Ramos, J. Rodríguez-Viejo, *Riv. Nuovo Cim.* (2022). https://doi.org/10.1007/s40766-022-00029-y
[3] T. Pérez-Castañeda, C. Rodríguez-Tinoco, J. Rodríguez-Viejo, M. A. Ramos, *Proc. Natl. Acad. Sci.* **111**, 11275 (2014).
[4] T. Pérez-Castañeda, R. J. Jiménez-Riobóo, M. A. Ramos, *Phys. Rev. Lett.* **112**, 165901 (2014).

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Casimir contribution to the interfacial Hamiltonian for 3D wetting

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Previous treatments of three-dimensional (3D) short-ranged wetting transitions [1-6] have missed an entropic or low temperature Casimir contribution to the binding potential describing the interaction between the unbinding interface and wall. This we determine by exactly deriving the interfacial model for 3D wetting from a more microscopic Landau-Ginzburg-Wilson Hamiltonian [7]. The Casimir term changes the interpretation of fluctuation effects occurring at wetting transitions so that, for example, mean-field predictions are no longer obtained when interfacial fluctuations are ignored. While the Casimir contribution does not alter the surface phase diagram [1], it significantly increases the adsorption near a first-order wetting transition and changes completely the predicted critical singularities of tricritical wetting [8], including the non-universality occurring in 3D arising from interfacial fluctuations. Using the numerical nonlinear renormalization group [8] we show that, for critical wetting, the asymptotic regime is extremely narrow with the growth of the parallel correlation length characterised by an effective exponent in quantitative agreement with Ising model simulations, resolving a longstanding controversy.

[1] H. Nakanishi and M. E. Fisher, *Phys. Rev. Lett*. **49**, 1565 (1982).
[2] F. P. Buff, R. A. Lovett, and F. H. Stillinger, *Phys. Rev. Lett.* **15**, 621 (1965).
[3] A. O. Parry, J. M. Romero-Enrique, and A. Lazarides, *Phys. Rev. Lett.* **93**, 086104 (2004).
[4] A. O. Parry, C. Rascón, N.R.Bernardino, and J.M. Romero-Enrique, *Phys. Rev. Lett.* **100**, 136105 (2008). Erratum: *Phys. Rev. Lett.* **100**, 259902 (2008).
[5] A. O. Parry,C. Rascón, N. R. Bernardino, and J. M. Romero-Enrique, *J. Phys.: Condens. Matter* **18**, 6433 (2006).
[6] J. M. Romero-Enrique, A. Squarcini, A. O. Parry, and P. M. Goldbart, *Phys. Rev. E* **97**, 062804 (2018).
[7] A. Squarcini, J. M. Romero-Enrique, and A. O. Parry, accepted in *Phys. Rev. Lett.* (2022).
[8] C. J. Boulter and F. Clarysse, *EPJE* **5**, 465 (2001).
[9] R. Lipowsky and M. E. Fisher, *Phys. Rev. B* **36**, 2126 (1987).

Simulating active agents under confinement with Dissipative Particles (hydro)Dynamics

C. Miguel Barriuso Gutierrez[1], **José Martín-Roca**[1,3], Valentino Bianco[3], Ignacio Pagonabarraga[4] and Chantal Valeriani[1,2]

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In this ongoing work we are developing a framework to simulate active agents taking into account both hydrodynamics and thermal fluctuations. Currently we are limiting our study to colloids and polymers although the framework will be applicable to agents with a wide range of structures. To achieve this we propose an extension of the widely known simulation software LAMMPS [1] that allows the implementation of hydrodynamic self-propulsion via force redistribution among solvent particles, this extension, in combination with the Dissipative Particle Dynamics (DPD) package [2], enables these kind of simulations. Similar approaches using lattice Boltzmann (LB) methods [3] and Multi-Particle Collision dynamics (MPC) [4] have been already well studied. With DPD and MPC dynamics we can easily simulate agents with more complex shapes taking into account thermal fluctuations, both of which are harder to implement using LB methods. Our approach takes advantage of the versatility of the LAMMPS code, being MPI-parallelizable and allowing the combination of our implementation with the wide range of features LAMMPS offers.

We are interested in the subsets of active matter systems known as active colloids and active polymers, which have very useful and broad applications. Their collective behaviour is rich and complex, and in many cases cannot be ascribed solely to the agents motion: hydrodynamic interactions need to be taken into account . This is the case, for example, of many self-propelled microorganisms, or *microswimmers*, whose movement is an essential aspect of life. A successful model for this systems is the so-called *squirmer*, in their simplest form these are hard spheres that take into account the propulsion induced by the beating cilia and flagella as a prescribed steady velocity of the solvent particles tangential to the surface of the sphere. This model serves as inspiration for our project.

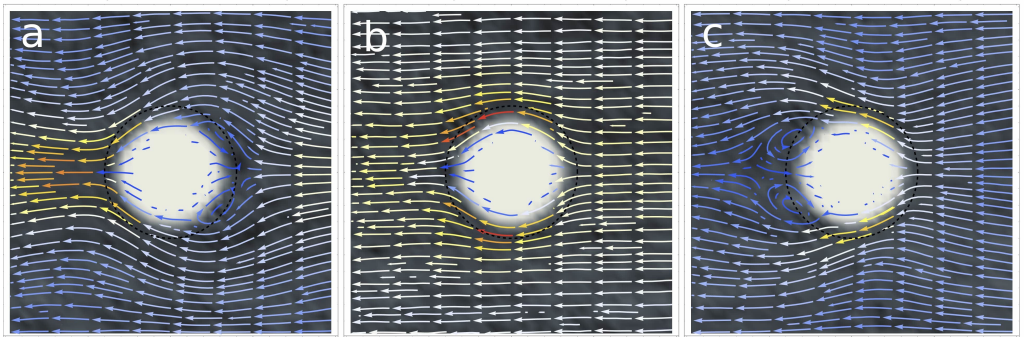

Figura 1: Solvent velocity field around a squirmer self-propelling in the positive x-axis in the colloid (left) and laboratory (right) reference frame, for $\beta = -5$ (*pusher*, left) and $\beta = 5$ (*puller*, right).

Referencias

[1] A. P. Thompson et al, Comp Phys Comm, **271** (2022) 10817.
[2] Groot and Warren, J Chem Phys, **107**, 4423-35 (1997)
[3] F. Alarcon, E. Navarro-Argemí, C. Valeriani, and I. Pagonabarraga, Phys. Rev. E **99**, 062602
[4] Zöttl, A., Stark, H. 2018, Simulating squirmers with multi-particle collision dynamics, *Eur. Phys. J. E* **41** 61

Collective behaviour of energy depot repulsive particles

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In this work we consider an active particle model, that reproduces the motion of microscopic biological objects, such as cells or bacteria, that is described with Langevin dynamics. The particles are able to take energy from their environment, store it into an internal energy depot and convert it into kinetic energy [1]. This model uses a velocity dependant friction function [2]. We have studied a two dimensional suspension of repulsive particles, where the interaction between the particles is implemented with a WCA potential.

$$\dot{\mathbf{v}} = -\gamma(\mathbf{v})\mathbf{v} - \frac{1}{m}\boldsymbol{\nabla} U(\mathbf{r}) + \mathcal{F}(t)\ , \quad \gamma(\mathbf{v}) = \gamma_0 - \frac{q_0 d_2}{c + d_2 \mathbf{v}^2}.$$

The parameters q_0, d_2 and c express the properties of the energy depot. We have studied both dynamical and structural features of the system. The pump rate of energy from the environment into the internal depot is q_0. d_2 is The rate of conversion of the internal depot energy to the particles kinetic energy, this implies that the particle is self propelling. c represents the internal dissipation, which takes into account the energy loss due to intern dissipative processes. In our study we fix the parameters d_2, and c, and we study the effect of different q_0 values.

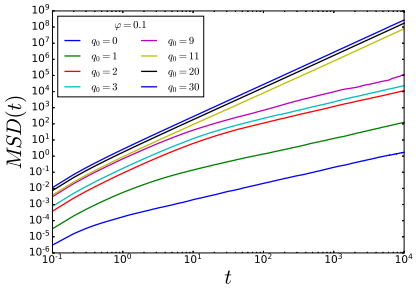

Figure 1. Mean squared displacement over time for different systems of $\varphi = 0.1$ and different values of q_0.

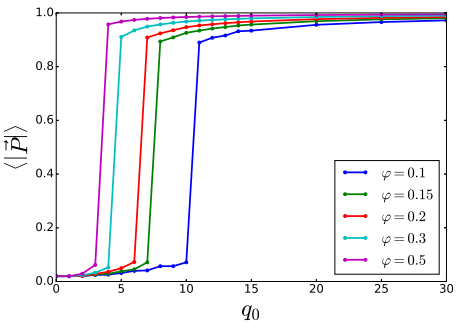

Figure 2. a) Mean polar order parameter as a function of q_0 parameter for the studied volume fractions φ.

The friction function will cancel at some velocity v_0, $\mathbf{v}_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d_2}$, this imposes two regimes onto the system; when $\mathbf{v} > \mathbf{v}_0$ the friction will be positive and the motion is damped. When $\mathbf{v} < \mathbf{v}_0$ we have negative friction, meaning that the motion of the slow particles is pumped as if the particles had an additional source of energy.

So far we have studied the diffusion through the mean squared displacement, finding different regimes as we increase q_0 (Fig.1). The main studied structural feature is a phase transition between an ordered an a disordered state for different volume fractions φ and values of q_0 (Fig.2).

The interest of this model comes from the fact that its able to mimic several properties of the biological microscopic matter, as self propulsion, collective motion or out of equilibrium phase transitions.

The interest in the model comes from the difference from other models such as Vicsek's or Active Brownian Particles, that address self-propulsion as a random process, while here the friction is the cause of this phenomenon.

[1] Schweitzer, F., Ebeling, W., & Tilch, B., *Physical Review Letters* **80(23)**, 5044 (1998).
[2] Erdmann, U., Ebeling, W., Schimansky-Geier, L., & Schweitzer, F., *The European Physical Journal B-Condensed Matter and Complex Systems* **15(1)**, 105-113 (2000).

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Dynamics of hard particles confined by an isotropic harmonic potential

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The dynamics of a system composed of elastic hard particles confined by an isotropic harmonic potential is studied. In the low-density limit, the dynamics is described by the Boltzmann equation and the system does not reach equilibrium except for some particular class of initial conditions. On the contrary, the system reaches a periodic in time state in which the velocity distribution function is Gaussian, but with the hydrodynamic fields oscillating in time with some specific profiles. It is shown that this so-called *breather* state is completely specified by the constants of the motion, the mean square displacement, $\langle r^2 \rangle$, at the initial time and its derivative with respect to time also at the initial time. This is due to the fact that, at this level of description, $\langle r^2 \rangle$ verifies a closed second order differential equation. For low but finite densities, the dynamics of the system is analyzed by taking into account the finite size of the particles. Under well-controlled approximations, a closed evolution equation for $\langle r^2 \rangle$ is derived, obtaining that it decays to its equilibrium value, oscillating with a frequency slightly modified with respect to the Boltzmann values. The time average of the oscillations is also renormalized. An excellent agreement is found between Molecular Dynamics simulation results and the theoretical predictions for the frequency and the time average of the oscillations. For the relaxation time, the agreement is not as good as for the two previous quantities and the origin of the discrepancies is discussed.

Trapping active particles up to the limiting case: bacteria enclosed in a biofilm

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Active matter systems are composed of constituents, each one in nonequilibrium, that consume energy in order to move [1]. A characteristic feature of active matter is collective motion leading to nonequilibrium phase transitions or large scale directed motion [2]. A number of recent works have featured active particles interacting with obstacles, either moving or fixed [3,4,5]. When an active particle encounters an asymmetric obstacle, different behaviours are detected depending on the nature of its active motion. On the one side, rectification effects arise in a suspension of run-and-tumble particles interacting with a wall of funnelled-shaped openings, caused by particles persistence length [6]. The same trapping mechanism could be responsible for the intake of microorganisms in the underground leaves [7] of Carnivorous plants [8]. On the other side, for aligning particles [9] interacting with a wall of funnelled-shaped openings, trapping happens on the (opposite) wider opening side of the funnels [10,11]. Interestingly, a cylindrical confinement considerably modulates the swimming features of an active colloidal swimmer [12], with respect to the colloid in bulk.

Active particles can be synthetic (such as synthetic active colloids) or alive (such as living bacteria). A prototypical model to study living microswimmers is P. fluorescens, a rod shaped and biofilm forming bacterium. Biofilms are microbial communities self-assembled onto external interfaces. Biofilms can be described within the Soft Matter physics framework [13] as a viscoelastic material consisting of colloids (bacterial cells) embedded in a cross-linked polymer gel (polysaccharides cross-linked via proteins/multivalent cations), whose water content vary depending on the environmental conditions. Bacteria embedded in the polymeric matrix control biofilm structure and mechanical properties by regulating its matrix composition. We have recently monitored structural features of Pseudomonas fluorescens biofilms grown with and without hydrodynamic stress [14,15]. Bacteria are capable of self-adapting to hostile hydrodynamic stress by tailoring the biofilm chemical composition, thus affecting both the mesoscale structure of the matrix and its viscoelastic properties that ultimately regulate the bacteria-polymer interactions [16].

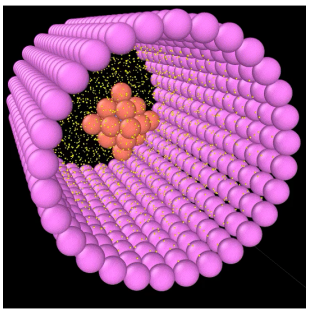

Figure 1. Active colloid in a cylindrical confinement.

[1] C. Bechinger et al., *Rev. Mod. Phys.* **88**, 045006 (2016).
[2] T. Vicsek, A. Zafeiris, *Phys. Rep.* **517**, 71 (2012).
[3] C. Bechinger et al., *Reviews of Modern Physics* **88**, 045006 (2016)
[4] R Martinez, F Alarcon, DR Rodriguez, JL Aragones, C Valeriani, *EPJ E* **41** 1 (2018).
[5] DR Rodriguez, F Alarcon, R Martinez, J Ramírez, C Valeriani, *Soft matter* **16**, 1162 (2020).
[6] C. O. Reichhardt and C. Reichhardt, *Annual Review of Condensed Matter Physics* **8**, 51 (2017).
[7] W Barthlott, S Porembski, E Fischer, B Gemmel, *Nature* **392**, 447 (1998).
[8] C B. Giuliano, R Zhang, R.Martinez Fernandez, C.Valeriani and L.Wilson (in preparation, 2022).
[9] R Martinez, F Alarcon, JL Aragones, C Valeriani, *Soft matter* **16**, 4739 (2020).
[10] P. Galajada, J. Keymer, P. Chaikin and R.Austin, *Journal of Bacteriology* **189**, 8704 (2007).
[11] M. Wan, C.O. Reichhardt, Z. Nussinov, and C. Reichhardt, *Physical Review Letters* **101**, 018102 (2008).
[12] C Miguel Barriuso Gutierrez, J Martin-Roca, V Bianco, I Pagonabarraga, C Valeriani, *arxiv* (2022).
[13] J N. Wilking , T E. Angelini , A Seminara , M P. Brenner , and D A. Weitz *MRS Bulletin* **36** 385 (2011).
[14]J Jara, F Alarcón, A K Monnappa, J Ignacio Santos, V Bianco, P Nie, M Pica Ciamarra, A Canales, L Dinis, I López-Montero, C Valeriani, B Orgaz, *Frontiers in Microbiology* **11**, 3460 (2021).
[15] P Nie, F Alarcon, I López-Montero, B Orgaz, C Valeriani, M Pica Ciamarra, *Soft Material* **0 1**, (2021).
[16] J Martin Roca, V Bianco, F Alarcon, A K. Monnappa, P Natale, F Monroy, B Orgaz, I Lopez-Montero, C Valeriani, *arxiv* (2022).

MIPS and Activity Cycles in Fire Ants

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Since its origin in the studies of bird flocks in the 1990's [1], active matter theory has sought to understand the behaviours of a broad class of systems that have energy added and dissipated at the single particle level [2]. In fact, most biological systems can be considered active systems, from schools of fish to intercellular fluids. Great strides have been made in understanding and predicting common features of these systems, such as collective motion, which is the tendency of local alignment interactions to lead to system-wide symmetry breaking, even in 2D [3], and motility induced attraction and phase separation, which is the tendency for motility effects to lead to the formation of dense stationary clusters in the absence of local alignment [4]. As the field has evolved, more and more remarkable predictions of active matter theory have been tested and proven in synthetic systems, which have the advantage of simpler interactions compared to the biological systems that originally launched the field. However, active matter theory's broadest impact likely remains in the study of biological systems. Here we seek to understand the crowd dynamics of *Solenopsis Invicta,* fire ants, which are social insects with complex interactions, within the framework of active matter.

We begin by studying the nature of interactions between pairs of ants, and show that one of the dominant effects in low-density groups of ants is motility-induced attraction. When the density of ants is increased, attraction can eventually lead to phase separation, such that the ants form dense, long-lasting clusters of stationary ants surrounded by a background of moving ants.

As we continue to increase the density of ants in our cells, the ants begin to exhibit spontaneous bursts of high activity, called activity cycles. While in an activity cycle, motility effects become less important in the crowd dynamics.

We show that the result of the suppression of motility effects is that the ants can now exhibit collective motion, which in large vertical columns, leads to the formation of spontaneous waves (Figure 2). The ants in the wave exhibit collective motion that is switched on and off not via density or rotational noise, as it has been in theory and experiments so far. Instead, local changes in the activity of the ants necessarily leads to alignment and propagates an "activity wave".

[1] Vicsek, T., et al., Novel Type of Phase Transition in a System of Self-Driven Particles, *Physical Review Letters* **75**, 1226 (1995).
[2] Marchetti, M. C., et al. Hydrodynamics of Soft Active Matter, *Reviews of Modern Physics* **85**, 1143 (2013).
[3] Toner, J. & Tu, Y. Long-Range Order in a Two-Dimensional Dynamical XY-Model: How Birds Fly Together, *Physical Review Letters* **75**, 4326 (1995).
[4] Cates, M. E. and Tailleur, J., Motility-Induced Phase Separation, *Annual Reviews of Condensed Matter Physics* **6**, 219 (2015).

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Collapse of magnetite-decorated pNIPAM microgels trapped with optical tweezers

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Microgels are versatile nanoparticles composed of crosslinked hydrogels which typically exhibit thermo-responsiveness. They are extensively used in applications that make use of their softness and ability to be swollen in an aqueous phase, e.g. as drug carriers or Pickering emulsion stabilizers [1]. In these applications, the systems inherit the thermo-responsiveness of the microgels [1,2]. Therefore, it is critical to understand the way in which the microgels collapse upon heating above their lower critical solution temperature (around 32 °C for pNIPAM and pVCL microgels). There is an open debate around the way in which this collapse happens, whether it is a first order transition. In fact, the usual diameter vs temperature plots produced by dynamic light scattering seem to hint to more complex transition phenomena [3,4]. In the present study, we use optical tweezers [5] to trap single microgels and measure this collapse upon self-heating in pure water and in the presence of conductive salts. The self-heating is achieved decorating the microgels with magnetite nanocubes that absorb radiation from the trapping laser (see Fig. 1). We find interesting features, such as partial collapses which produce bistable trapping dynamics, and collapses that seem to hint to a first order transition.

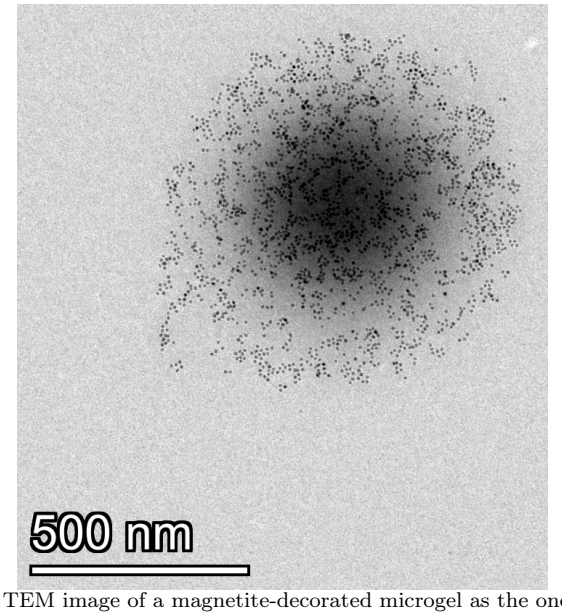

Figure 1. TEM image of a magnetite-decorated microgel as the ones we trap with optical tweezers.

[1] M.A. Fernandez-Rodriguez, A. Martin-Molina, & J. Maldonado-Valderrama, *Advances in Colloid and Interface Science* **288**, 102350 (2021).

[2] I. Navarro Arrebola, L. Billon, & G. Aguirre, *Advances in Colloid and Interface Science* **287**, 102333 (2021).

[3] R. Keidel *et al.*, *Science Advances* **4**, eaao7086 (2018).

[4] S. Bocheneck *et al.*, *Langmuir* **35**, 16780–16792 (2019).

[5] J. Gieseler *et al.*, *Advances in Optics and Photonics* **13**, 74–241 (2021).

Acknowledgements: The Authors acknowledge financial support from FEDER/Junta de Andalucía-Consejería de Transformación Económica, Industria, Conocimiento y Universidades/ Proyecto P18-FR-3583. MAFR acknowledges financial support from the project PID2020-116615RA-I00 and grant IJC2018-035946-I funded by MCIN/AEI/10.13039/501100011033.

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Phase behaviour and dynamics of colloidal cuboids: paving the path to biaxial nematic liquid crystals

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Colloidal cuboids have an especially rich phase behaviour [1, 2] and the potential to self-assemble into biaxial nematic (N_B) liquid crystals [3]. Over the last few decades, several theoretical works have predicted the existence of a wide region of the phase diagram where biaxial nematics would be stable, but imposed rather strong constraints on the particle rotational degrees of freedom, which artificially enhance the stability of the N_B phase [4, 5, 6].

In this contribution, we present molecular simulation results that clarify the relevance of fully unfreezing the rotational degrees of freedom to accurately determine the range of stability of the N_B phase. Our results show that only a large size dispersity or the presence of an external field can induce the formation of thermodynamically stable biaxial nematics [7, 8]. In particular, surprisingly weak field strengths are able to spark a uniaxial-to-biaxial phase transition at the self-dual shape, where prolate and oblate geometries fuse into one, suggesting a path to exploit low-energy uniaxial-to-biaxial order switching.

Motivated by this scenario, we have also simulated the unsteady-state reorientation dynamics when a field is applied (uniaxial-to-biaxial switching) and then removed (biaxial-to-uniaxial switching) [9]. We detected a strong correlation between the response time, being the time taken for the system to reorient, and particle anisotropy, which spans from rod-like to plate-like geometries. Interestingly, self-dual shaped cuboids, theoretically considered as the most suitable to promote phase biaxiality for being exactly in between prolate and oblate particles, exhibit surprisingly slow response times.

[1] A. Cuetos, M. Dennison, A. Masters, A. Patti, *Soft Matter* **13**, 4720 (2017).
[2] A. Patti and A. Cuetos, *Mol. Simul.* **44**, 516 (2018).
[3] E. van den Pol, A. Petukhov, D. Thies-Weesie, D. Byelov, G. Vroege, *Phys. Rev. Lett.* **103**, 258301 (2009).
[4] M. P. Taylor and J. Herzfeld, *Phys. Rev. A* **44**, 3742 (1991).
[5] S. Belli, A. Patti, M. Dijkstra, R. van Roij, *Phys. Rev. Lett.* **107**, 148303 (2011).
[6] Y. Martínez-Ratón, S. Varga, E. Velasco, *Phys. Chem. Chem. Phys.* **13**, 13247 (2011).
[7] A. Cuetos, E. M. Rafael, D. Corbett, A. Patti, *Soft Matter* **15**, 1922 (2019).
[8] E. M. Rafael, A. Cuetos, D. Corbett, A. Patti, *Soft Matter* **16**, 5565 (2020).
[9] E. M. Rafael, L. Tonti, D. Corbett, A. Cuetos, A. Patti, *Phys. Fluids* **33**, 067115 (2021).

Acknowledgements: E.M.R. acknowledges the Malaysian Government Agency *Majlis Amanah Rakyat* for funding his Ph.D. at the University of Manchester. A.P. and L.T. acknowledge the Leverhulme Trust Research Project Grant RPG-2018-415, the assistance given by Research IT and the use of the Computational Shared Facility at The University of Manchester. A.C. acknowledges the Spanish Ministerio de Ciencia, Innovación y Universidades and FEDER for funding (Project No. PGC2018–097151-B-I00) and C3UPO for the HPC facilities provided. A.P. is supported by a "Maria Zambrano Senior" distinguished researcher fellowship, financed by the European Union within the NextGenerationEU program.

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Nematics in 3-tori: Doubly twisted structures and defect-populated configurations

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Nematic liquid crystals are partially ordered fluids characterized by an apolar vector field, called director, that represents the average orientation of its anisotropic building blocks. Confining a nematic liquid crystal can frustrate its order, leading necessarily to the presence of topological defects which are regions where the alignment is not defined. Each topological defect can be characterized by a quantity called topological charge. Mathematically, the Poincaré-Hopf index theorem relates the total topological charge to the confining topology [1]. For instance, a 2-sphere must have a total topological charge of +2, so that the presence of defects is mathematically required.

In the case of the 2-torus, the total topological charge must be equal to 0, and thus defect free configurations of the material are allowed. In prior experimental work in our group, we filled a 3-torus with a nematic liquid crystal and found spontaneous chiral symmetry breaking without defects [2]. In this talk, we will report on alternative configurations populated by defects. Those appear as s=±1 pairs, with the s=+1 and s=-1 defects most often located in regions of positive and negative Gaussian curvature respectively. There are, however, other defect structures we observe.

[1] H. Hopf, *Math. Ann.* **96**, 209 (1926).
[2] E. Pairam et al, *Proceedings of the national academy of sciences* **110**, 9295 (2013).