ESPCI PARIS | PSL

UMR 7083 Gulliver

Experimental and Theoretical Travels in Soft Matter

2023-2024

Topics

Programmable matter

Interfaces in soft matter

Active matter and collective effects

Topological soft matter

Information and stochastic dynamics

Numerical and analytical methods

Controlling active flows through “smart confinement”

Encadrante:
T. Lopez-Leon (Gulliver)

Possibilité de thèse: Oui
Financement: Oui

Contact: *teresa.lopez-leon@espci.fr*

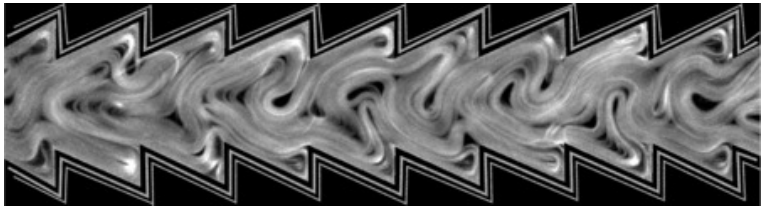


Figure. Active nematic confined to a two-dimensional micro-channel: the pattern of the wall induces directional flows and transport along the channel.

Résumé

Active liquid crystals are bio-inspired materials combining biofilaments and motor proteins. When confined to an interface, these biofilaments form bundles that locally orient parallel to each other, developing long-range orientational order, also called nematic order. The motor proteins bring the biofilaments bundles into motion by consuming ATP. This results in a fascinating system with autonomous motion, which continuously reorganizes its structure and flows over time. This distinctive behavior conceals another significant feature of active liquid crystals: their capability to adapt to the environments where they reside.

Geometrical confinement tends to control active flows, replacing their intrinsic chaotic dynamics by more regular flow configurations. Using high resolution 3D-printing, we have shown the emergence of spontaneous directional flow when the active nematic is confined inside a two-dimensional channel with open ends (see figure). This result is the first step towards the realisation of active flow networks (AFNs), that is, networks of connected channels in which an active fluid spontaneously flows. Recent theoretical works have provided design tools to create AFNs that are programmed to perform specific tasks, for instance, simple logical operations. The goal of the internship is to experimentally implement these ideas. First, we will study how the active fluid behaves at a bifurcation, and then, we will consider more complex configurations.

This study will be relevant for potential applications, including autonomous microfluidic devices or bio-inspired micro-machines, and in assessing the pertinence of the concepts of active matter in the description of biological systems. This work will be done in the Gulliver lab at ESPCI, in collaboration with the University of Barcelona and the University of Chicago.

[1] T. Sanchez et al., Nature 491, 431 (2012)

[2] J. Hardoüin et al., Communication Physics (2019)

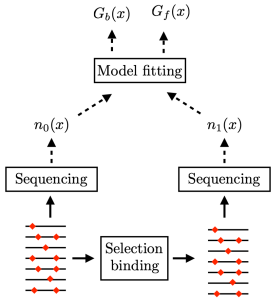
Keywords: active nematics, programmable matter, confinement, channel networks

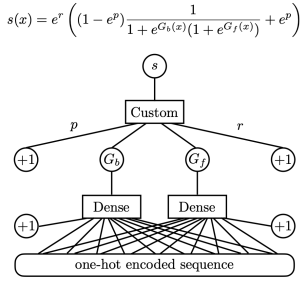
Physics-based statistical models of protein sequences

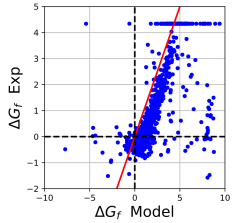
Encadrant:
O. Rivoire (Gulliver)

Possibilité de thèse: Oui
Financement: Non

Contact: olivier.rivoire@espci.fr
Webpage: http://statbio.net/







Abstract

Understanding the connection between a protein's amino acid sequence and its function remains a significant challenge. Traditional biophysics methods address the 'sequence→3D structure' problem but not the 'sequence→function' problem. Recent data-driven approaches analyze protein evolution to build statistical models of this relationship. These models, rooted in statistical physics and machine learning, enable the design of new functional protein sequences. A current challenge is imbuing physical interpretability into these models, to understand how sequences correspond to different physical properties of proteins, and to design proteins with specific properties. The goal of the internship is to advance these models in this direction using data from natural or/and experimental evolution.

Keywords: biophysics, machine learning, proteins, evolution

Investigating nucleation at mesoscale and condensation in complex media

Encadrantes:
A. Bouillant (MSC) & M. Reyssat (Gulliver)

Possibilité de thèse: Oui
Financement: Non

Contacts: *ambre.bouillant@u-paris.fr* & *mathilde.reyssat@espci.fr*

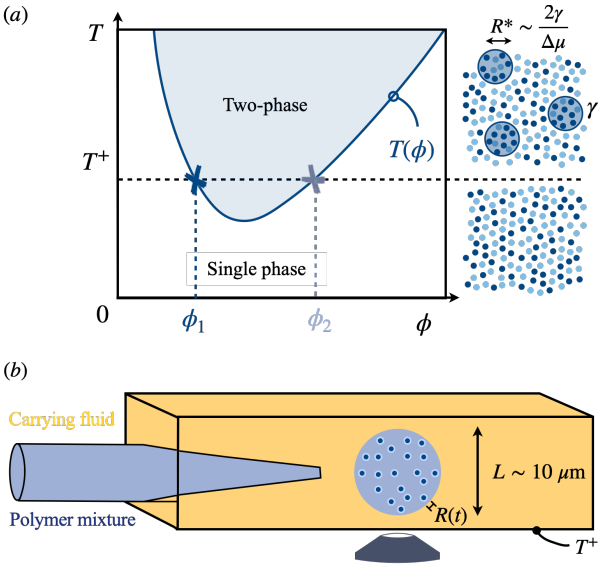


Figure (*a*) : Binary diagram giving a polymer blend demixing conditions. Above the temperature $T(\phi)$, droplets nucleate with a radius R^* and grow.

(*b*) Microfluidic model experiments to investigate homogeneous nucleation at a mesoscopic scale and to mimic the formation of bio-condensate in cells.

Résumé

Nucleation, the emergence of new phase structures, is ubiquitous in nature and fundamental in a broad spectrum of domains. These encompass atmospheric physics (*cloud formation*), biology (*protein crystallization*), catalytic processes (*alloy precipitation*), technological applications (*dislocation-free semiconductors*) and the food industry. Despite its fundamental relevance, this process is poorly understood. The Classical Nucleation Theory (CNT) is indeed notoriously defected by experiments, primarily due to the nanometric size of nuclei, which compromises direct observation of nucleation events and verification of the CNT. This internship aims to **study experimentally nucleation and condensation in polymer mixtures**, where nuclei appear at a mesoscopic, hence, observable scale to directly test the CNT.

Living cells are actually exploiting this phase transition to bring order and regulate intracellular reactions. As shown recently, many of cell compartments are liquid droplets (the so-called *biocondensates* BCs) assembled by homogeneous liquid-liquid condensation of biomolecules. Yet, the formation of BCs defies the classical rules of phase transition, notably by their arrested growth and fixed density, making them remarkably stable. While studies on BC focused on identifying them and their biological functions, the conditions for the formation, stability, and interactions with their environment remain to be understood. This internship will lead to a Ph.D program that will tackle the role of the medium complexity (confinement, macromolecular crowding and elasticity) on condensation, to explain the BCs starling stability and ultimately, to develop tuneable biomimetic emulsions with unusual stability.

Keywords: phase transition, nucleation, condensation, soft matter, interfaces, bio-inspired synthetic polymers, biomimetic emulsions

Fibrous microfluidics: from self-assembly to micro-dressings

Encadrants:

J. McGraw & M. Labousse (Gulliver)

Possibilité de thèse: Oui
Financement: Non

Contact:

Joshua.mcgraw@espci.fr
matthieu.labousse@espci.fr

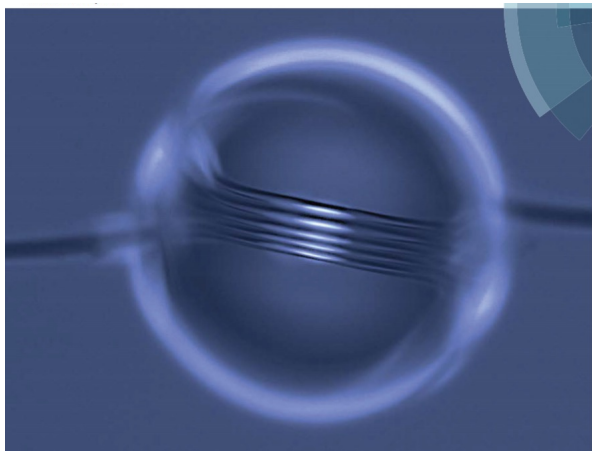


Figure 1 Elasto-capillary self-assembly. At small scale capillary forces are sufficient to overcome elastic stresses and spontaneously create 3D structures (picture from Schulman *et al.* (2017))

Résumé

A liquid drop wants to minimize its surface. It has have shown that thin sheets and fibers could be bent by a liquid drop as a result of capillary forces. Wrapping a drop decreases the total surface energy, which is preferred, but this has to be balanced with the cost of bending an elastic object, which is not preferred. This building strategy is called elastocapillary self-assembly and is used to build micrometric coils. An experimental submillimetric coiled droplet is shown in Figure 1.

However the relaxation dynamics is completely unknown. During this internship, we will study the relaxation dynamics of such a structure until equilibrium is reached. This internship can lead to a PhD project which would be supervised by Matthieu Labousse and Joshua D. McGraw. The work will take place at the Institut Pierre-Giles de Gennes (IPGG) in Paris. IPGG is the technological platform dedicated to the development of microfluidic-based projects, while Gulliver is an UMR which topics range from fluid at interfaces, active matter, molecular programming, to statistical physics. Theory and modelling will be done either at IPGG or in the Ecole Supérieure de Physique et de Chimie Indutrielles (ESPCI) whereas the experiments will be do carried out at IPGG.

An candidate with an experimental profile in fluid mechanics and soft matter is the most welcome to apply. An interest in the biotech sector as well as a curiosity in the creation of start-ups would be a plus.

Keywords: microfluidics, capillary interaction, micro-fabrication, micro chemical reactor

Entrance effects in osmotic nanofluidics for Blue Energy

Encadrants:
C. Trégouët (CBI)
A. Colin (CBI)
T. Lopez-Leon (Gulliver)

Possibilité de thèse: Oui

Financement: Non

Contact: *corentin.tregouet@espci.fr; annie.colin@espci.fr*
teresa.lopez-leon@espci.fr

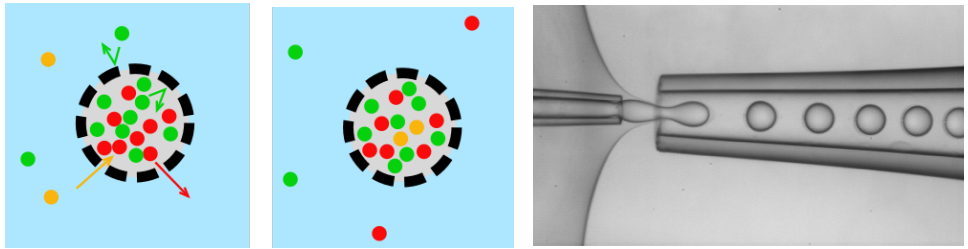


Figure. Working principle: osmotic forces drive the red cations out, which creates an electric field that pushes the orange cations inside the capsules (left). Glass- capillary device to produce core-shell droplets in a controlled way (right).

Résumé

Osmosis is the phenomenon responsible for spontaneous liquid transfer through membranes separating water volumes of different salt concentrations. Osmotic effects are of outmost importance in water desalination and biology. New understanding of these phenomena, acquired in the past 20 years, has opened the doors for promising applications, including energy production or depollution.

It is indeed possible to use ion-exchange membranes to force salt fluxes by using controlled gradients of another salt (see figure, left). Consequences are numerous, from depollution to pH control through physical mechanisms. To do this, a promising path is to fabricate capsules made of ion-exchange membranes.

The aim of the internship is to use a method of controlled capsule fabrication (see figure, right) to individually study the behavior of the capsules, and then, develop a microfluidic method to scale up the fabrication process.

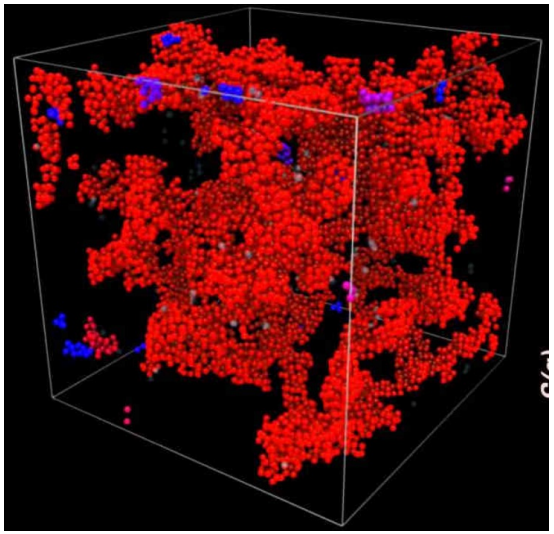
Keywords: osmosis, membranes, blue energy, nanofluidics

Boltzmann inversion : measuring forces by watching movies

Encadrant:
Ludovic Berthier (Gulliver)

Possibilité de thèse: Oui
Financement de thèse: Sous réserve d'un financement ANR

Contact: ludovic.berthier@espci.fr



Confocal microscopy image of a colloidal gel. The goal is to infer directly from these images the particle interactions leading to the formation of this material.

Résumé

Statistical mechanics traditionally starts from microscopic interactions: given microscopic rules, interactions, equations of motion, one tries to make predictions about the emerging physical behaviour. It is sometimes useful to work backwards and ask the opposite question. Given a specific experimental system, say a complex fluid or a biological system, what are the rules governing the behaviour of that particular system? This amounts to addressing the inverse problem of guessing the model from the observed physics.

The inverse problem has a long history across various fields from statistical mechanics to soft matter and computational studies of complex systems with applications from self-assembly to non-equilibrium phase transitions in driven systems. Our broad goal is to develop an efficient method to guess particle interactions of a broad range of physical systems simply from watching movies. Earlier work mainly used techniques such as Iterative Boltzmann Inversion which requires a painful iterative process involving a new Monte Carlo simulation for each step of the iteration until convergence.

We will develop a method based on formal but straightforward manipulations of the pair correlation function to efficiently iterate towards the correct result. Mathematically, the method is well-defined and simple and necessarily leads to the correct solution. Preliminary results show that robustly inferring forces from a set of images involves solving a number of practical obstacles when only a finite number of data is available. Several exciting applications of the method will then be explored, involving both equilibrium and non-equilibrium physics with applications to active matter, biological systems and disordered systems.

The work will make use of basic concepts of statistical mechanics, and will explore different physical systems in colloidal physics and active matter. Watching lots of movies will also be required.

Keywords: statistical mechanics, colloids, active matter

Morphoswarm robotics

Encadrant:
Olivier Dauchot (Gulliver)

Possibilité de thèse: Oui
Financement de thèse: Sous réserve d'un financement ANR

Contact: *olivier.dauchot@espci.fr*

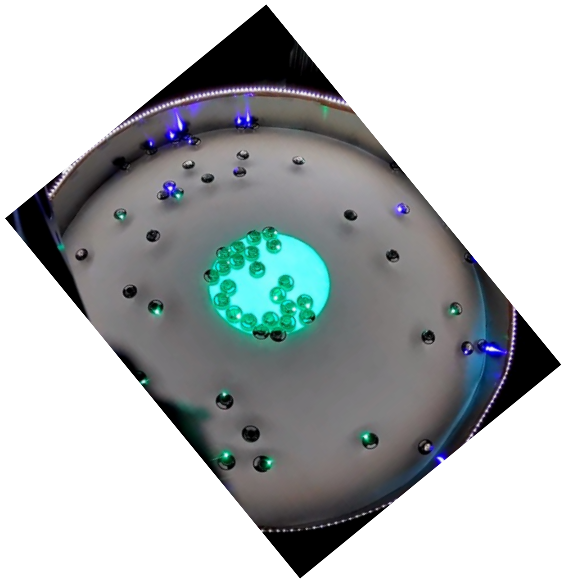


Figure. A swarm of morphobots performing phototaxy

Résumé

We are interested in swarm robotics, where a large number of robots with limited computation and communication power are considered.

Our goal is to propose new design methods, with a particular focus on considering the role of physical interactions among individuals. Embodiment is critical and useful for programming self-organizing collective systems. We thus propose to achieve collective decision making using both morphological and logical computation in swarm robotics.

To do so, we will take advantage of the design of a new kind of swarm robotics set-up together with a numerical model describing the swarm of robots in a faithful way, which we successfully developed in the paste three years.

The goal of the PhD research plan will be to obtain specific educated collective behaviors: starting from the spontaneous phase obtained from the purely physical interaction of the robots and applying minimal control from embodied capabilities on each robot, we will induce collective behavior, which we will refer to as operational phases. Optimization of such behavior will allow for the realization of complex collective tasks.

Examples of such tasks include phototaxy, harvesting objects, escaping mazes etc…

In all cases a special attention will be paid to the respective role of morphological and logical computation. Making connection with the typical phenomenology of active liquids will serve as a general guiding principle.

Keywords: active matter, swarm robotics, etc…

Dynamic self-assembly of bacteria in liquid crystals

Encadrantes:
T. Lopez-Leon (Gulliver)
A. Lindner (PMMH)

Possibilité de thèse: Oui
Financement: Non

Contact: *teresa.lopez-leon@espci.fr*
anke.lindner@espci.fr

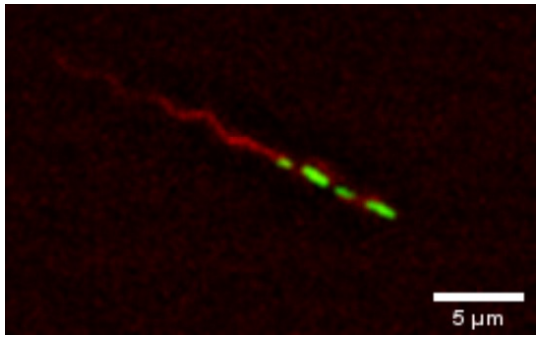


Figure. A chain of bacteria swimming in a liquid crystal. The flagella (in red) of individual bacteria self-assemble into a super bundle that is capable to propel the whole chain. Image from Martyna Góral.

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Résumé

In nematic liquid crystals, bacteria have been shown to swim along the nematic director field [1]. Interestingly, when we increase the concentration of these active particles, bacteria attract each other due to elastic forces arising from the distortions they induce in the liquid crystal. These elastic forces lead to the formation of chains of bacteria, as it has been observed for passive particles [2]. In contrast to passive systems, bacteria self-propel and their activity can overcome the attractive forces induced by the liquid crystal, resulting in an interleading dynamics of chain assembling and breaking. We experimentally investigate this problem using E. coli bacteria swimming in a nematic liquid crystal confined to a microfluidic chamber. We track their dynamics using fluorescent microscopy [3]. The goal of this study will first be to characterize the distribution of the chain length of bacteria and compare it to the distribution of passive particles, here E.-coli bacteria that have been stripped of their flagella. Then, the study will focus on the self-propulsion of these chains, studying the relationship between chain length and velocity. Specific attention will be paid to the propulsion mechanism provided by the super bundle (see figure) that is formed by the flagella of all the different bacteria of the chain, grouped in a unique helix rotating in synchrony.

The internship will be performed jointly between the Gulliver and PMMH labs.

[1] S. Zhou et al., PNAS, 11, 1265 (2014)

[2] P. Mushenheim et al , Soft Matter, 10, 88 (2014)

[3] M. Goral et al. Interface focus, 12, 20220039 (2022)

Keywords: bacteria, active matter, nematic order, self-assembly, swimming

Reconfigurable active matter in 3d

Encadrant:
C. P. Royall (Gulliver)

Possibilité de thèse: Oui
Financement: Oui

Contact: *paddy.royall@espci.fr*

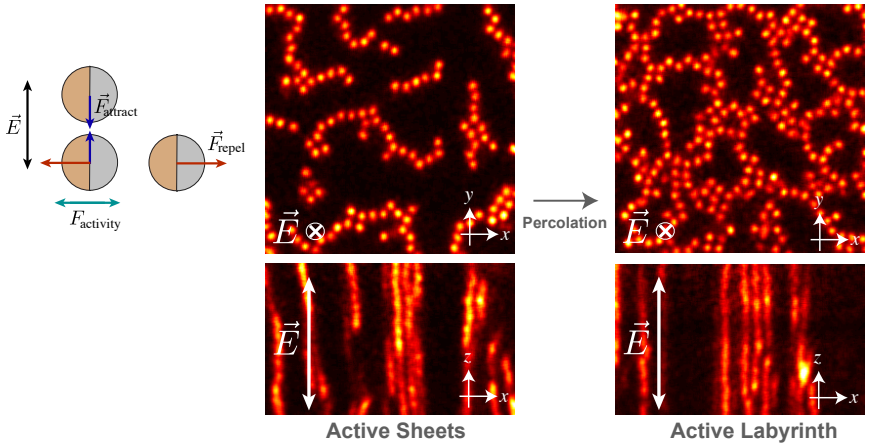


Figure. Active colloids in 3d. (left) The electric field E provides the activity in the *xy* plane. It also induces dipolar interactions, an attraction in *z* and repulsion in *xy*. (right) Snapshots of new phases of matter using 3d confocal microscopy. Top xy planes showing sheet phase labyrinth. Botton xz planes .

Résumé

Active systems exhibit fascinating pattern formation, and collective dynamics not seen in conventional materials. A key consequence of our improving understand of active matter the potential for the application to biological systems, from collective behaviour in fish to insect swarms, such as, as these in general are active due to processing of energy.

Yet to make progress in understanding active matter, simple, controllable and well-characterized systems play a key role and among these are active micron-sized particles (colloids). Here the interactions between the particles are well-understood [1]. In particular, colloidal particles assemble in to a variety of structures, which can be interpreted with statistical mechanics [2]. However almosy all work with active colloids has used (quasi) 2d systems.

We have developed a 3d active colloidal system of dipolar particles which are active in the *xy* plane and which have already produced two new phases (see Figure) [3]. This project proposes to investigate further the behaviour of this exotic, and yet well-controlled system. The project may be carried out in experiment, or in computer simulation as we have also developed a simulation model of the same system [3].

[1] Mauleon Amieva et *al Sci. Adv*. 9 eadf5144 (2023).

[2] Royall et al *ArXiV* 2305.02452 (2023).

[3] Sakaï N and Royall CP, *ArXiV* 2010.03925 (2020).

[4] Moore FJ et al , *J. Chem. Phys*. **158** 104907 (2023).

Keywords: active mater, active colloids, self-assembly, phases of matter

Colloid Nucleation: the « second-biggest discrepancy in physics »

Encadrants:
C.P. Royall (Gulliver), F. Smallenburg (Laboratoire de Physique des Solides, Universite Paris Sud)

Possibilité de thèse: Oui
Financement de thèse: Oui
Contact: *paddyroyall@gmail.com*

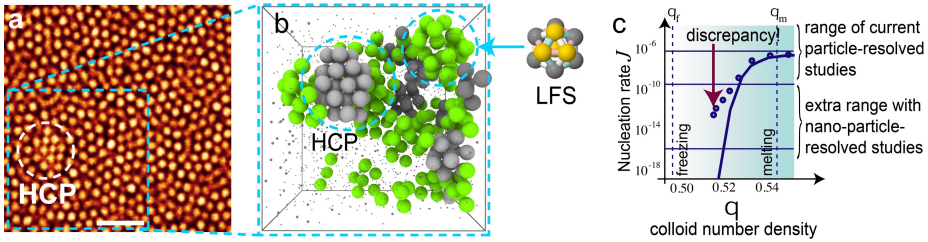


Figure. (a) Crystal nucleating in a liquid of colloids. 3d Confocal microscopy image. Bar=20μm. (b) 3d rendering of particle coordinates: grey hexagonal close-packed crystal, green liquid locally favoured structure. (c) Nucleation rate in hard spheres. Line – prediction from computer simulation, data points, experimental data.

Résumé

How does a liquid transform into a crystal? Remarkably, even now this everyday process is poorly understood. One challenge with studying the birth of a crystal, the process of nucleation, is that it is hard to see such tiny groups of a few atoms or molecules. Mesoscopic colloidal particles follow the same laws of statistical mechanics and form crystals just like atoms. Early work with colloids used indirect scattering methods, to measure the rate of formation of crystal nuclei (Fig. 1c). Very surprisingly, when the rate of formation J is low, experiments find a rate that is more then *ten orders of magnitude* faster than the prediction from computer simulation, "the second-biggest discrepancy in physics".

Now it is possible to see the colloidal particles in a confocal microscope, which can image in 3d (Fig 1a). This is a very useful experimental method to investigate nucleation, because we can directly see the nucleus and track the coordinates of the colloids – *particle-resolved studies* (Fig. 1b). Here, we will study colloid nucleation with a new technique, "nano—particle resolved studies". This method uses much smaller colloids than is usual. This is important, because these "nano--particles" move 1000s of times faster than normal, which means that we can investigate nucleation in the regime where the discrepancy is found.

The precise content of the internship, performed at Gulliver and also in collaboration with Frank Smallenburg(LPS, Paris Sud) will be discussed with the candidate to fit his/her interests and knowledge.

Keywords: colloids, nucleation, confocal microscopy

Tackling the Glass Challenge

Encadrant:
C. P. Royall (Gulliver)

Possibilité de thèse: Oui
Financement: Oui

Contact: *paddy.royall@espci.fr*

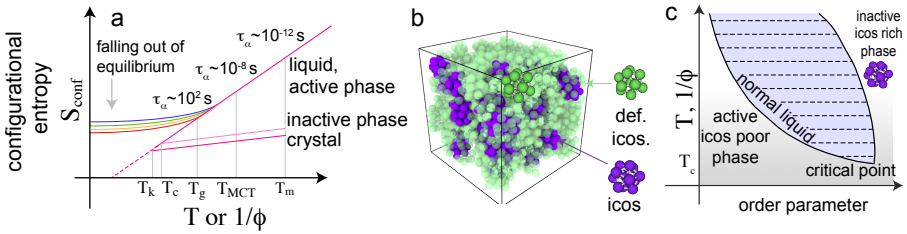


Figure. **a** The thermodynamic interpretation of the glass transition, configurational entropy drops with temperature, faster in the liquid than the crystal. **b** Particles in a glassy liquid organise into icosahedra (icos) and defective icosahedra which are locally favoured structures. **c** The dynamic interpretation of the glass transition: a glassy inactive phase rich in icosahedra coexists with the normal liquid.

Résumé

Glasses have been part of our everyday life for 4000 years, yet the process by which a liquid transforms into an amorphous solid (glass) remains one of the deepest mysteries of condensed matter physics. The glass transition is a rare example of *a scientific revolution* in the sense of Thomas Kuhn [1]. In brief, these means that there are mutually incompatible theories which give equally good descriptions of experimental measurements.

One, the *thermodynamic* approach (Fig. **a**), posits that the glass transition is due to a drop in configurational entropy in the (glassy) liquid upon cooling. At the Kauzmann temperature T_k, the liquid configurational entropy becomes less than that of the crystal, the Kauzmann paradox (a paradox as entropy is conventionally thought of as a measure of disorder so how can a liquid be less disordered than a crystal?). This drop in entropy is related to locally favoured structures such as icosahedra (Fig. **b**) [2].

The other, *dynamical* approach (Fig. **c**) posits that the glass transition arises through a special mind of phase transition, a *dynamical phase transition* between the liquid and a glassy state. The inactive glass phase is rich in icosahedra.

This project looks at ways to unify these two incompatible theories of the glass transition and thus end the scientific revolution. To do so, we need new data, which is either from new experiments with colloids [2] or new computer simulations with GPUs [3]. This project may be either computational or experimental.

[1] Kuhn T, *The Structure of Scientific Revolutions*, (first published). 1962.

[2] Hallett J. *et al Nature Communications* **9** 3272 (2018).

[3] Ortlieb L. *et al Nature Communications* **14** 2621 (2023).

Keywords: glass transition, colloids, super-resolution imaging GPU computer simulation

Self-organization of rod-shaped viruses in a spherical shell

Encadrants:
T. Lopez-Leon (Gulliver)
E. Grelet (CRPP, Bordeaux)

Possibilité de thèse: Oui
Financement: Non
Contact: *teresa.lopez-leon@espci.fr*
eric.grelet@crpp.cnrs.fr

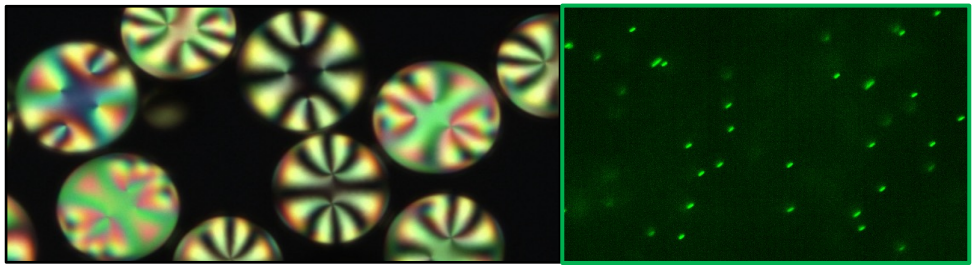


Figure. Liquid crystals confined to a spherical shell (left). Rod-like viruses forming a nematic phase; note that only a few viruses are fluorescently labelled (right)

Résumé

Liquid crystals can self-organize in fascinating ways when confined to a spherical shell, due to the impossibility of establishing their preferential orientational *molecular* order everywhere on the sphere [1]. One of the most outstanding consequences of this spherical confinement is the presence of topological defects in the ground state of the system (https://twitter.com/TheLuProject/status/803530225850208256?s=20&t=x9BS-bmHtRDj6C9RKSznnA). These defects can be optically detected by using cross-polarized microscopy, as shown in the picture below (left), where defects appear as singular spots where black lines cross.

In this joint project between ESPCI and the CNRS/University of Bordeaux, we aim at creating shells of *colloidal* liquid crystals using filamentous rod-like viruses. Replacing the liquid crystal molecules by colloidal rods will enable the visualization, at the single particle level, of the liquid crystal organization, as illustrated by the picture above (right), where the alignment of 1µm long viruses can be observed by fluorescence microscopy [2]. The scaling up of the particle size (from molecular to colloidal) will allow us to have direct access to the dynamics and structure of topological defects for the first time, opening the way for a better understanding of the role of geometrical confinement in self-organization processes.

The student will produce the liquid crystal shells using microfluidic techniques and study the resulting defect structures by means of polarizing and fluorescence optical microscopy.

[1] T. Lopez-Leon et al., Nature Phys. 7, 391 (2011).

[2] A. Repula and E. Grelet, Phys. Rev. Lett. 121, 097801 (2018).

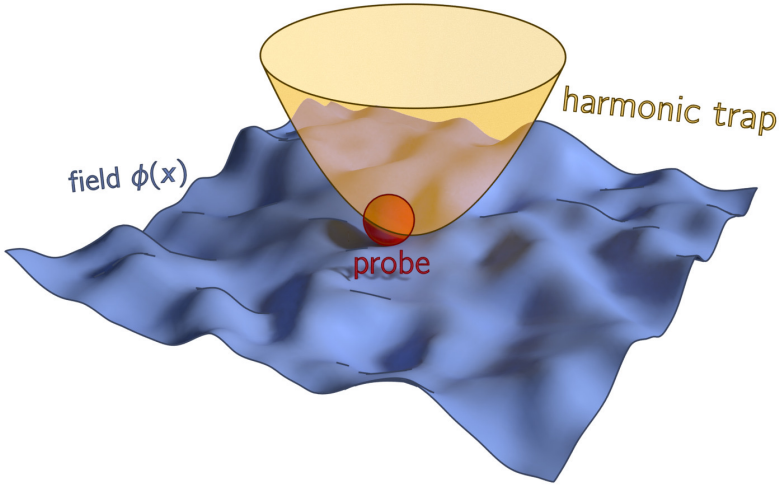
Keywords: liquid crystals, colloids, viruses, topological defects, confinement, microfluidics

Diffusion with a non-reciprocal coupling to the environment

Encadrant:
V. Démery

Possibilité de thèse: Oui
Financement: Non

Contact: vincent.demery@espci.psl.eu



Abstract

Non-reciprocal interactions between particles, such as the ones arising between catalytically active colloids, can lead to the formation of self-propelled molecules [1]. This active behavior enhances the diffusion of tracer particles, and, the system being out-of-equilibrium, the Einstein relation between the diffusion coefficient and the mobility is not satisfied [2]. The long time diffusion coefficient has been computed theoretically for soft interactions [2], shedding light on the mechanisms and the relevant parameters leading to the diffusion enhancement. However, a complete characterization of the dynamics of the tracer particle would require the calculation of the mean squared displacement (MSD) at all times, and not only at very large times. Computing the MSD theoretically for soft interactions is the goal of this internship. This calculation has been done with a path-integral approach for a colloid held in a harmonic trap [3]. We will use the same approach with non-reciprocal interactions. We will finally compare our results with numerical simulations.

[1] Self-Assembly of Catalytically Active Colloidal Molecules: Tailoring Activity Through Surface Chemistry, Soto and Golestanian, PRL 112, 068301 (2014).

[2] Enhanced diffusion of tracer particles in non-reciprocal mixtures, Benois, Jardat, Dahirel, Démery, Agudo-Canalejo, Golestanian and Illien, arXiv 2307.05408 (2023)

[3] Non-Gaussian fluctuations of a probe coupled to a Gaussian field, Démery and Gambassi, arXiv 2307.07721 (2023)

Keywords: stochastic processes, out-of-equilibrium systems, path-integral methods, numerical simulations

Growth and adaptation to an uncertain environment

Encadrant:
D. Lacoste (Gulliver)

Possibilité de thèse: Oui
Financement de thèse: Non

Contact: *david.lacoste@espci.fr*
Web: https://www.pct.espci.fr/~david/

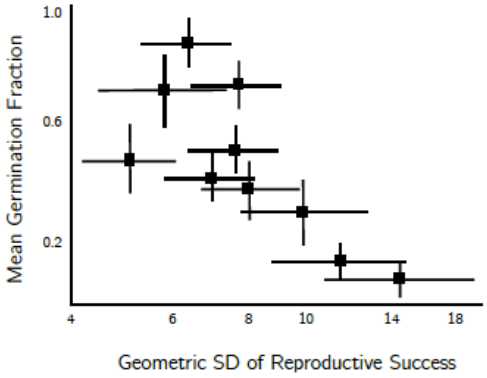


Figure. Left: a species of wildflower of the southwestern United States believed to implement a bet-hedging strategy. Right: An inverse relationship between the germination fraction and the standard deviation in reproductive success in deserts. From D. Venable, Ecology (2007)

INFORMATION AND STOCHASTIC DYNAMICS

Résumé

In recent work of the group, we have studied evolutionary strategies used by biological or ecological populations to cope with uncertain environments by drawing analogies with a model of gambling known as Kellys's model.

In this model, a gambler strives to maximize his/her capital growth by placing appropriate bets. The strategy of maximizing the long term growth rate of the capital is optimal but risky in practice. Recently, we have revisited this model by including a penalization due to the risk, measured in practice by the fluctuations of the growth rate, and we have studied the corresponding trade-off between growth and risk [1]. We found the same trade-off to be also relevant for a biological population in a fluctuating environment with individuals stochastically switching between two phenotypes [2].

In biology, individuals take decisions (for seeds this can mean whether to germinate or not as illustrated in figure) in order to adapt to a possibly harmful environment. Individuals also often sense their environment and use that information to survive or grow in a process called adaptive sensing. In a simple illustration of that idea, the learning process can be modeled using Bayesian inference [3].

The goal of this internship/thesis is to further extend these ideas using methods from Non-equilibrium Statistical Physics. We ask what are the fundamental limits of adaptation or sensing from the point of view of thermodynamics and information theory ? Under what conditions do these strategies emerge ? How general is the trade-off between growth and risk mentioned above ?

The work will be mainly fundamental and theoretical but we also plan to model an experiment carried out by colleagues in a nearby institute, in which colonies of yeast cells growing in a reactor are exposed to a fluctuating environment.

[1] Phase transitions in optimal betting strategies, L. Dinis, J. Unterberger and D. L., Eur. Phys. Lett., 131, 60005 (2020).

[2] Pareto-optimal trade-off for phenotypic switching of populations,L. Dinis, J. Unterberger and D. L., J. Stat. Mech. (2022) 053503.

[3] Adaptive strategies in Kelly's horse race model, A. Despons, L. Peliti, and D. L., J. Stat. Mech. (2022) 093405.

Keywords: bet-hedging, evolution, adaptation

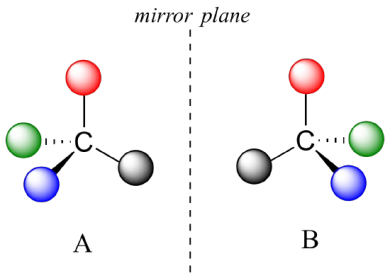
Emergence of homochirality in complex media

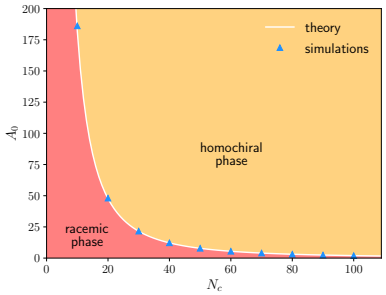
Encadrants:
D. Lacoste (Gulliver)
M. Castellana (Institut Curie)

Possibilité de thèse: Oui
Financement de thèse: Non

Contact: *david.lacoste@espci.fr*
michele.castellana@curie.fr

Web: https://www.pct.espci.fr/~david/





Left: illustration of the mirror symmetry between two chiral enantiomers. Right: phase diagram in the plane (N_c the number of chiral species, and A_0 the injection of energy) [1].

Résumé

Homochirality, also called biological asymmetry, is a long-standing problem in the research on the origins of life. Many mechanisms have been proposed to explain it, but none is fully accepted by the community. It is important to progress on this issue because homochirality could be an important biomarker for the detection of life outside Earth, and it is also a central issue in model experiments designed to mimic the complexification of living matter. The pioneering paper by Frank in 1953 presented a simple mathematical model based on autocatalytic reactions, which provides an amplification mechanism leading to homochirality. The model is rather simple because it contains only a few species and assumes a well-mixed environment. These two hypotheses do not fit well with experiments in prebiotic chemistry, which typically involve a large number of species and non-well-mixed systems.

In a previous work of the group, we have introduced a generalization of Frank's model containing a large number of chiral species [1]. This study shows that homochirality can emerge robustly in a large class of autocatalytic chemical networks, provided the network is large enough (in terms of the number of its chiral species) and driven sufficiently far from equilibrium.

In this project, we propose to build models for the homochirality emergence by including spatial inhomogeneities and repulsive interactions between molecules. Our model will also introduce new methods to take into account the chemical complexity of prebiotic systems, which comes from having a large number of species involved together in autocatalytic cycles [2], with unknown kinetics and topology.

[1] Emergence of homochirality in large molecular systems, G. Laurent, D. Lacoste, and P. Gaspard, Proc. Natl. Acad. Sci. U.S.A., 118, (2021)

[2] Universal motifs and the diversity of autocatalytic systems, A. Blokhuis, D. D. Lacoste, and P. Nghe, PNAS, 117, 25230 (2020).

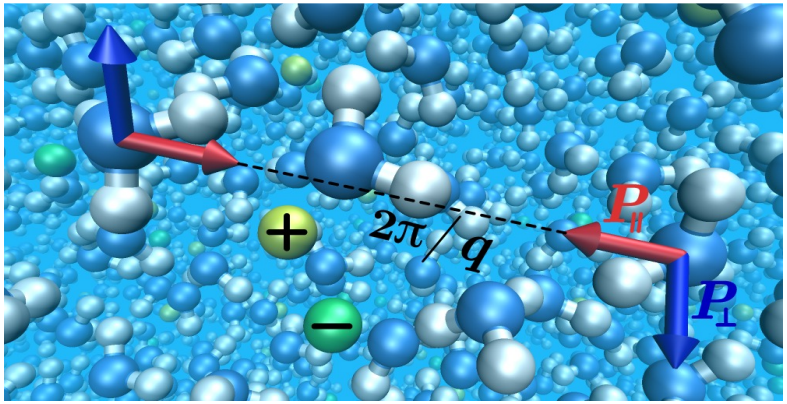
Keywords: homochirality, origin of life, chemical networks

Properties of electrolytes at the nanoscale

Encadrants:
H. Berthoumieux (Gulliver)
A. Kornyshev (Imperial College)

Contact: helene.berthoumieux@*espci.fr*

Possibilité de thèse: Oui
Financement: Non



Sketch of electrolyte at the nanoscale. Water acts as a nonlocal nonlinear dielectric medium to the presence of ions.

Résumé

The properties of confined electrolytes focus a lot of attention. They play a key role in controlling reactivity and transport in confinement. These processes are omnipresent in *in vivo* metabolic pathways and in nanofluidic devices developed to produce non-intermittent green energy. As the properties of the fluid at the nanoscale differ drastically from the macroscopic ones, a theory based on a linear local description of the fluid, such as the Poisson-Boltzmann theory or the method of image charge breaks down at this scale and a new framework is necessary to describe these systems [1,2,3]. In this internship, we will investigate the interplay between the structure of the fluid, the correlations of the ions and the geometry and the physical properties of the confining surface on the dielectric properties of the liquid. Via standard tools of statistical physics and field theory we will derive analytically the properties of this system and will extract the coupling between fluid molecular structure and confinement. Molecular dynamics simulations will be performed to parametrize the field theory model and validate the analytical results.

1. L. Fumagalli,et al. Anomalous low dielectric constant of confined water, Science, 360 1339 (2018)
2. G. Monet, et al. The nonlocal dielectric response of water in nanoconfinement, Phys. Rev. Lett. 126 216001, (2021)

3. A. Robert et. al. Coupled Interactions at the Ionic Graphene-Water Interface, Phys. Rev. Lett. 130 (7), 076201, (2023)

Keywords: electrolytes, confinement, field theory

People


H. Berthoumieux


O. Dauchot


V. Démery


M. Fruchart


G. Gines


M. Labousse


D. Lacoste


L. Leibler


T. Lopez-Leon


A. C. Maggs


J. McGraw


E. Raphaël


M. Reyssat


O. Rivoire


Y. Rondelez


P. Royall


M. Schindler


K. Sekimoto


Z. Zeravcic