

2024, Nov 03 – Nov 6

Centro de Ciencias de Benasque Pedro Pascual

https://www.benasque.org/2024ssm/

Application deadline: Sep 15





Organizers: Juan L Aragones (IFIMAC-UAM) Laura R Arriaga (IFIMAC-UAM) Alberto Fernandez-Nieves (UB-ICREA) Miguel Ruiz-Garcia (UCM)

Schedule	Sunday, November 3 rd
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
	Fisica I Quimica)
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, November 4 th
9:00 - 9:45	Opening by Alberto Fernandez-Nieves and
	Invited Talk by Soledad Le Clainche
9:45-11:25	Session on Structure and Dynamics of Polymers and Colloids
11:25-11:55	Coffee
11:55-13:35	APS Sponsored Session on Active/Driven Particles
13:35-15:00	Break
15:00-15:30	Coffee
15:30-16:10	APS Sponsored Session on Active/Driven Particles (Part II)
16:10-17:30	Session on Liquid Crystals
17:30-19:00	Poster Session
19:00	Welcome reception and posters

Schedule	Tuesday, November 5 th
9:00 - 9:40	Invited Talk by Pedro Tarazona
9:40-10:40	Session on Drops, Vesicles, Cells and Grains
10:40-11:30	Coffee
11:30-12:10	Session on Drops, Vesicles, Cells and Grains (Part II)
12:10-12:50	Invited Talk by Juan Colmenero
12:50	Adjurn

Schedule	Wednesday, November 6 th
9:00	Bus from Benasque to Barcelona



Schedule	Program on Monday, November 4 th
9:00 - 9:45	Opening by Alberto Fernandez-Nieves and
	Invited Talk by Soledad Le Clainche
	Machine learning for reduced order modelling
	Session on Structure and Dynamics of Polymers and Colloids
9.45-10:05	1. Structure and dynamics in model vitrimers: Looking for microscopic evidences of
	the topological transition. Arantxa Arbe
10:05-10:25	2. Interplay of linking chirality and heterogeneous flexibility in mechanically bonded
	membranes. Juan Luengo-Márquez
10:25-10:45	3. Conformational effects of polypeptide precursors on the collapse into
	nanoparticles. Paula Malo de Molina
10:45-11:05	4. Static-Dynamic decoupling in soft-colloid suspensions. José Ruiz-Franco
11:05-11:25	5. Does surface tension depend on gravity? Luis G. MacDowell
11:25-11:55	Coffee
	APS Sponsored Session on Active/Driven Particles
11:55-12:15	 Magnetic control of driven colloids dispersed in liquid crystals. Joel Torres- Andrés
12:15-12:35	2. Shakers at a fluid interface: Bridging the gap between 2D and 3D Dynamics.
	Alvaro Dominguez
12:35-12.55	3. Enhancement of effective diffusion in active colloids with time-dependent
	propulsion velocity. Carles Calero
12:55-13:15	4. Brownian dynamics and spontaneous rotation of a Janus particle in a polymer
	solution. Marco De Corato
13:15-13:35	5. Smart magnetic microrobots learn to roll with deep reinforcement learning.
42.25.45.00	David G. Calatayud
13:35-15:00	Break
15:00-15:30	Coffee
15:30-15:50	6. The carnivorous plant Genlisea harnesses active particle dynamics to prey on
15.50 16.10	microtauna. Jose Martin-Roca
12:20-10:10	7. Cluster formation in a system of photoactive macroscopic particles. Sara Levay
16.10 16.20	1 Active nemetic defects exhibit hunerunifermity, hethickrei Nembisen
16:10-16:30	Active nematic defects exhibit hyperuniformity. Jyothishraj Nampisan Searching for the bioxiel nematic liquid crustel phase. A journey between
10.50-10.50	2. Searching for the blackal hematic liquid crystal phase. A journey between molecules and colloids. Alessandre Patti
16.50-17.10	3 Anchoring transition of a smeetic film and nattern formation of focal conic
10.50 17.10	domains in liquid crystal flow cell geometry. Olga Bantysh
17.30-19.00	Poster Session
17.50 15.00	1. Ionic self-phoresis maps onto correlation-induced self-phoresis. Alvaro
	Domínguez
	2. Depletion forces in dipolar polymer brushes and dipolar colloidal systems:
	external field modulation of system properties. Joan J. Cerdà
	3. Walls and boojums in nematic toroidal droplets. Javier Rojo-González
	4. Soft matter for biotech applications: microfluidic generation of chitosan gels for
	biological pest control. Adria Meca
	5. Self-Assembly of Active Bifunctional Patchy Particles. Caterina Landi
	6. Rolling rebels: counteractive transport of microrollers in an obstacle lattice. Galor
	7. Optimal transport of active colloids through depp reinforcement learning. Arin E. Ortiz
	8. Protein-mediated adhesion of polymer vesicles. Berta Tinao
	9. Capillary instabilities and hysteresis of multiphase flow in disordered media.
	Ramon Planet
1	10. E. coli motion in double emulsion droplets. Richard A. Campusano

	11. Dissipative self-assembly of FtsZ over confined lipid bilayers. Marc Vergés Vilarrubia
	12 Polymer informatics tools for sustainable polymers and 3D printing Petra Bačová
	13 Transient motion of a Eutertic Indium-Gallium dron inside a canillary subject to
	an oscillatory voltage Javier Rodríguez Rodríguez
	14 Sampling from athermal suspensions: averages distributions and fluctuations
	Guillaume Briand
	15. Swelling of ionizable alginate hydrogel under the presence of NaCl and $CaCl_2$
	salts. Marta Gil-Fraca
	16. Probing the dynamics of responsive microgel with respect to concentration with 3DDLS techniques. A Arenas-Gullo
	17 Unsteady emptying of a capillary: A model system for solat painting Lorène
	Champougny
	18. Exploring microfluidics for the development of controlled microfabrication of
	blood clot. Herrera Restrepo
	19. Active self-organisation of dense nematic structures in the actin cytoskeleton.
	Alejandro Torres-Sanchez
	20. What sculpts vascular network organization? Flow vs. shape. Prasanna
	Padmanaban
	21. Casimir contribution to the interfacial Hamiltonian for 3D wetting. José Manuel
	Romero-Enrique
	 Exact equilibrium properties of hard-core disks in single-file confinement. Ana M. Montero
	23. Derivation of a universal law for ac hysteresis area with applications in
	biosensing. Pablo Palacios-Alonso
	24. Broad Adaptability of Coronavirus Adhesion Revealed from the Complementary
	Surface Affinity of Membrane and Spikes. Pablo Ibáñez-Freire
	25. Single cell death triggers local avoidance response in the cosmopolitan
	picoeukaryote Micromonas. Marco Polin
	26. Density and inertia effects on two-dimensional active semiflexible filament
	suspension. Giulia Janzen
	27. Water turbidity prediction in desalination plants using machine learning-based
	models. Samuel Lozano Iglesias
	28. A self-averaging method to fit parameters in coarse-grained models. Carlos
	Monago
19:00	Welcome reception and posters

Schedule	Program on Tuesday, November 5 th
9:00 - 9:40	Invited Talk by Pedro Tarazona
	Protein filaments as active polymers
	Session on Drops, Vesicles, Cells and Grains
9:40-10:00	1. Effect of Particle Shape on the Flow of an Hourglass. Raúl Cruz Hidalgo
10:00-10:20	2. Fluid dynamics of a respiratory droplet in the context of viral dynamics. Javier
	Martínez-Puig
10:20-10:40	3. Membrane-enabled transduction of internal flows into vesicle motion. Paula
	Magrinya
10:40-11:30	Coffee
10:40-11:30 11:30-11:50	4. Active flow networks and their complex dynamics. Rodrigo Fernandez-Quevedo
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Plenary Contributions

MACHINE LEARNING FOR REDUCED ORDER MODELLING

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One of the greatest challenges our society encounters is addressing climate change. To alleviate its impacts, it is essential to investigate various alternatives and create new technologies capable of reducing atmospheric pollution. Fluid mechanics, a science with numerous applications, can be harnessed for this purpose, such as enhancing the efficiency of combustion systems, examining methods to diminish air pollution in urban environments, and optimizing the design of aircraft to improve their efficiency. To examine these issues, reduced-order models (ROMs) grounded in physical principles are proposed, employing (i) modal decompositions (singular value decomposition – SVD, higher-order dynamic mode decomposition - HODMD), and (ii) machine learning techniques (neural networks) integrated with these decompositions. This research applies these methods to tackle the aforementioned challenges while also presenting new approaches to develop efficient and accurate ROMs for different applications, such as accelerating computational fluid dynamic (CFD) numerical simulations, data assimilation, flow control and studying the flow physics in big databases.

REFERENCES

Hetherington, A., Corrochano, A., Abadía-Heredia, R., Lazpita, E., Muñoz, E., Díaz, E., Maiora, E., López-Martín, M., Le Clainche, S., ModelFLOWs-app: data-driven post-processing and reduced order modelling tools, Comp. Phys. Com, 301, 109217, 2024.

Hetherington, A., Le Clainche, S., Low-cost singular value decomposition with optimal sensor placement, arXiv:2311.09791, 2023.

PROTEIN FILAMENTS AS ACTIVE POLYMERS

Pedro Tarazona, Depto. Física Teórica de la Materia Condensada, IFIMAC Condensed Matter Physics Center, Universidad Autónoma de Madrid, Madrid 28049, Spain pedro.tarazona@uam.es

Some proteins, both in bacteria and in eukarvota, have been evolutionarily designed to form filamentary structures that play several crucial roles in the cell. The best known example are the microtubules, formed by tubulin, that are essential for the cell division of eukaryota and also for the active transport within the cells. A peculiarity of tubulin, shared by other filament forming proteins in eukaryota and bacteria, is their GTPase activity: Each bond between protein monomers includes a GTP molecule, but once the bond is formed that (high enthalpy) molecule is hydrolyzed to form the (lower enthalpy) GTD, and the strength of the bond is severely reduced. Why these proteins have been selected to "burn" (hydrolyze) the "glue" (GTP) that they require to form and keep those filaments, crucial for their role in the cell? From a physicist's point of view, the answer for tubulin comes in the need of a most peculiar dynamics for the polymerization/depolymerization of those protein structures. In the appropriate biochemical environment, both in vivo and in vitro, microtubules grow steadily with polymerization rates that may be tuned by the concentration of protein, GTP, etc..., but their growth is interrupted by "catastrophic" depolymerization events that suddenly shorten the length of the microtubule. Simple physical models may capture the essentials of these complex dynamics, as the result of a fine-tuning of the protein monomers to crystallize in ordered tubular structures, stabilized by the bonds with all the neighbours and therefore weaker at the ends, where the monomers have fewer neighbours, compensated by the fact that the bonds at the ends are likely to be more recently formed, and therefore to be stronger, since the hydrolysis of the GTP molecules has had less time to act.

FtsZ, a protein that plays a crucial role in the bacterial cell division [1], seems to be a bacterial ancestor of tubulin. They share crucial structural motives, the need of GTP to form bonds and also the GTPase activity that weakens the bonds between protein monomers along the filaments. However, the FtsZ aggregates are much more disordered and flexible than tubulin microtubules. Compared with the crystalline order of the finely tailored tubulin monomer in eukaryotic cells, the primitive FtsZ aggregates in bacteria show a typical soft-matter character that makes much uncertain the possible biological role for the need and the hydrolysis of GTP at FtsZ bond. *In vitro* experiments, under a broad range of conditions, have shown a wide polymorphism of FtsZ, with some claims of *threadmilling*, i.e. of the directional kinetics of the polymerization at one of the ends and depolymerization at the other end of the filaments [1]. This talk explores how that behaviour may appear and what could be it biological function. The combination of soft-matter structures (flexible polymers anchored to lipid membranes) and the out of equilibrium process of GTP hydrolysis and replacement lead to simple models in which the breaking of the spatial and time symmetry may produce that threadmilling effect in *active polymers* that, though the "burning" of the (externally provided) GTP "fuel" may produce global movements.

[1] Pablo Mateos-Gil; Pedro; Marisela Vélez (2019), FEMS MICROBIOLOGY REVIEWS, **43**, 73-87; and references there in.

UNVEILING THE COLLECTIVE DYNAMICS OF LIQUIDS AND POLYMER MELTS AT THE MESOSCALE BY NEUTRON SPECTROSCOPY WITH POLARIZATION ANALYSIS AND MD-SIMULATIONS

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Soft-matter systems in general show a hierarchy of different dynamical processes taking place at different time/frequency and length sales. The collective dynamics at the so-called 'intermediate scales' (or mesoscales) are of paramount importance to understand, for instance, the role of specific interactions -as hydrogen bondsand the formation of dynamic aggregates of supramolecular nature. However, due to inherent difficulties, the mesoscopic range is still a rather 'white area' in the relaxation map of these systems. In principle, quasi-elastic neutron scattering (QENS) is the ideal technique with which to directly observe the collective relaxation of liquids and glass-forming systems in a wide Q-range (Q: momentum transfer) due to the high energy resolution currently available. The problem is that the measured intensity always contains a combination of coherent and incoherent contributions, which can be very relevant at the mesoscopic range. The only way to clearly separate coherent and incoherent contributions is to apply polarization analysis techniques, which, for spectroscopy, still are rather scarce. As a first step, by means of the recently implemented neutron polarization analysis on a wide time-of-flight spectrometer (LET @ ISIS), we have recently measured coherent and incoherent dynamic structure factor of heavy water (H-bonded system) [1] and deuterated tetrahydrofuran (van der Waals system) [2] with sub-meV resolution in a wide Q-range. The results obtained were interpreted with the help of massive MD-simulations [3]. This work has convincingly proved the power of neutron spectroscopy with polarization analysis that can hugely impact the progress of microscopic dynamic investigations in different fields. Unfortunately, the spectrometers with polarization analysis currently available do not allow to extend this kind of studies to polymers and more complex systems. In this direction, we are exploring the possibilities of using wide angle spin echo techniques (WASP) for such investigations. In this talk I will give an overview of the current status of this topic.

[1] A. Arbe, G. J. Nilsen, J. R. Stewart, F. Alvarez, V. García-Sakai and J. Colmenero, Phys. Rev. Research 2020, 12 022015(R)

[2] A. Arbe, G. J. Nilsen, M. Devonport, B. Farago, F. Alvarez, J. A. Martínez González and J. Colmenero, J. Chem. Phys. 2023, 158 184502

[3] F. Alvarez A. Arbe and J. Colmenero, J. Chem. Phys. 2021, 155 244509

ORAL Contributions

APS Sponsored Session on Active/Driven Particles

STRUCTURE AND DYNAMICS IN MODEL VITRIMERS: LOOKING FOR MICROSCOPIC EVIDENCES OF THE TOPOLOGICAL TRANSITION

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In addition to the glass transition, vitrimers undergo a topological transition from viscoelastic liquid to viscoelastic solid behavior, when the network rearrangements facilitated by dynamic bond exchange reactions freeze. The microscopic observation of this transition is elusive. Model polyisoprene (PI) vitrimers based on imine dynamic covalent bonds were synthesized by reaction of α , ω -dialdehyde-functionalized polyisoprenes and a triamine. In these dynamic networks nano-phase separation of polymer and reactive groups leads to the emergence of a relevant length scale characteristic for the network structure. We have exploited scattering sensitivity to structural features at different length scales to determine how dynamical and topological arrests affect correlations at segmental and network levels. Chains expand obeying the same expansion coefficient throughout the entire viscoelastic region, i. e., both in the elastomeric regime as well as in the liquid regime. The onset of liquid-like behavior is only apparent at the mesoscale, where the scattering reveals the reorganization of the network triggered by bond exchange events. The such determined 'microscopic' topological transition temperature is compared with differential scanning calorimetry. We show that using proper thermal (aging-like) protocols, this transition is also nicely revealed by the latter [1].

In addition, applying broadband dielectric spectroscopy, we have studied the polymer dynamics from the segmental to the whole chain scale, taking advantage of the fact that PI belongs to the class of molecules that exhibit a net dipole moment associated with the end-to-end vector. Three distinct relaxation phenomena are identified. The fastest relaxation is attributed to the segmental PI dynamics with a small influence of the crosslinking. An intermediate relaxation attributed to the dipolar character of the crosslinker is also observed. The slowest identified relaxation component, corresponding to fluctuations of the end-to-end PI chains, is found to be determined by the dynamics of the cluster formed by the crosslinkers with a time scale orders of magnitude faster than that of the terminal relaxation as inferred from the viscous flow [2].

[1] A. Arbe, A. Alegría, J. Colmenero, Saibal Bhaumik, Konstantinos Ntetsikas and Nikos Hadjichristidis, ACS Macro Letters 2023, 12 1595-1601

[2] A. Alegría, A. Arbe, J. Colmenero, Saibal Bhaumik, Konstantinos Ntetsikas and Nikos Hadjichristidis, Macromolecules 2024, 57 5639-5647

Interplay of linking chirality and heterogeneous flexibility in mechanically bonded membranes

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Salvatore Assenza, Universidad Autónoma de Madrid, Madrid, Spain Cristian Micheletti, International School for Advanced Studies (SISSA), Trieste, Italy

Chain entanglement in polymer systems often results in unusual kinetic and static properties. In recent years, mechanically bonded membranes - quasi two-dimensional networks of interlocked rings - have gained substantial attention both because of their interest as a promising class of meta-materials and due to their intriguing natural occurrence, i. e. kinetoplast DNA.

In this work [1], we address two open questions concerning the large-scale impact of network connectivity and its interplay with ring flexibility. We perform Molecular Dynamics simulations of mechanically bonded membranes composed of copolymer rings with flexible and rigid fragments of variable length (Fig. 1). We examine the effect of network connectivity by tuning the linking chirality between pairs of rings. We observe that linking pattern and ring flexibility have independent large-scale reverberations, the former determining the shape and curvature while the latter fixing the size of the membranes. Notably, this finding opens the way to utilize these properties as complementary control parameters for the rational design of mesoscopic membranes.



Figure 1 – Model for mechanically bonded membranes, composition of ring copolymers and global effect of link chirality.

[1] J. Luengo-Márquez, S. Assenza, C. Micheletti, Soft Matter, 20, 6595-6607 (2024)

CONFORMATIONAL EFFECTS OF POLYPEPTIDE PRECURSORS ON THE COLLAPSE INTO NANOPARTICLES

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Single chain nanoparticles (SCNPs) are individual polymer chains that fold or collapse through intramolecular cross-linking under high dilution, resulting in sparse conformations and a topological polydispersity akin to intrinsically disordered proteins (IDPs). There is growing interest in adapting this technology to biodegradable and biocompatible polymers, including proteins. We synthesized bovine serum albumin (BSA) nanoparticles by intramolecular cross-linking of denatured BSA with disuccinimide ester linkers that predominantly react with lysine residues in polypeptides. Small-angle neutron scattering (SANS) measurements revealed that cross-linking induces a progressive compaction of the denatured protein, with a corresponding decrease in the scaling exponent, allowing control over the size of the BSA nanoparticles.¹

To further extend SCNP technology to polypeptides, it is crucial to understand how the conformation of the precursor chain influences the resulting nanoparticle morphology. We systematically varied solvent conditions (pH, salt, and denaturant concentrations) of BSA and polylysine solutions, as well as the cross-linker concentration, and analyzed the resulting nanoparticles using dynamic and static light scattering, along with SANS. Our results demonstrate that the precursor conformation significantly impacts nanoparticle morphology; specifically, more extended precursor chains tend to undergo greater collapse with increased intramolecular cross-linking. Furthermore, the use of longer cross-linkers enhances chain compaction by facilitating the formation of larger intramolecular loops.²

- (1) Malo de Molina, P.; Le, T. P.; Iturrospe, A.; Gasser, U.; Arbe, A.; Colmenero, J.; Pomposo, J. A. Neat Protein Single-Chain Nanoparticles from Partially Denatured BSA. ACS Omega 2022, 7 (46), 42163– 42169.
- (2) Le, T. P.; Cavalcanti, L.; Tellam, J. P.; Malo de Molina, P. Effect of the Protein Chain Conformation on the Collapse into Nanoparticles. *Biomacromolecules* **2024**.

DOES SURFACE TENSION DEPEND ON GRAVITY?

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The surface tension is a fundamental parameter in capillary theory and interface science. But is the interface tension an *intrinsic* parameter of the two phase system, or could it also depend on the external field applied to the interface?

In standard applications, the free energy of an interface is described in terms of the surface tension, assumed as an intrinsic property, plus additional contributions corresponding to the applied surface tension [1]. However, microscopic studies of the interface structure suggest that higher order terms in the free energy expansion can lead to effective field dependent surface tensions [2,3]. A particularly interesting case is the gravity field, which is present in all interfaces. Unfortunately, the role of second order contributions under such a weak external field appear to be unmeasurable in ordinary fluids [3].

This situation can be remedied in the special case of colloidal suspensions, which have an extremely weak surface tension. In a recent study, we reanalized experiments of two dimensional colloidal monolayers at two phase coexistence, and found results consistent with a linear dependence of surface tension with the gravity field predicted by theory [4]. Was this result a mere coincidence related to experimental uncertainty?



In this paper we will report ongoing computer simulations of model colloidal suspensions aimed at shedding further light into the question.

Verification of this hypothesis is of general interest to interfacial science, as it would allow to identify corrections to the fundamental equation of equilibrium capillarity and shed light on the microscopic origin of the celebrated Kardar-Parisi-Zhang equation of interfacial growth [4].

Figure 1 – Surface tension of colloidal monolayer suspensions on a plate as a function of tilt angle [4]. Symbols are experimental results from Thorneywork et al.. Phys. Rev. Lett. **118**,158001 (2017).

[1] de Gennes, Brochard-Wyart, Quèrè, Capillarity and wetting phenomena, Springer, New York (2004).

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ORAL Contributions

APS Sponsored Session on Active/Driven Particles

MAGNETIC CONTROL OF DRIVEN COLLOIDS DISPERSED IN LIQUID CRYSTALS

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Nanotecnologia de la Universitat de Barcelona (IN²UB), Universitat de Barcelona, Universitat de Barcelona

Driven colloids are a class soft matter system in which micrometer-sized particles are propelled using an external force, such as an electric field. This soft matter system has been widely studied when the continuous phase is a simple (Newtonian) fluid. Now, the focus has shifted to uncovering new phenomena that arise when

the continuous phase is changed from a simple to a complex (non-Newtonian) fluid. Liquid crystals (LCs) are complex fluids that feature long range orientational order, and studying the propulsion of colloidal entities within them is of interest for their capacity to respond to external stimuli. When colloids are dispersed and driven in LCs, new propulsion phenomena emerge due to the inherent anisotropy of the liquid phase¹. Furthermore, orientational waves (waves formed by changes in the orientation of molecules within the material) can be generated and propelled through the material^{2,3}. Particularly, studies have shown the possibility to generate solitonic waves that exhibit behavior close to that of solid colloids: they can move, collide without annihilation, or display Brownian motion. While the motion of solitonic waves and solid particles within liquid crystals has been explored, there is a lack in in-situ control of their directionality-both individually and collectively-using simple experimental setups while performing observations. In this work, we show simple arrangements based on the application of fixed external magnetic fields to control solid polystyrene (PS) particles and two types of solitary waves, skyrmions and butterflv defects. in confined both and unconfined LCs. We demonstrate that degeneration in motion directionality can be broken by applying an in-plane fixed magnetic field while running experiments both with particles and solitonic waves, showing that, for the case of skyrmions, the magnetic field has a



Figure 1 - a) Rotating mill conformed of polystyrene (PS) particles around a +1 defect inside a nematic LC cell. The defect is created by applying a ring magnet under the presence of an AC electric field. The background color refer to the mean velocity modulus in the field of view. **b**) Velocity modulus variation of the PS particles as a function of mill radius. **c**), **d**) Normalized velocity variation of skyrmions when passing through microfluidic channels. The motion direction of the solitonic waves is controlled by the application of an in-plane fixed magnetic field, they are propelled by a modulated AC electric field with a 100% of duty cycle.

direct effect on their shape and velocity. In addition to this, we show how to attain dense regions of PS particles in the form of rotating mills, by generating topological defects on the surrounding LC using magnetic fields, enabling the collective study of particle flocks. Moreover, some of these colloidal entities are introduced and steered inside microfluidic channels. It is in these systems where we observe a dependency of skyrmions' velocity on the channel width, a clear phenomenon related to lateral confinement imposed by walls. Consequently, this work, gives an approach into the field of colloidal control in complex fluids by magnetic fields.

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- [2] Ackerman, P.J.; et. al. Nat. Commun., 2017, 8:673, p. 1-13.
- [3] Li, B.X.; et. al. Nat. Commun. 2019, 10:3749, p. 1-9.

SHAKERS AT A FLUID INTERFACE: BRIDGING THE GAP BETWEEN 2D AND 3D DYNAMICS

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It is long known that the spatial dimensionality can affect dramatically the dynamics of complex systems. A colloid at a fluid interface looks like a two--dimensional (2D) system, but the hydrodynamic interactions are mediated by the three--dimensional (3D) flows in the surrounding fluid. Even though this 3D flow is incompressible, the 2D flow projected on the interface and experienced by the colloid is compressible, which has a relevant impact on the collective dynamics, e.g. Fick's law of diffusion breaks down [1-4].



This configuration can serve as a testbed for understanding the dependence of the dynamics on the spatial dimensionality, and it is qualitatively different from the purely 2D models for a colloidal monolayer residing on a wall or trapped between two walls.

We consider active shakers trapped at a deformable interface and address the collective dynamics driven by the competition between the capillary attraction and the compressible hydrodynamic interactions. We study a kinetic model analytically and numerically that accounts for these two ingredients [5-7]. Most interestingly, the hydrodynamic flows induced by activity can halt the capillary collapse and, in a range of parameter values, lead to an evolution resembling spinodal decomposition.

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ENHANCEMENT OF EFFECTIVE DIFFUSION IN ACTIVE COLLOIDS WITH TIME-DEPENDENT PROPULSION VELOCITY

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Self-propelled or active colloids are currently the focus of considerable attention. These comprise swimmers which cyclically deform in a non-reciprocal manner (be it by internal consumption of energy or by external actuation) and particles which propel due to self-phoretic mechanisms [1, 2]. Understanding their collective dynamics is of interest both from a fundamental perspective and due to their potential applications, such as drug delivery vectors or non-invasive microsurgery devices.

Depending on their mechanism of self-propulsion, active colloids can exhibit a time-dependent, often periodic, propulsion velocity [2, 3]. The precise propulsion velocity profile determines their mean square displacement and their effective diffusion coefficient at long times. Here we demonstrate that any periodic propulsion profile results in a larger diffusion coefficient than the corresponding case with constant propulsion velocity [4]. We investigate in detail the case of periodic exponentially decaying velocity pulses, expected in propulsion mechanisms based on sudden absorption of finite amounts of energy. We show both analytically and with numerical simulations that in these cases the effective diffusion coefficient can be arbitrarily enhanced with respect to the case with constant velocity equal to the average speed. Our results may help interpret from a new perspective observations on the diffusion enhancement of active colloids.



Fig. 1 -- The effective diffusion of active colloids propelling through periodic exponentially decaying velocity pulses (green line on right panel) is always larger than the case with constant velocity equal to the average speed (blue line). The effect of the time dependent velocity profile is appreciated in the 2D trajectories in the left panels.

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Brownian dynamics and spontaneous rotation of a Janus particle in a polymer solution

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The development of engineered active colloids that harness the chemical energy of the environment to move has enabled one to mimic and dissect mechanisms in biological systems while opening doors to multiple applications: bioremediation, micromixing, micromachinery, drug delivery, and more. However, the application of active colloids for biomedical applications must consider the complex nature of most biological fluids, which contain large macromolecules and display viscoelastic and non-Newtonian rheology.



Figure 1 – Streamlines around a squirmer that spontaneously rotates when propelling through a polymer solution. The contour levels show the polymer concentration relative to its equilibrium value.

Recent experiments showed that active colloids propelling through a polymer solution experience a drastically enhanced rotational diffusion ¹and can rotate spontaneously due to an instability the origin of which is not understood². Earlier work suggests that the instability arises from the advection of polymers around the colloid and requires a fore-aft asymmetric interaction between the particle and the polymers³.

Here, we go beyond the study of the instability and we employ a fluctuating hydrodynamics approach developed in our group⁴ to study the Brownian dynamics and the spontaneous rotation of a spherical Janus active particle moving through a polymer solution. We model the evolution of the polymer concentration using a stochastic advection-diffusion equation that includes the thermal fluctuations of the polymer concentration. The results show that driving a Janus particle out of equilibrium in a polymer solution has a profound impact on its Brownian dynamics. In agreement with the experiments, we find that the rotational diffusion coefficient is drastically enhanced before the onset of the spontaneous rotation. Our work demonstrates the importance of considering the colloidal nature of polymer solutions and highlights the challenges of controlling active matter in a complex fluidic environment.

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SMART MAGNETIC MICROROBOTS LEARN TO ROLL WITH DEEP REINFORCEMENT LEARNING

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Accurate control of micron-scale robots, or microrobots, requires addressing unique challenges, including the difficulties associated with achieving motion in a non-inertial fluid dynamics regime, the development of real-time control strategies, and the presence of complex and dynamic environments. Unlike their macroscopic counterparts, microrobots are subject to Brownian motion, which randomizes their position and orientation. Deep reinforcement learning is a promising method for autonomously developing robust controllers to create smart microrobots, providing them with the capability to adapt their behavior to operate in uncharacterized environments without the need to model system dynamics. In this work, we report the development of smart magnetic-driven spherical particles that harness lubrication forces to facilitate rolling on a substrate. We use real-time control of these rollers to train a reinforcement learning model that generates an actuation policy to direct their motion in a simple standard navigation problem whose optimal solution can be derived from the underlying physics. The model's performance is analyzed under different sets of physically-informed system states. As a hallmark of the microscopic world, we characterize the influence of Brownian motion on the learning process by using particles of different sizes. Although the field of microrobotics has not yet reached the evolutionarily honed refinement of microscopic living organisms, deep reinforcement learning is a promising approach that is likely to enhance the capabilities of the next generation of microrobots.



Figure 1: Schematic representation of the microrobot control process using deep reinforcement learning. From left to right: microscope image input, deep neural network for policy learning, rotating magnetic field actuation, and resulting roller motion.

The carnivorous plant Genlisea harnesses active particle dynamics to prey on microfauna

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Carnivorous behavior in plants is a rare characteristic that has independently evolved multiple times throughout evolutionary history. Plants from the Genlisea genus are carnivorous and capture microorganisms living in the soil using specialized underground leaf structures. A diverse range of microfauna, including ciliates, amoebae, and soil mites, has been found in the digestive chambers of these plants.

In this study, we propose through experiments and simulations that Genlisea uses active matter physics to direct bacterial movement, creating a local flow of bacteria toward the plant's digestion vesicles. In contrast, larger macromolecular digestion products can diffuse away from the vesicle, generating a carbon source gradient that attracts larger microorganisms deeper into the plant. Our findings suggest this process is localized, with no evidence of large-scale movement of digested materials.



Figure 1. (a) Photograph of a *G. hispidula* plant: Photosynthetic leaf (L), digestive vesicle (V), trap neck (N), trap bifurcation (B), and the characteristic `corkscrew' structure containing the trap openings (T). **(b)** Image showing the interior of one of the traps. The detentive hairs point upwards along the rhizophyll's central channel towards the digestive vesicle. **(c)** Trajectories of simulated bacteria within the rhizophyll of Genlisea, with dimensions taken from experiments.

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CLUSTER FORMATION IN A SYSTEM OF PHOTOACTIVE MACROSCOPIC PARTICLES

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Active matter refers to systems of interacting, self-propelled agents that convert energy into mechanical motion, representing a nice example of out-of-equilibrium systems. The energy can come from the particles themselves or an external source. This area of study has gained significant attention due to its applications in physics, chemistry, biology, and robotics. Examples of active matter systems include microrobots, cells, Janus particles, bacterial systems, robot swarms, bird flocks, and human stampedes. Despite the diversity of constituents and their interactions, these systems share common properties at the group level. Accordingly, several models have been developed to describe the emergence of collective behavior.

In our work, we focus on active granular matter, where macroscopic (~5 cm) agents interact solely through physical contact. These agents are photoactive, meaning that the energy converted to their motion comes from a light source. To realize this experimentally, we modified Hexbug nano particles by adding a solar cell to the top of each particle (see Fig. 1 left). This allows the agents to move only when there is a sufficient amount of light, and by adjusting the light intensity, we can control the particle activity. To serve as the light source, we constructed a large programmable LED panel. Which allows us to change the illumination pattern and, consequently, the particle activity in space and time.



Figure 1 – Left: scheme of the experimental setup and picture of the photoactive bug. Right: snapshot of an experiment with five clusters (groups of more than 3 particles contacting each other) displayed with different colors.

This setup offers two main advantages: (1) We have external control over the activity of the internally excited agents, which is a scenario common in microscopic systems but a new approach in macroscopic ones. (2) Because of the macroscopic size of the agents and their sole interaction through collisions, we can precisely adjust the experimental parameters and easily reproduce the same experimental conditions. This can be challenging in biological systems or in systems where there is hydrodynamic and/or social interaction among the agents. As a result, our experiment can serve as a genuine limit case for more complex active systems.

Our research investigates the clustering behavior of these agents under homogeneous illumination (see Fig. 1 right). By varying the illumination intensities and changing the population of the system, we observed a power-law-like distribution for both the cluster sizes and durations. We identified a transition from unstable to stable clusters, as indicated by the divergence of average cluster durations. Higher particle activity and lower populations led to the creation of unstable clusters, which disassociated relatively easily. On the other hand, lower particle activity and higher populations resulted in large, stable clusters that persisted over time. In this contribution, we aim to present and explain this transition with the help of a simple model capturing the most important processes involved in cluster dynamics.

ORAL Contributions

Session on Liquid Crystals

ACTIVE NEMATIC DEFECTS EXHIBIT HYPERUNIFORMITY

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Theoretical and experimental studies of active matter often involve characterizing the fluctuations in the number density of the active particles. The fluctuation-compressibility theorem states that in equilibrium, the number variance σ^2 of *N* particles within an observation region of size *R* is proportional to the volume of the region R^d , with d the dimensionality of space. Out-of-equilibrium systems typically deviate from this with an exponent $\alpha > d$, leading to giant number fluctuations (GNFs), which are often considered to be a hallmark of active matter. The opposite behaviour corresponds to systems exhibiting suppression of number fluctuations relative to the equilibrium situation. In this case, $\alpha < d$, and the system is said to be hyperuniform (HU) [1].

HU systems have been extensively studied via the mathematical analysis of point configurations and have been observed in cellular layers, driven particles, jammed packings, and even vortices in type II superconductors [1]. In our work, we report hyperuniformity in a system of topological defects in an active nematic formed by microtubule filaments and kinesin-streptavidin motor proteins [2]. While the observation of hyperuniformity is itself exciting, our work is more significant as these active particles self-propel and explore the available phase space, subject to defect-defect interactions and creation-annihilation events, all while still exhibiting HU as an intrinsic property. We perform experiments with the active nematic in 2D flow cells, imaged by fluorescence confocal microscopy, and identify the defect charge and positions over time via our image analysis algorithms. This system of active defects has been shown to develop short-range correlations without any global order, with features independent of defect density [3]. We then quantify the HU exponents in experimental data and achieve good agreement with numerical simulations. Using a theory based on active-vs-absorbing state phase transitions, we rationalize these effects and understand the origin of hyperuniformity in such an active system, one we believe to be the first complete attempt in this regard. We show that the active recycling of defects via creation-annihilation events, combined with defect-defect interactions and subsequent unbinding, causes likesigned defects to spread out more than uniform points, thus in effect, hyperuniformizing the entire system continuously over time.

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Searching for the Biaxial Nematic Liquid Crystal Phase: A Journey Between Molecules and Colloids

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Liquid crystals represent a fascinating family of materials with physical properties that lie between those of liquids and crystalline solids. They flow like liquids, but their components—molecules or colloidal particles, generally defined as mesogens—exhibit an ordered spatial distribution reminiscent of crystalline structures. When this order is primarily orientational, with mesogens aligned along a common direction, nematic phases are observed. In contrast, more complex phases, such as smectic or columnar, form when a degree of positional order is added in one or two dimensions.

Of particular technological and fundamental interest are liquid crystals formed by mesogens with significantly more sophisticated geometries than disc-shaped or cylindrical molecules or particles. Cuboidal, ellipsoidal, or banana-shaped mesogens, generally defined as biaxial, have a broader spectrum of positional and orientational degrees of freedom, leading to rich phase behaviour often predicted by theory and later corroborated experimentally. However, despite these theoretical advancements, achieving a rigorous and precise agreement between predictions and experimental observations remains challenging. The case of the biaxial nematic (N_B) phase is a prime example of this ongoing quest.

Colloidal cuboids, in particular, demonstrate especially rich phase behaviour and the potential to self-assemble into N_B liquid crystals [1, 2, 3]. Over the past few decades, numerous theoretical studies have predicted a wide region of the phase diagram where biaxial nematics would be stable. However, these studies often impose strong constraints on the particle rotational degrees of freedom, artificially enhancing the stability of the N_B phase [4, 5, 6]. In this contribution, we present simulation results that elucidate the conditions necessary for the formation of N_B liquid crystals at the colloidal scale [7, 8]. Furthermore, we use these findings to guide our investigation into the existence of biaxial nematics at the molecular scale, presenting the results of our molecular simulations [9].

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ANCHORING TRANSITION OF A SMECTIC FILM AND PATTERN FORMATION OF FOCAL CONIC DOMAINS IN LIQUID CRYSTAL FLOW CELL GEOMETRY

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Liquid crystals (LC) are anisotropic fluids composed of elongated organic molecules (mesogens) that tend to align along a common director, **n**, and displaying a number of mesophases. After a phase transition or the application of an externally imposed stimulus, reorganization of molecular order usually leads to the formation of topological defects, either as kinetically trapped metastable objects or as components of free energy-minimizing configurations [1]. Understanding and controlling defects in LCs is important to many technological applications.

The most common LC phases are the nematic (N) and smectic A (SmA). In the first one mesogens preserve only the orientational order characterized by a director field. The SmA phase possesses a density wave resulting in a layered structure, where **n** is normal to equally spaced smectic layers, thus this phase preserves both orientational and translational order. In the presence of an interface, the spatial symmetry of N LC breaks, and the surface influences the orientation of its director field. This phenomenon is known as anchoring of LC on a surface. The chemical composition and the structure of the surface determine preferred anchoring directions for the LC molecules, both with respect to the surface normal and to an in-plane projection. Changing of the molecular anchoring is named anchoring transition. This phenomenon has been studied mostly in nematic films, and there are only few reports of anchoring transitions in a smectic film formed either between two soft (water and air) [2] or two solid interfaces [3].

In this work we present a new approach to create thin, relatively large and flat films of 8CB LC enclosed between solid (glass) and fluid (water solution) interfaces, where the LC anchors homeotropically and planarly, respectively. Upon cooling, the N-SmA phase transition takes place, accompanied by a drastic reorganization of the director field geometry and formation of focal conic domains (FCDs) [4]. These events are followed by an anchoring transition in which the SmA layer changes from planar to homeotropic at the water interface, leading to the disappearance of the FCDs. By locally removing

regions of the hydrophobic silane coating from the glass surface, we create the regions, where FCDs anchor and persist during said anchoring transition. Such a simple way of controlling the spatial arrangement of FCDs may be used in applications based on regularly ordered micro- and nanosystems [5].



Figure 1 – Temperature driven anchoring transition in 8CB LC resting on the top of an active gel inside a flow cell.

Besides, relaxation towards the final pattern of FCDs can be expedited by the local stirring of the aqueous subphase, which we have realized here using an active gel of microtubules and kinesin motors.

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ORAL Contributions

Session on Drops, Vesicles, Cells and Grains

Effect of Particle Shape on the Flow of an Hourglass

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The flow rate of a granulate out of a cylindrical container is studied experimentally and numerically as a function of particle shape for flat and elongated ellipsoids. We find a nonmonotonic dependence of the flow rate on the grain aspect ratio. Starting from spheres, the flow rate grows and has two maxima around the aspect ratios of $a/b\approx 0.6$ (lentil-like) and $a/b\approx 1.5$ (ricelike). For even more anisometric shapes, the flow rate drops. Interestingly, particles with slightly nonspherical shapes not only form a better packing in the silo but also move faster through the orifice than spheres. We also show that the resistance of the granulate against shearing increases with the aspect ratio for both elongated and flat particles; thus, the change in the effective friction of the granulate due to changing particle shape does not coincide with the trend in the flow rate. To our knowledge, no systematic experimental tests have been performed to measure how the discharge rate changes with particle shape when all other parameters (surface roughness, density, hardness, etc.) are identical.



Fig. The experimental setup and a snapshot of the 3D numerical simulation

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Fluid Dynamics of a Respiratory Droplet in the Context of Viral Dynamics.

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The COVID-19 pandemic highlighted important knowledge gaps in the airborne propagation of pathogens. A fundamental question, with important applications in the development of disease transmission models, is where are virions found inside the dry residue of respiratory droplets [1].

By means of experiments and simulations, we shed some light on this complex microfluidic transport problem. We evaporate sub-microliter respiratory-like droplets in a humidity-controlled chamber to measure simultaneously the velocity field inside the droplet (using particle tracking methods) and the evaporation rate. We use these experimental measurements to validate our theoretical and numerical framework quantitatively. We use this model to predict the morphology and chemical composition distribution of the drop residue once the different phases have segregated at the end of the evaporation process. Our model agrees with preliminary experiments using fluorescence microscopy.



Figure 1. Panel a) displays a respiratory-like droplet inside a humidity-controlled chamber. Panel b) presents a fluorescent image of the residue from a respiratory droplet. Panel c) shows the experimental radial velocity measured with particle tracking. Panel d) presents a snapshot of our simulations. We present, in dimensionless units, the radial velocity inside the droplet and the vapour concentration outside the droplet.

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MEMBRANE-ENABLE TRANSDUCTION OF INTERNAL FLOWS INTO VESICLE MOTION

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Cytoplasmatic streaming is key in the biological functions of cells, including the circulation and mixing of nutrients or organelles, as well as cell motility. The self-contained nature of cytoplasm fluid mechanics within the cell membrane makes its character complex, and a detailed physical description of the coupling between them remains elusive. Therefore, we constructed a minimal cell model, using droplet-microfluidics [1], to measure and explore the connection between confined flows and the mechanical properties of the cell membrane. The model consists of a single ferromagnetic microparticle encapsulated within vesicles with variable membrane compositions, as illustrated in Figure 1. Under the actuation of an external rotating magnetic field, we study the dynamics of the rotating particle enclosed within the vesicle. We show that the interaction of particle and vesicle, mediated by the flows generated by the rotating particle, depends on the membrane's mechanical properties. Moreover, we show that such flows can induce conformational changes in phase-separated membranes. Finally, the hydrodynamic coupling between the particle and the vesicle results into vesicle rotation, enabling it to roll on a substrate. These observations may have implications for the development of motile vesicles that leverage frictional forces to accurately target specific locations.



Figure 1: schematic representation of the experimental set-up.

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Active flow networks and their complex dynamics

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Flow networks are essential to understand systems such as the animal and plant vasculature, or the power distribution network. In this project we present a system including active elements that can pump fluid (active pores [1]) and regions that can accumulate volume (elastic reservoirs). We use a flow network including nodes and connections as a phenomenological model [2–3] to understand our active flow network. We show numerically how as the system evolves, a soliton-like structure emerges spontaneously from a disordered system. Time permitting, we will discuss how the continuum limit of the system allows us to understand its behaviour analytically.

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A MATHEMATICAL AND COMPUTATIONAL MODEL TO STUDY THE ROLE OF THE EXTRACELLULAR MATRIX DURING MORPHOGENESIS

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During vertebrate heart morphogenesis, an internal structure of muscular ridges develops in the ventricles. This structure, called trabeculae, helps the heart to properly pump blood to the rest of the body and is formed from the delamination of myocardial cells at early stages of development. One of the key components of this process is the dynamics of the extracellular matrix, also known as cardiac jelly, located between the myocardium and endocardium layers during embryonic development. Besides its viscoelastic properties, the cardiac jelly's thickness inhomogeneities during these stages are crucial for correct development. Experimental data in zebrafish have shown a strong correlation between these inhomogeneities, or fractures, and the process of delamination that forms the internal structure of the heart's ventricle.

In this study, we introduce a detailed mathematical model to describe the dynamics and damage of the cardiac jelly. Our model captures the intricate interplay between its elasticity, viscosity, time-dependent deformation, and material damage. This approach allows us to delve deeper into the physical properties that govern the cardiac jelly's behavior during embryonic development. We solve our physical model using a higher-order finite element method, in which we simulate a 3D reconstruction of the geometry of the heart in which the cardiac jelly lies and captures the real geometry of the system. The main application of our model is to investigate fracture generation within the cardiac jelly and enables us to study the generation of fracture patterns depending on the geometrical and material properties of the system and to compare our results with experimental observations in zebrafish embryos.

Posters

IONIC SELF-PHORESIS MAPS ONTO CORRELATION-INDUCED SELF-PHORESIS

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Self-phoresis denotes the motion of a force-free particle under the action of a self-generated gradient (in chemical concentration, temperature, or other thermodynamic field). Self-phoretic particles have become a customary experimental realization of an artificial swimmer, whereby the catalytic activity of the particle's surface induces concentration gradients in the surrounding solution.

We address the self-phoresis of a particle that releases pairs of ions into an electrolyte solution [1]. We show analytically that, in the linear regime, the mathematical description of this system maps onto that of the recently proposed mechanism of correlation–induced self-chemophoresis of neutral solutes [2]. This connection blurs the distinction between phoresis in electrolytes and in non-electrolytes, respectively, providing a unifying perspective of the two phenomena: what matters is a non-vanishing range of the solute-solute interaction, regardless of whether electrostatic or of any other kind.

One recovers and extends recent predictions in ionic self-phoresis as particular instances of the correlation– induced chemophoresis. Conversely, ion-phoretic particles are identified as candidates for experimental investigations into the rich variety of motility patterns predicted by the theoretical model of correlation-induced chemophoresis.



Phoretic diagram. The source of phoresis is a gradient, either externally imposed or selfgenerated. The mechanism responsible for a non-vanishing drift velocity of the particle is either the solute interaction with the particle (adsorption) or the solute-solute interactions (correlations).

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DEPLETION FORCES IN DIPOLAR POLYMER BRUSHES AND DIPOLAR COLLOIDAL SYSTEMS: EXTERNAL FIELD MODULATION OF SYSTEM PROPERTIES

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In this contribution we show via Langevin Dynamics numerical simulations how the properties of both dipolar polymer brushes and dipolar colloidal solutions can be strongly modulated through external applied fields. In the case of dipolar polymer brushes external fields can be used to modify force profiles and favor the entrapping and retention of colloidal particles inside them for a later release [1]. Alternatively, by choosing right external field strengths it is also possible to develop force barriers that prevent colloidal particles from reaching the surface where polymers forming the brush are attached. In the case of solutions of dipolar colloids, external applied fields can be used to modify the depletion force profiles among two large non-dipolar particles immersed in the dipolar solution. The modulation of the orientation and strength of the external field allows the possibility to use these suspensions as funneling tools to create aligned clusters of non-magnetic colloidal particles, colloidal tweezers able to control the distance between two large colloidal particles, and ratchets [2].

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Walls and boojums in nematic toroidal droplets

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Liquid crystals, including nematic liquid crystals, allow studying the fascinating world related to topological defects, which can be characterized by their dimensionality into point defects (0D), disclination lines (1D) and walls (2D). While point defects and disclination lines can be observed in most systems, wall defects are unstable and most commonly split into disclination lines. Non-singular walls, called alignment inversion walls [1], can nevertheless form in the presence of magnetic or electric fields. They are also usually either unstable or metastable requiring of external fields to introduce the energy barrier required for their stability.

Topological defects can be forced by confining the nematic liquid crystal with boundaries having non-trivial geometries and topologies and certain imposed anchoring conditions. In nematic droplets or shells with parallel anchoring, defects are necessary as demanded by the Poincaré-Hopf index theorem [2]. When confining a nematic liquid to a toroidal droplet with planar anchoring, this same theorem allows defect free configurations which have been observed in previous work [3]. Interestingly, when melting the nematic into the isotropic phase, and after cooling back to the nematic phase, stable defect-populated configurations consisting of pairs of ± 1 boojums appear and are stabilized by the high energy barrier that must be crossed to transition to the defect free state [4].

In the presence of magnetic fields, parallel anchoring, and for the cases with and without prior defect pairs in our nematic toroidal droplets, we find that stable alignment inversion walls form. These walls are not metastable, but rather equilibrium states of the toroidal droplet under a magnetic field. Moreover, we observe different types of walls and the evolution of one into the other as a result of the mobility of the boojum pair. Our results also illustrate how to move defect pairs using magnetic fields by means of the movement of a wall, and how to generate nematic tori with a controlled number of defect pairs.

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SOFT MATTER FOR BIOTECH APPLICATIONS: MICROFLUIDIC GENERATION OF CHITOSAN GELS FOR BIOLOGICAL PEST CONTROL

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Our collaboration with biotech company Agrobio focuses on developing a scalable method for producing spherical polymer gels that can serve as containers for liquid diets used to feed insect predators in intensive biological pest control. These gels, made from chitosan, are designed to be monodisperse in size and structure, ensuring consistency in application.

In the initial phase of the project, we developed a single-injector microfluidics setup to produce spherical chitosan gels polymerized under UV light. The gels were shown to significantly increase the life expectancy of the biological predators when used as containers for their diet, marking a significant step toward an efficient and cost-effective method for mass-producing them.

Building on this success, our current research involves scaling up the production process. We are developing a parallelized, multi-injector system that can operate at higher flow rates to produce larger quantities of gels simultaneously. This work is centered around optimizing the design of a lab-scale prototype, which includes multiple custom-made components created with 3D printing. Key aspects of this effort involve refining the injector assembly and conducting extensive tests to ensure consistent drop formation across multiple injectors.

Additionally, to best serve their purpose, the gels must sufficiently retain water and have the right mechanical properties. We have studied water retention over time, which is essential for maintaining the viability of the diets during shipping and storage of the predators, and optimized their mechanical rigidity, to ensure they are soft enough for predators to consume the diet while rigid enough to withstand transport. This talk will summarize our results in this project.

Self-Assembly of Active Bifunctional Patchy Particles

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Colloidal self-assembly represents one of the most exciting topics in soft matter. In this context, activity emerges as a powerful tool, as it gives rise to a remarkable range of interesting collective behaviors. While most research on active colloidal matter has focused on suspensions of active particles interacting via isotropic potentials [1], the field has recently branched out to explore the interplay between activity and anisotropic interactions [2]. Considering the "patchy particle" model as a practical model to study anisotropic interactions [3], we intend to investigate a system made of active patchy particles that form linear chains [4].

With the intent of exploring the polymerization of active patchy particles in linear chains, we study a twodimensional suspension of active bifunctional Brownian particles (ABBPs).

At all studied temperatures and densities, ABBPs self-assemble in aggregating chains, in contrast to the uniformly space-distributed chains observed in the corresponding passive systems [4]. The main effect of activity in the system, other than inducing chain aggregation, is to reduce the average chain length and to increase the probability of two ABBPs to bond with the same orientation.

Interestingly, at the lowest temperature studied, as density increases, we observe a novel state, which we term MIPS (Motility-Induced Spiral Phase). In this state, chains aggregate to form spirals characterized by a finite angular velocity, as illustrated in the left panel of Figure 1. On the contrary, at the highest temperature, density, and activity chains aggregate forming a different novel state characterized by a compact and hexagonally ordered structure, both translating and rotating (right panel of Figure 1). The rotation arises from an effective torque generated by the presence of competing domains where particles self-propel in the same direction.



Figure 1 – Steady state configurations of the investigated system: MISP (left panel) and spinning crystal (right panel).

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ROLLING REBELS: COUNTERACTIVE TRANSPORT OF MICROROLLERS IN AN OBSTACLE LATTICE.

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The ability to control transport at the microscale is crucial for a variety of applications, from controlling bacterial flow for mitigating infection risks to navigation of microrobots for micro-surgical and drug delivery purposes. Microrollers, which are microscopic particles driven into rolling motion by an external field, are viable candidates for such transport purposes since they can be driven in a non-invasive manner. However, in the case of complex microscale environments, such as in biologically relevant systems, accurately steering microrollers is challenging due to hydrodynamic interactions between the microroller and the surrounding environment. In our work, we use an ordered obstacle array as a model system and study the dynamics of a microroller suspended between the obstacles (See Fig 1 a & b). We observe a counterintuitive phenomenon: under certain conditions, the microroller traverses the lattice in the opposite direction of its rolling motion (See Fig. 1 c). We show that a microroller's direction of motion depends on its size, height above the surface, and the distance between the obstacles in the array. Our findings offer critical insights into precise control over microroller dynamics and could be implemented to design strategies for steering microrollers in more complex and biologically relevant systems, advancing applications in targeted drug delivery and microscale transport.



FIG. 1: (a) & (b) Top-down and side views of the obstacle post array. (c) Schematic of the experimental system - a microroller suspended on a substrate comprising an ordered obstacle array, moving in the opposite direction to its rolling motion. (d) Microroller trajectories inside and outside the the obstacle array, showing motion in opposite directions.

OPTIMAL TRANSPORT OF ACTIVE COLLOIDS THROUGH DEEP REINFORCEMENT LEARNING

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Transport multitude biological of active driven particles plays crucial role in of processes ranging from or а а all systems electrons solids. In is controlled structure and properties of the to in these systems transport by the environment. То achieve controlled transport these particles must respond to their environment Our goal is to emulate this hiahly efficient systems that are often found in nature. Therefore. we propose to optimize the transport properties of surface-enabled micro-robots in complex environments. empowering them with sensina capabilities

system Specifically, active rotating spinners, containing our consists of particles, or on substrate of а arravs fixed obstacles. The spinners can only translate in 2D along the plane perpendicular to their rotation. In square lattices, steady-state obstacle constant angular different spinners rotating at frequency are trapped in one of two trajectories. but time modulation of that frequency can break this confinement. achieving transport. We use а coarse-grained the (DRI) hvdrodvnamics model of spinners and deen reinforcement learning techniques to train a neural network and find the optimal frequency modulation to achieve ballistic in variety situations transport а of ranging from an ordered square obstacle lattice to disordered obstacle arravs: or free and fixed transport direction goals

available Although the training the neural network uses simulations. the input data is also our of on will experimental setup through real-time tracking of the spinners and obstacles. We that work open expect our new possibilities for the control of driven colloids and the study of the effects of complex environments on active and driven colloid transport.



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: optimal policy to achieve ballistic transport in the +y direction in a square obstacle array. The colour represents the optimal rotational frequency of the spinner at every point of the unit cell. The white circles represent obstacles.

Protein-mediated adhesion of polymer vesicles.

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Keywords: Microfluidics • Vesicles • Proteins • Adhesion

Cell adhesion is a widely observed feature during tissue development. While at the molecular scale, this phenomenon involves the precise coordination of numerous protein interactions, at the cellular scale, adhesion relies on membrane mechanical properties enabling cellular global shape changes from an unbound state to the bound state. To understand the importance of the elastic nature of membrane deformation upon adhesion, we design a minimal experimental model consisting of microfluidic produced polymer vesicles capable of interacting with avidin proteins. This polymer-protein interaction promotes the adhesion of vesicles to protein coated glass surfaces. The interplay between the number of proteins and the excess membrane available, let us explore different vesicle adhesion regimes, and therefore, gain physical insight into this polymersome-protein system that can further be used as the building blocks of a synthetic tissue-like material.



Figure 1. Confocal images of the vertical cross sections of a vesicle in a) the strong adhesion regime, and b) the weak adhesion regime. Polymer membrane is fluorescently label with DOPE-Rh and protein coating is fluorescently with FITC. Scale bars are 100 µm.

CAPILLARY INSTABILITIES AND HYSTERESIS OF MULTIPHASE FLOW IN DISORDERED MEDIA

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Two-phase fluid displacements in porous and fractured materials occur through the invasion of individual pores or gap openings, often driven by sudden interfacial motions caused by capillary instabilities. These localized jumps lead to fluid rearrangements, which can trigger further instabilities, creating cooperative, spatially-extended fluid avalanches known as Haines jumps. These irreversible events result in large-scale hysteresis, with significant implications for various natural and engineering processes, such as soil irrigation, carbon sequestration, and oil recovery.

Current models for pressure-saturation hysteresis cycles at large scales typically rely on phenomenological or semi-empirical approaches. In contrast, we present a model based in the physical principles of local pressure balance at the fluid-fluid interface. The model resolves a sequence of equilibrium configurations corresponding to local energy minima. Numerically, this is implemented using simple, synchronous rules that offer high computational efficiency. All the parameters involved have physical meaning and can be measured experimentally. The model and the results from our simulations are validated against laboratory experiments of quasi-static displacements in a slightly inclined Hele-Shaw cell with variable depth, an experimental analogue of a rough fracture where the stabilizing effect of gravity suppresses viscous fingering.

Our approach offers a physically grounded description of the nonequilibrium, metastable nature of multiphase flow in porous and fractured media, as well as the memory effects associated with partial wetting-dewetting cycles.



Figure 1 – LEFT: Schematic of the model and its experimental realization. RIGHT: Simulated and experimental Pressure-Saturation cycles in terms of external head H and wet area Sw in the imperfect Hele-Shaw cell shown in the left panel.

E. COLI MOTION IN DOUBLE EMULSION DROPLETS

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E. coli is a prototypical microswimmer and a model organism widely used in the study of bacterial motility and biofilm formation [1]. *E. coli* microswimmers accumulate near solid flat surfaces [2], and at the oil/water interface when encapsulated in aqueous drops with diameters smaller than the bacteria persistence length [3]. At high bacteria densities, they exhibit collective turbulent-like motion, capable of propeling the drops [4]. The behavior of *E. coli* in larger droplets and lower densities remains unexplored. Here, we study this regime to understand the principles driving the formation of bacteria clusters, which could potentially inform about the initial steps of biofilm formation. For this, we culture *E. coli* W3110 (wild type) bacteria, containing the pBTCherry plasmid that encodes the expression of the red fluorescent protein mCherry, and encapsulate them during the stationary phase, when their pathogeneity increases, in water/oil/water double emulsion drops using microfluidics. The drops are then confined between two flat glass slips separated (25 ± 1) µm, forming oblates with radii ranging from 10 to 70 µm. We then use epi-fluorescence microscopy to track the motion of the individual bacteria at the oblate equatorial plane under these confinement conditions (Figure 1). This approach enables capturing the rich dynamics of bacterial suspensions, including scattering events with other bacteria or the interface, which could help understanding bacteria accumulation near walls and biofilm formation.



Figure 1. Equatorial plane of an oblate drop with a radius of 68 μ m. **a**) Bright-field image; **b**) epifluorescence image; **c**) overlaid temporal sequence of epifluorescence images acquired during 30 s; **d**) instantaneous velocity profile, with an average velocity of (7 ± 3) μ m/s.

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DISSIPATIVE SELF ASSEMBLY OF FTSZ OVER CONFINED LIPID BILAYERS

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FtsZ is a protein directly involved in bacterial cell division. This study observes the behavior of FtsZ under twodimensional confinement and lateral spatial restrictions as an alternative to the three-dimensional confinement FtsZ is exposed to within a bacterium. We developed two protocols to restrict this lateral movement of the protein in bilayers containing a lipid mixture of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) with 5% Nitrilotriacetic acid (NTA). The first protocol is based on creating micrometer-sized corrals using bovine serum albumin (BSA) / Polyethylene Glycol (PEG)-impregnated seals on pre-cleaned glass, then introducing the bilayer into these corrals and subsequently adding the FtsZ protein [1]. The second protocol involves generating bilayer islands using a solution of Giant Unilamellar Vesicles (GUVs) [2] at very low concentration on an



Figure 1 – Corral where FtsZ has been deposited, illustrating the opening new avenues for FtsZ confinement intention to completely "trap" FtsZ between the walls of our corrals.

atomically flat mica surface [3]. Once FtsZ exposed to this two-dimensional is restriction, we studied its behavior in confined spaces through observation with Atomic Force Microscopy (AFM) [4]. The results obtained represent an advance in the FtsZ confinement protocol [5], although we encountered significant challenges, especially in the first process. Furthermore, the confinement allowed us to observe distinct behaviors in the folding and distribution of FtsZ. These observations suggest the capacity of FtsZ to modify and generate NTA patches in the fluid bilayer,

methods and the development of protocols that will improve our understanding of how FtsZ behaves in the bacterial membrane,

contributing to the understanding of bacterial division mechanisms and the potential design of future antibiotics.

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Polymer Informatics Tools for Sustainable Polymers and 3D printing

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Biodegradable polymers are intended to replace the synthetically produced polymers, however, their wider usage is limited by their moderate thermal and mechanical properties. In order to elucidate the structureproperties-performance relationship of these materials, we design a bottom-up approach, combining multiple computational tools, with the ultimate goal to facilitate their characterization and property optimization during the additive manufacturing. We use the poly(lactic acid) (PLA) as the model polymer, which due to its chirality and wide popularity in 3D printing represents an ideal candidate to test the developed methodology. In the first stage of the bottom-up approach, we produced an extensive data set consisting of atomistic trajectories of different stereoisomers of PLA in melt. We used those data to build a chemistry-specific coarse-grained (CG) model to extend the time and length scales to those relevant in the experimental studies. In addition, to close the loop, we implement a machine-learning based methodology to reinsert the atomistic details into CG models of different stereochemistry [1]. Since the computational techniques are considered to be a more sustainable alternative to the experimental characterization, we aim to extend the simulation practices commonly used for synthetic polymers to more complex bio-based polymers. By combining different computational techniques, we provide a consistent set of open-access tools [2,3] with the ultimate goal to facilitate the usage of multiscale computational analysis in the fast-growing field of biodegradable materials and additive manufacturing.



[1]A Physics-informed Deep Learning Approach for Re-introducing Atomic Detail in Coarse-Grained Configurations of Multiple Poly(lactic Acid) Stereoisomers, E. Christofi, P. Bačová, V. Harmandaris, Journal of Chemical Information and Modeling, 2024 64 (6), 1853-1867 [2]https://github.com/SimEA-ERA/PLA-BackMap-CG [3]https://github.com/pbacova/ PLA analysis tools.git

Figure 1 – Schematic illustration of the implementation of the computational tools

Transient motion of a Eutectic Indium-Gallium drop inside a capillary subject to an oscillatory voltage

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Gallium alloys are liquid at ambient temperature. This makes these materials ideal to build electronic devices that need to change their configuration while in service (e.g. liquid antennas) or that need to sustain large deformations (e.g. biomedical wearables). Continuous electrowetting allows the manipulation of liquid metals using low voltages (around 1 V) without the need of mechanical pumps. While it is relatively simple to estimate the speed at which a drop translates in steady state [1], there is no theory to determine how fast a drop responds to a change in the excitation voltage. This is a crucial piece of information as, in small electronic devices, what limits the time it takes to reposition a drop is not the steady speed that it can reach, but rather how fast it responds to a change in the excitation voltage. To the best of our knowledge, there is no theory based on first principles to describe the transient motion of liquid metal drops. Such a theory is much needed in the design, for instance, of liquid-metal antennas [2]. With this motivation, we carry out an experimental and theoretical investigation on how fast a long drop of Eutectic Indium-Gallium alloy (EGaIn) immersed into a long capillary tube responds to an oscillatory excitation voltage (Fig. 1a). Using this canonical configuration we sideline the geometrical complexity found in real applications, which allows us to focus on the physical mechanisms at play during the transient motion of the drop.





When a current flows through the liquids inside the capillary, the caps of the drop act as capacitors [3], that is, a charge double layer is created on them. The presence of the charges reduces the surface energy which, in turn, lowers the surface tension as predicted by Lippmann's law. The fact that the current flows asymmetrically on both ends of the drop (from buffer to metal in one cap and from metal to buffer in the other) creates an imbalance between their surface tensions. This translates into a capillary pressure gradient inside the drop that drives the flow. We model the flow driven by the resulting oscillatory pressure gradient using an equation similar to that proposed to describe the transient imbibition of a liquid in a capillary [5]. We characterize experimentally the equivalent electrical circuit without drop (electrodes plus buffer). Also, the physical properties of EGaIn are taken from the literature [4]. Thus, our theory has no free parameters.

Fig. 1b displays the peak velocity reached by the drop in every oscillation, V_{max} , as a function of the excitation frequency for two different voltages E_0 . The theory predicts that at a critical frequency (around *f*=1 Hz) the liquid inertia becomes comparable to viscous friction. At lower frequencies viscous friction dominates and the velocity becomes independent of the frequency. Conversely, as the frequency increases, inertia dominates, which causes the drop to stop responding to the electric current. We show that $V_{max} \sim f^{-1}$ in this regime, akin to the behavior observed in the so-called Womersley flow. These results are essential to understand how fast we can displace an EGaIn drop in a capillary using electrowetting. Moreover, it provides researchers and electronic engineers with a simple theory to predict how fast liquid metal drops can be manipulated.

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Sampling from athermal suspensions: averages, distributions and fluctuations

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Statistical physics works perfectly well at equilibrium to provide results for the averages and fluctuations of observables in the thermodynamic limit. However, working out of equilibrium and very far from the thermodynamic limit can be challenging when attempting to control the averages of observables accurately.

In this study, we aim to address the extent to which it is possible to obtain a good estimate of the average particle number concentration in athermal suspensions by performing only a few sampling measurements of certain volume in situations a priori not far from equilibrium.

Our control parameters are the volume fraction of beads, ϕ , and the sampling volume, V_s , using a pipette. We take six aliquots from the entire sample, which was assumed to be in a homogeneous state, and measure the number of beads, N_s , in each aliquot. We then quantified the average over aliquots $\langle N_s \rangle$ and the mean squared fluctuations, $\sigma_{N_s}^2 = \langle N_s^2 \rangle - \langle N_s \rangle^2$. By plotting $\langle N_s \rangle$ as a function of ϕ for a given V_s , we expected to obtain a linear relationship since $\langle N_s \rangle = \frac{V_s}{v_{beads}}\phi$. However, for all the V_s tested, our results did not show a linear relationship between $\langle N_s \rangle$ and ϕ , but rather an affine relationship $\langle N_s \rangle = a\phi + b$. The intercept, b, could be assumed to arise from fluctuations relative to the homogeneous state. Additionally, the measured slope, a, was consistently well below the expected theoretical value.

By implementing a minimal numerical model to sample a homogeneous state from a Poissonian process, we concluded that the deviation of the slope could be due to skewed noise in the particle measurement.

Repeating similar measurements in more controlled experimental setups would likely be more informative for understanding the estimation of macroscopic averages of observables far from the thermodynamic limit.

Swelling of ionizable alginate hydrogel under the presence of NaCl and $CaCl_2$ salts

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Alginate-based hydrogels are highly versatile. Due to their bio-compatibility, these gels have many applications and are used, for example, in the pharmaceutical industry and in molecular gastronomy. They are ionic gels and can swell and deswell in interesting ways in the presence of various types of salts. Opposed to traditional belief, alginate gels remain stable when stored in ultra-pure water. We here report on work with three type of gels –capsules made in the absence and presence of sodium dodecyl sulphate (SDS), and spherical gels– in the presence of various [CaCl2], [NaCl] and pH. The behavior is consistent with that of permanently cross-linked ionic gels, with no signal of gel degradation. Our results thus suggest that cross-linking in these gels is not ionic, contrary to what one often finds in the literature.

Probing the dynamics of responsive microgel with respect to concentration with 3DDLS techniques

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Abstract

The dynamics of a microgel suspension is highly dependent on its particle concentration, as well as particle size and softness. We perform 3D dynamic light scattering experiments with a system consisting of NIPAM and AAc (crosslinked with pEG-d) at a temperature and pH range to analyze its swelling behaviour. Next, we focus on its relaxation time dependence with concentration. At higher concentrations, two different time scales show up, associated to a diffusive and a structural relaxation regimes. This shows up as a two step decay, the second of which is modeled through a stretched exponential. We analyze the dependence of the structural relaxation time, τ_{α} , as well as the stretching exponent as the particle concentration increases above the glass transition.

UNSTEADY EMPTYING OF A CAPILLARY: A MODEL SYSTEM FOR SPLAT PAINTING

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In art, splat painting consists in accelerating a paint-loaded brush (for example by "flicking" it or tapping its handle) to detach paint filaments or droplets. These are projected onto the canvas, leaving aesthetic filamentary or spotty patterns (Fig 1a). In previous work, we characterized experimentally how the amount of paint detached and its final spatial distribution on the substrate depend on liquid viscosity and brush acceleration. Ultimately, these quantities of artistic interest depend on the flow in the bundle of bristles, which is very hard to measure directly in a real brush. To shed light on those flow regimes, we perform new experiments on a simplified system, consisting of a flexible capillary tube clamped at the tip of a rigid rod (Fig 1b). This model geometry – representing one pore in the actual bundle – has two main advantages. First, it allows us to track in real-time the liquid front in the capillary, and thus to correlate its motion to the time-varying acceleration imposed to the brush. Second, the simplified geometry makes it possible to aim at one-to-one comparison with an analytical model we develop for the unsteady emptying of a capillary. Together, experiments and theory reveal the subtle role of surface tension in different flow regimes observed with the real brushes.



Figure 1 – (a) Artwork based on splat painting by Caroline Champougny. "Sunday Afternoon" (acrylic paint on paper, 15 x 20.5 cm), 2022, used with permission. (b) Liquid ejection caused by an impact on brush handle for a round commercial brush loaded with a 20% glycerol/water mixture (top), and for a "simplified brush", made of a flexible capillary tube of internal diameter 0.2 mm, filled with water (bottom).

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Exploring microfluidics for the development of controlled microfabrication of blood clot

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The pursuit of enhanced drug testing for the treatment of diseases has led scientists to develop methodologies for delivering drugs into controlled and localized spaces. Blood-like substances have shown promise as noninvasive solutions [1]. Although individual blood cells have been investigated as drug carriers for various treatments, they face challenges in terms of drug release, targeting, and production. An alternative approach involves the use of blood clots as carrier entities by exploiting their natural formation process [2]. Recent studies have examined in vitro coagulation processes [3]. However, these investigations have neglected important factors, such as blood clot dimensions and composition, which are crucial for developing new controlled materials. Microfluidic mixing technologies enable mass transport governed solely by diffusion, allowing reactions to occur in a non-convective transport environment [4]. The application of these technologies permits the creation of products of various shapes and structures through controlled mixing [5]. In this study, we demonstrate a microfluidic method that effectively controls blood clot size and structure using a 5 inlet Y-junction-like device. Homogeneous and heterogeneous blood clots were constructed following our approach, highlighting the versatility of manufacturing clots using microfluidic approaches.

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The actin cytoskeleton is remarkably adaptable and multifunctional. It often organises into nematic bundles such as contractile rings or stress fibres. However, how a uniform and isotropic actin gel self-organises into dense nematic bundles is not fully understood. Here, using an active gel model accounting for nematic order and density variations, we identify an active patterning mechanism leading to localised dense nematic structures. Linear stability analysis and nonlinear finite element simulations establish the conditions for nematic bundle self-assembly and how active gel parameters control the architecture, orientation, connectivity and dynamics of self-organised patterns. Finally, we substantiate with discrete network simulations the main requirements for nematic bundle formation according to our theory, namely increased active tension perpendicular to the nematic direction and generalised active forces conjugate to nematic order. Our work portrays actin gels a reconfigurable active materials with a spontaneous tendency to develop patterns of dense nematic bundles.

WHAT SCULPTS VASCULAR NETWORK ORGANIZATION? FLOW VS. SHAPE

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Vascular networks exhibit remarkable diversity in both flow patterns and structural shape across living systems. Understanding the intricate coordination between vascular architecture and flow dynamics is essential for uncovering the mechanisms that drive development and adaptation. Studies have demonstrated that blood flow modulation, shear stresses within vessels, and interstitial flows within influence vascular tissues can development. remodelling, and regression in a tissue-specific manner [1-3]. However, the roles of external flows outside blood vessels and the shape of the surrounding tissue architecture in governing these processes remains poorly understood. In two separate studies using the chick chorioallantoic membrane model, we revealed that both external fluid flows [4] and the geometry of surrounding tissues [5] play active roles in directing vascular development, remodelling, Computational models further and regression. confirmed that these vascular changes are predominantly driven by mechanical forces that are induced by external flows and shapes.



This unprecedented approach offers a powerful predictive framework for unravelling the complex interplay between structure and function in vascularization processes, with potential applications in modeling both healthy and pathological conditions.

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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 [7,8]. 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 [9], including the non-universality occurring in 3D arising from interfacial fluctuations. Using the numerical nonlinear renormalization group [10] 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.

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EXACT EQUILIBRIUM PROPERTIES OF HARD-CORE DISKS IN SINGLE-FILE CONFINEMENT

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Experiments with confined quasi-one-dimensional colloidal liquids have revealed the presence of an attractive potential well in the effective colloid-colloid interaction [1]. However, a clear methodology to study both thermodynamic and structural properties of confined fluids with that kind of interaction potential from a theoretical point of view is still lacking.

In this study, we present exact thermodynamic and structural analyses of highly confined square-well and square-shoulder disks. Utilizing a novel mapping technique, we transform the original system into a onedimensional polydisperse mixture of nonadditive rods [2]. This approach enables the derivation of all confined system properties using standard liquid theory applied to its one-dimensional counterpart. Key properties including the equation of state, internal energy, radial distribution function (illustrated in Fig. 1), and structure factor are obtained. Moreover, this technique facilitates exploration of additional interesting properties, such as partial radial distribution functions capturing inter-particle correlations at different transverse positions, and the asymptotic behavior of the radial distribution function revealing discontinuous structural changes in spatial correlations. Exact analytical expressions for the second virial coefficient are also provided.

The approach developed in this investigation, though presented for the square-well and square-shoulder potentials, can be applied to a wider variety of interaction potentials.



Figure 1. Radial distribution function at a linear density of 0.6 and various temperatures for (a) the square-well and (b) the square-shoulder potentials. Monte Carlo simulation results are depicted by circles

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DERIVATION OF A UNIVERSAL LAW FOR AC HYSTERESIS AREA WITH APPLICATIONS IN BIOSENSING

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The hysteresis area measured in oscillatory magnetometry is very sensitive to variations in the size of ferromagnetic colloids. This fact is already being use to detect the presence of biomolecules in solutions using bioconjugated nanoparticles. While analytical expressions for the hysteresis area exist in the linear regime (characterized by low magnetic fields and high frequencies), the greatest sensitivity is often observed in the non-linear regime, where precise predictions demand complex and time-consuming simulations. To address this challenge, we have derived a phenomenological analytical expression for the hysteresis area by solving the non-linear Fokker-Planck equation, resulting in a physically grounded model that accurately describes the magnetization cycle of dilute ferromagnetic nanoparticle solutions. This expression has been validated using both Brownian simulations and experimental data across a wide range of conditions, establishing its universal applicability.



Figure 1 – Variation in the magnetic area of AC magnetization cycles as a function of field frequency for different types of particles: (a) uncoated particles, (b) particles coated with dextran, (c) dextran-coated particles functionalized with a receptor, and (d) receptor-functionalized particles immersed in a solution containing a protein that specifically recognizes the receptor. Symbols indicate experimetal measures and lines fits with the presented theory.

This analytical model is further integrated into a Monte Carlo algorithm, allowing the estimation of system parameters by matching the theoretical and experimental hysteresis areas over different frequencies and field intensities. As a result, this approach allows AC magnetometry to function as stand-alone technique, capable of measuring with exceptional precision the average size, size distribution (polydispersity) and magnetic moment of bioconjugated ferromagnetic nanoparticles, This method has been successfully applied to detect nanometer-scale changes in particles hydrodynamic size which result from proteins adsorbed on their functionalized coatings.

Broad Adaptability of Coronavirus Adhesion Revealed from the Complementary Surface Affinity of Membrane and Spikes.

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Coronavirus stands for a large family of viruses characterized by protruding spikes surrounding a lipidic membrane adorned with proteins. The present study explores the adhesion of transmissible gastroenteritis coronavirus (TGEV) particles on a variety of reference solid surfaces that emulate typical virus-surface interactions. Atomic force microscopy informs about trapping effectivity and the shape of the virus envelope on each surface, revealing that the deformation of TGEV particles spans from 20% to 50% in diameter. Given this large deformation range, experimental Langmuir isotherms convey an unexpectedly moderate variation in the adsorption-free energy, indicating a viral adhesion adaptability which goes beyond the membrane. The combination of an extended Helfrich theory and coarse-grained simulations reveals that, in fact, the envelope and the spikes present complementary adsorption affinities. While strong membrane-surface interaction lead to highly deformed TGEV particles, surfaces with strong spike attraction yield smaller deformations with similar or even larger adsorption-free energies.

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SINGLE CELL DEATH TRIGGERS LOCAL AVOIDANCE RESPONSE IN THE COSMOPOLITAN PICOEUKARYOTE MICROMONAS

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Phytoplankton cell death has been identified as contributing to the largest carbon transfers on the planet moving 109 tonnes of carbon in the oceans every day. During a cell death organic matter is released into the local environment which can act as both a food source and a warning signal for nearby organisms. Here we present a novel motility response in populations of the cosmopolitan pico-eukaryote Micromonas sp., where the death of a single cell triggers the escape of cells in the surrounding area. These so-called "burst events" follow a simple model based on the release of a diffusive species with an estimated diffusion constant typical of molecules. Laser ablation of single cells reproduces the observed avoidance response, confirming that Micromonas sp. has evolved a motility allowing it to escape from regions where cell lysis takes place. This behaviour has potential implications for the spread of viral infections in Micromonas communities.

DENSITY AND INERTIA EFFECTS ON TWO-DIMENSIONAL ACTIVE SEMIFLEXIBLE FILAMENT SUSPENSIONS

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Filamentous and polymeric structures are essential in both biological and artificial systems, spanning scales from microscopic elements such as microtubules and actin filaments in the cellular cytoskeleton to bacterial filaments and macroscopic robotic systems. In this study, using detailed numerical simulations, we investigate the influence of density and inertia on the structural transitions between chain and spiral configurations in planar assemblies of active semiflexible filaments. Specifically, we examine how variations in density and Péclet numbers drive activity-induced transitions to spiral states in self-avoiding, semiflexible active polymer chains. Our findings indicate that spiral configurations become unstable at higher densities, leading to a transition back to a motile, chain-like state (Fig. 1). This density-dependent reentrant phase transition occurs as tightly coiled spirals extend into open chains. The underlying mechanism is attributed to inertial effects at the single polymer level, where increased persistence length due to inertia drives polymer unfolding.

Additionally, our two-dimensional simulations reveal that reducing the damping coefficient initiates the partial unwinding of spirals, resulting in longer, more extended filament arms. In a suspended state, interactions between these elongated arms can trigger a full unwinding of spirals, primarily driven by the combined effects of increased density and inertia [1]. Furthermore, we demonstrate that this reentrant phase transition persists even when different models of active forces are used. By comparing the structural and dynamic behavior of active filaments in two dimensions under tangential [2] and push-pull force [3, 4] models, we find that adjusting for differences in mean active force produces nearly identical behavior across both models [5].

These findings provide new insights into the dynamic behaviors of active filaments and have broader implications for the design of smart materials and active matter systems.



Figure 1. Phase diagram in the (ρ, Pe) -plane. Different phases are represented by distinct symbols: stable open chains without spirals (green triangles), stable chains with metastable loops and spirals (blue squares), stable open chains coexisting with stable spirals (red dots), spirals coexisting with metastable loops (red diamonds), stable spirals (orange stars), and stable compact chains with metastable spirals (blue pentagons).

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Water Turbidity Prediction in Desalination Plants Using Machine Learning-Based Models

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Machine learning is an advanced artificial intelligence technique extensively employed for predicting time-dependent phenomena, which we apply to the estimation of water turbidity in desalination plants. Turbidity, a critical physical parameter, is influenced by factors such as wind, ocean currents, temperature, salinity, and various water characteristics, which makes its analytical description complex and not fully understood. However, the characterization and forecasting of water turbidity are essential in numerous contexts, particularly in the production of potable water. High turbidity events pose significant challenges for desalination facilities, as membrane-based processes and reverse osmosis systems cannot operate effectively under elevated turbidity levels, leading to operational shutdowns. Consequently, we aim to develop a classification model capable of predicting the turbidity levels of desalination plant water two hours in advance, using historical turbidity data alongside relevant environmental variables. To address the requirement for a model that correlates historical and current data, we have designed an LSTM (long short-term memory) neural network trained via supervised learning, which has demonstrated adequate accuracy for preliminary implementation in several desalination plants.



A Self-Averaging Method to Fit Parameters in Coarse-Grained Models

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We introduce a parameter estimation method that utilizes microscopic data, specifically correlations or covariances of selected microscopic observables, to determine the parameters of a stochastic differential equation (SDE) governing coarse-grained (CG) degrees of freedom. The method is not limited to static parameters found in the reversible part of the CG dynamics, such as those in the CG free energy function or potential of mean force, but also extends to dynamic parameters, including friction coefficients. The coupled system self averages, according to Anosov's theorem, in such a way that the final state of the parameters gives coincidence between the microscopic and mesoscopic averages or correlations of CG variables. The method is validated in a simple case study of a Brownian particle in a harmonic potential. Additionally, it is applied to a more challenging problem involving a molecular dynamics (MD) simulation of a protein in water from which the microscopic averages and correlations are extracted. We present a particular CG model for the protein in terms of beads or blobs [1]. The Langevin dynamics for this model incorporate a reversible force, represented by an elastic network with adjustable elastic constants and Coulomb interactions, and irreversible friction forces. These irreversible forces stem from the intrinsic dissipation due to coarse-graining the protein into blobs and the dissipative interactions between the blob proteins and the surrounding water solvent. Our results demonstrate that the method effectively estimates the parameters for this blob-based model, confirming its applicability and accuracy. In particular, we observe that the internal friction between beads, representing internal dissipation, is numerically just as significant as the solvent dissipation caused by Stokes friction.



Figure 1 – (a) The Bovine Pancreatic Trypsin Inhibitor protein (BPTI), displaying both the atomic structure and the coarse-grained (CG) beads. (b) A representation of the elastic network, where the width of each link corresponds to its elastic constant (c) Average VACF over all beads for the microscopic (black) and for different mesoscopic models. The grey area indicate the standard deviation of the VACF over different beads.

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