



# Experimental and Theoretical Travels in Soft Matter

2024-2025

# TOPICS

STATISTICAL PHYSICS

TOPOLOGICAL SOFT MATTER

ACTIVE MATTER & COLLECTIVE  
EFFECTS

PROGRAMMABLE MATTER

INTERFACIAL SOFT MATTER

## PEOPLE



L. Berthier



H. Berthoumieux



O. Dauchot



V. Démary



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. Zeravic

# Nonlinear response functions in glassy fluids: What do they probe?

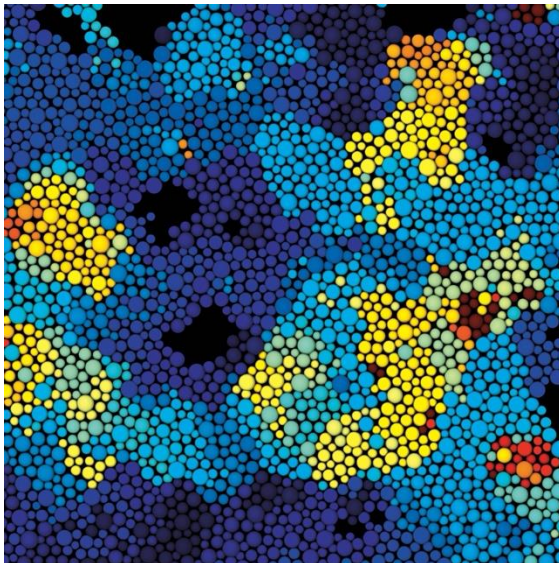
**Encadrant: Ludovic Berthier (Gulliver)**

**Collab: C. Scalliet (LPENS), JP Bouchaud (CFM), F. Ladieu (CEA)**

**Possibilité de thèse: Oui**

**Financement de thèse: Candidature à l'EDPIF**

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Dynamic heterogeneities close to the glass transition revealed by computer simulations. How to detect correlated domains via nonlinear response functions?

## Résumé

Dense liquids solidify at low temperatures through a process called the glass transition. While well-understood macroscopically, little is known from direct experiments about molecular dynamics near this transition. A microscopic understanding remains an active research problem despite decades of studies [1].

Over the past 10 years, non-linear dielectric measurements in molecular systems have emerged as a way to probe glassy correlations [2]. In parallel, new simulation techniques reveal a complex hierarchy of correlated molecular motion in dense glassy fluids [3]. Although the emergence of correlations in liquids near the glass transition is accepted, their nature remains debated. Are these correlations linked to an underlying phase transition, or are they purely dynamic, reflecting the movement of molecules without a structural transition?

This thesis will employ novel numerical approaches to measure non-linear response functions while resolving the molecular dynamics in space and time. By systematically analyzing static and dynamic correlations, this work aims to provide a microscopic interpretation of these functions. The ultimate goal is to bridge the gap between competing theoretical models and experimental results. The project will take place at Gulliver (ESPCI UMR 7083 CNRS) under the supervision of L. Berthier (DR, CNRS), with expertise in disordered materials and numerical simulations [4]. Collaborators include C. Scalliet (LPENS), J-P. Bouchaud (CFM), and F. Ladieu (CEA Saclay), combining expertise in theory, simulations and experiments [1-5].

[1] L Berthier et al, RMP 83, 587 (2011). [2] S Albert et al, Science 352, 6291 (2016). [3] B Guiselin et al, Nature Phys. 18, 468 (2022). [4] [4] L Berthier and DR Reichman, Nature Reviews Phys. 5, 102 (2023). [5] JP Bouchaud and G Biroli, PRB 72, 064204 (2005).

**Keywords: statistical mechanics, glassy dynamics, computer simulations**

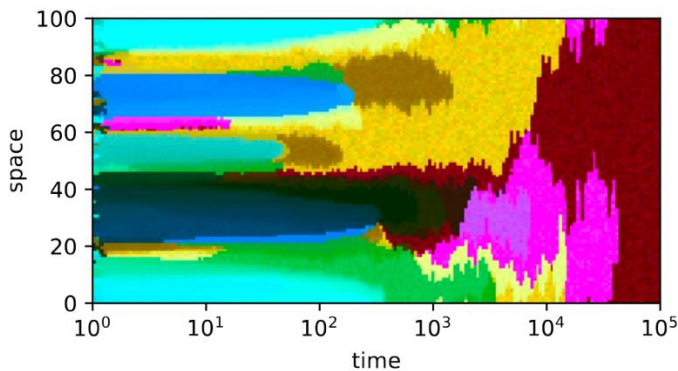
# Physics models for the origins of Darwinian evolution

**Encadrant: Olivier Rivoire (Gulliver)**

**Possibilité de thèse:** Oui

**Financement:** Oui

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Spatio-temporal dynamics of one of our models. This model is defined in a one-dimensional space (y-axis). At each point in time and space, different molecules are present in different concentrations. The colors represent different compositions, with similar colors representing similar compositions. As time passes (x-axis, in logarithmic scale), some compositional states appear, disappear, or expand at the expense of others in a process that bears analogy to Darwinian evolution.

## Abstract

Life is understood to be both the result and the engine of Darwinian evolution. Darwinian evolution, also known as evolution by natural selection, occurs when three key ingredients are present: (1) Variation: a population of individuals exhibits different traits; (2) Inheritance: these individuals reproduce and pass on their traits, at least in part, to their offspring; (3) Differential reproduction: some traits lead to greater survival and reproductive success than others. When these conditions are present, natural selection can occur, leading to changes in the population over time.

In modern life forms, the mechanisms underlying variation, inheritance, and differential reproduction are complex and themselves the products of billions of years of Darwinian evolution. At the origin of life, however, Darwinian evolution must have emerged from simpler processes. What were these processes? We approach this question from a physics perspective, aiming to define and study models of simple physical and chemical processes that can give rise to Darwinian evolutionary dynamics beyond the specific pathway that led to life on Earth.

## References

- Sakref, Y. & Rivoire, O. (2024). *Design principles, growth laws, and competition of minimal autocatalysts*. Commun. Chem. 7, 239.
- Sakref, Y., & Rivoire, O. (2024). *On the exclusion of exponential autocatalysts by sub-exponential autocatalysts*. J. Theor. Biol. 579, 111714.
- Charlat, S., Hems, T., & Rivoire, O. (2023). *Is natural selection physical? In Evolutionary Thinking Across Disciplines: Problems and Perspectives in Generalized Darwinism* (pp. 287-296). Springer International Publishing.

**Keywords:** evolution, origin of life, non-equilibrium dynamics, stochastic processes

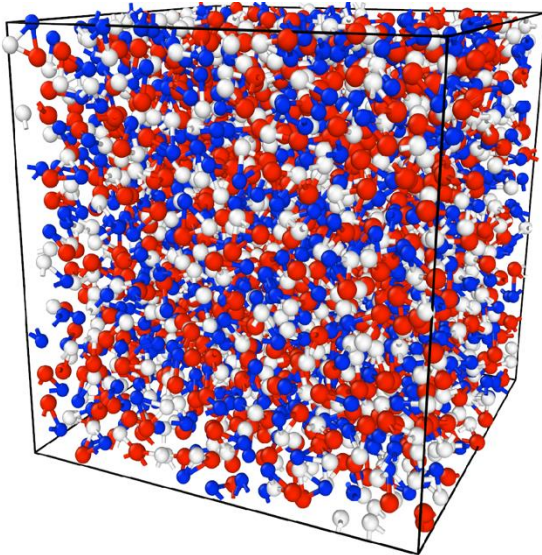
# Numerical study of the equilibrium Kauzmann transition between a liquid and a disordered glass

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**Possibilité de thèse: Oui**

**Financement de thèse: Candidature à l'EDPIF**

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This molecular fluid transforms at low temperatures into a non-equilibrium glass state. Is this process controlled by an underlying equilibrium phase transition?



# STATISTICAL PHYSICS

## Résumé

Most liquids gradually solidify at low temperature via a physical process called the glass transition towards a non-equilibrium disordered state of matter. This process is well-known experimentally at the macroscopic scale. At the fundamental level, however, the statmech description is much less advanced, as it took several decades of difficult analytic work to recently derive a solid mean-field transition of the liquid-glass transition, which is now reaching completion. The effect of fluctuations in disordered systems is typically very important but theory is for now unable to capture them. In the last 10 years, considerable progress was also made to develop simple yet realistic atomistic models for glass transition studies, as well as numerical methods to more efficiently sample the configuration space which is known to be highly complex.

State-of-the-art theory and simulations suggests that an equilibrium phase transition between liquid and glass states could exist in model liquids in finite dimensions, but demonstrating the existence of the transition and studying the associated properties (universality, exponents, characteristic lengthscales) has not been possible so far, leading some researchers to claim that this is an impossibly difficult task. We wish to solve this difficult problem.

In this thesis, we will develop and combine numerical approaches to systematically investigate the nature of the transition between liquid and glass states in equilibrium conditions. By carefully choosing simple glass models, and starting with modest system sizes, we will develop computational approaches to very efficiently explore complex energy landscapes and cross the equilibrium liquid-glass Kauzmann transition for bulk systems. In a second step, we will investigate whether the findings in small systems extend to larger ones, in order to eventually develop finite size scaling methods to approach the thermodynamic limit. Ultimately, this work will provide a definitive answer to a mystery that has haunted the field of disordered systems for more than fifty years by demonstrating whether a glass state of matter can truly be defined in three-dimensional glass-forming liquids.

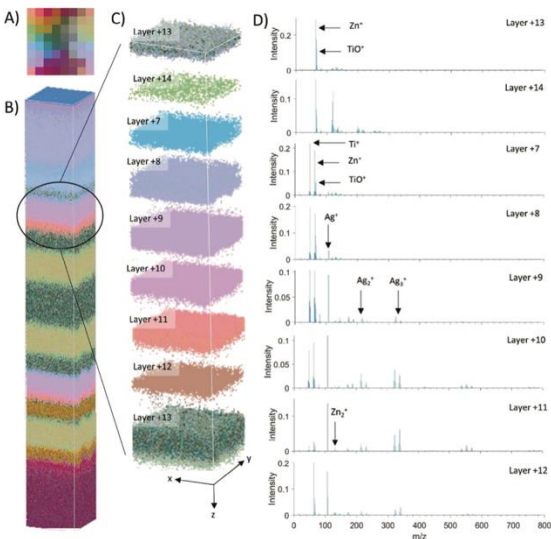
# Deformulation of complex glass-like materials through statistical analysis of Raman spectra

Encadrants: **Hélène Berthoumieux & Olivier Rivoire (Gulliver)**

Possibilité de thèse: Oui

Financement: ?

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Deformulation of a multilayer silver-glass coating from time-of-flight secondary ion mass spectrometry data using unsupervised machine learning for visualization (from Ref [3]).

## Abstract

The characterization of complex materials, in particular obtaining a three-dimensional map of their chemical composition and phases, represents a major challenge with important applications in industry. In the field of glasses, the analysis of Raman spectra is commonly used to identify the molecules present from individual peaks [1]. However, this approach does not take into account the correlations between peaks, which contain essential information on collective effects. Advances in machine learning now enable more sophisticated data analysis. These approaches open up new possibilities in analytical chemistry, which are only just beginning to be explored [2]. For glasses, the application of classic data projection tools has enabled the reconstruction of cutting profiles [3]. However, the interpretation of these profiles is still based on visual inspection, which limits the automation and quantification of the analysis. In collaboration with the Surface Verre Interface (SVI) laboratory associated with Saint-Gobain, we propose to develop a more in-depth approach to the analysis of Raman spectra. The aim is to automate data interpretation and assign a confidence score, enabling more robust and quantitative analysis of complex materials.

## References

- [1] Ben Khemis, S., Burov E., Montigaud H., Skrelic D., Gouillart E., Cormier L., (2021). Structural analysis of sputtered amorphous silica thin films: A Raman spectroscopy investigation. *Thin solid films*, 733, 138811.
- [2] Debus, B., Parastar, H., Harrington, P., & Kirsanov, D. (2021). Deep learning in analytical chemistry. *Trends in Analytical Chemistry*, 145, 116459.
- [3] Bamford, S. E., Jones, R. T., Gardner, W., Muir, B. W., Winkler, D. A., & Pigram, P. J. (2024). Profiling a Low Emissivity Glass Coating with ToF-SIMS and Machine Learning. *Advanced Materials Interfaces*, 11(3), 2300645.

# Properties of electrolytes at the nanoscale

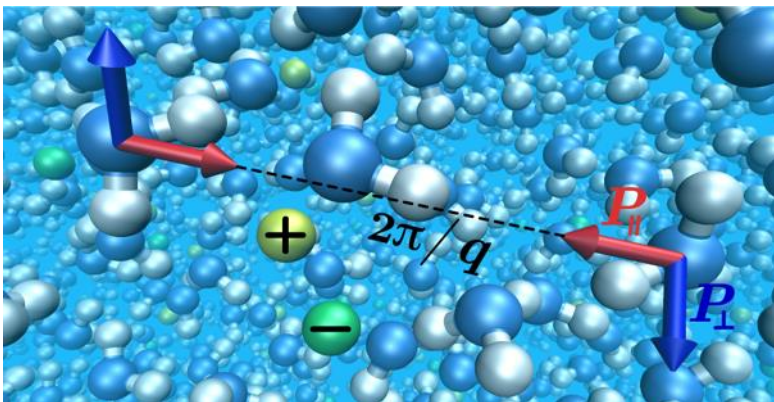
**Encadrants:**

**H. Berthoumieux (Gulliver)**

**A. Kornyshev (Imperial College)**

**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)

# Singularities in thin elastic sheets

**Encadrants:**

**V. Démery (Gulliver)**

**M. Adda-Bedia (ENS de Lyon)**

**Possibilité de thèse :** Oui

**Financement :** Non

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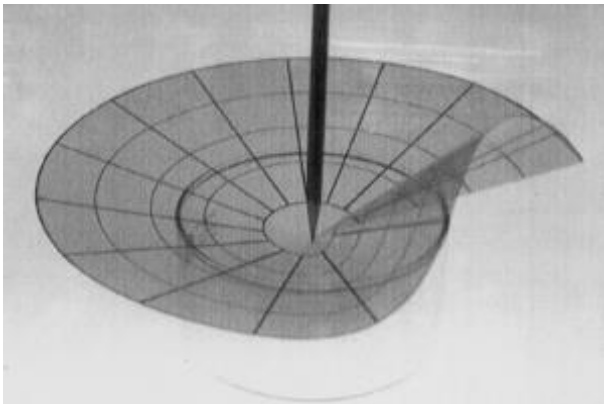


Figure. Conical singularity in an indented sheet.

## Résumé

Thin elastic sheets deform either by stretching or by bending, the latter offering less resistance by a factor  $(t/L)^2$ , where  $t$  is the thickness of the sheet and  $L$  its lateral extension. Moreover, the bending energy involves spatial derivatives of higher order than the stretching energy, yielding singular equations in the limit  $t/L \rightarrow 0$ . As a consequence, conical (Figure) and ridge singularities may form, whose extension is intermediate between  $t$  and  $L$ . Understanding these singularities may also require the adequate treatment of the geometrical nonlinearities of the governing equations, which are often neglected.

In this project, we aim to develop novel theoretical approaches to study such singularities. The goal is to investigate in various situations how the nonlinear elastic response of the material modifies the behavior of elastic fields in the vicinity of these singularities and how it affects their shape and mechanical response. Our exploration will rely on simplified geometries that capture fundamental and generic aspects of the proposed problems.

The internship will be performed jointly between Gulliver (ESPCI) and the Laboratoire de Physique (ENS de Lyon), in collaboration with Marcelo Dias (University of Edinburgh) and Dominic Vella (University of Oxford).

**Keywords:** thin sheets, mechanics, geometry, nonlinear physics

# Phase Waves in Active Solids

**Encadrants:**

**Olivier Dauchot (Gulliver)**

**Possibilité de thèse: selon les avancements du projet**

**Financement de thèse: potentiellement**

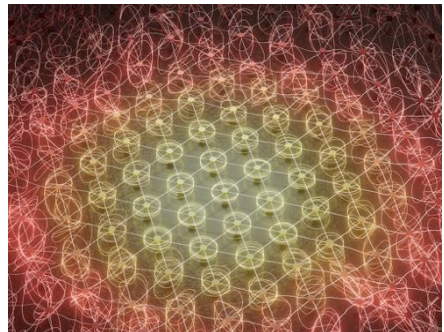
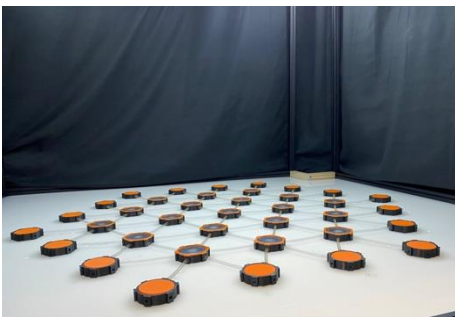


Figure. Active elastic lattices and Collective Actuation



# ACTIVE MATTER & COLLECTIVE EFFECTS

## Résumé

Active matter describes systems in which the elementary constituents consume energy to produce work. In active liquids, this work is turned into motion and the interactions lead to fascinating collective motion, as widely observed in nature, from bird flocks to cellular cytoskeletons.

In active solids, the elementary constituent are embedded in an elastic matrix in which they exert local stresses. These stresses deform the matrix. The induced strain in turn acts on the active units. As a result of this retro-action one observes spontaneously oscillating solids. Eventually, designing the elastic matrix and its coupling to the active units, one could program a new type of functional materials.

In the past three years we have tailored an artificial system that combines activity and elastic architecture and demonstrated that selective and collective actuation is a hallmark of active solids <https://twitter.com/i/status/1561626005520932864>. These results open a brand-new avenue of research, from further experimental and numerical investigations to theoretical analysis.

During this internship we would like to study **the propagation of waves in such solids**. These waves are phase waves of the oscillations, that emerge when the activity is large enough.

Depending on the personal taste of the intern, the project can be mostly experimental, or numeric, or theoretical. In all cases, we will take advantage of our existing set-up as well as our « walking grains », a system of self-propelled particles, which we have developed and extensively used in the past ten years. We also have good numerical models of these systems, which can be useful in examining the large-scale physics.

**Keywords: active matter, elastic lattices, waves, etc...**

# Mechanical Response of Active Solids

**Encadrants:**

**Olivier Dauchot (Gulliver)**

**Possibilité de thèse: non**

**Financement de thèse:**

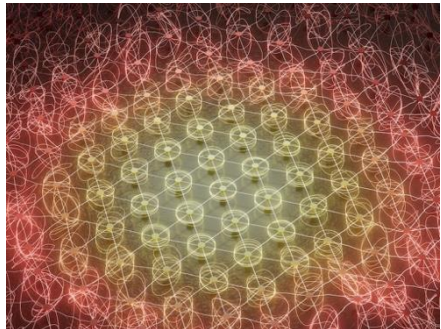
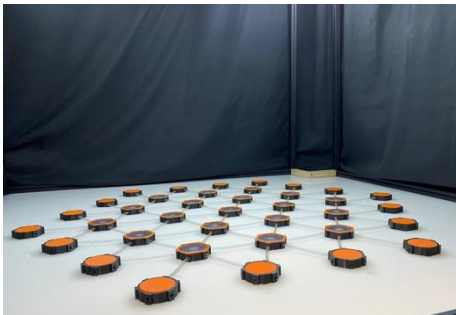


Figure. Active elastic lattices and Collective Actuation

# ACTIVE MATTER & COLLECTIVE EFFECTS

## Résumé

Active matter describes systems in which the elementary constituents consume energy to produce work. In active liquids, this work is turned into motion and the interactions lead to fascinating collective motion, as widely observed in nature, from bird flocks to cellular cytoskeletons.

In active solids, the elementary constituent are embedded in an elastic matrix in which they exert local stresses. These stresses deform the matrix. The induced strain in turn acts on the active units. As a result of this retro-action one observes spontaneously oscillating solids. Eventually, designing the elastic matrix and its coupling to the active units, one could program a new type of functional materials.

In the past three years we have tailored an artificial system that combines activity and elastic architecture and demonstrated that selective and collective actuation is a hallmark of active solids <https://twitter.com/i/status/1561626005520932864>. These results open a brand-new avenue of research, from further experimental and numerical investigations to theoretical analysis.

During this internship we would like to study **the mechanical response of such solids**. Preliminary observations reveal **extremely anomalous elasticity**, with mechanical response in the direction orthogonal to the stimulus!

Depending on the personal taste of the intern, and the progress of the project, the internship can be mostly experimental, or numeric, or theoretical. In all cases, we will take advantage of our existing set-up as well as the good numerical models of these systems.

**Keywords: active matter, elastic lattices, mechanics, etc...**

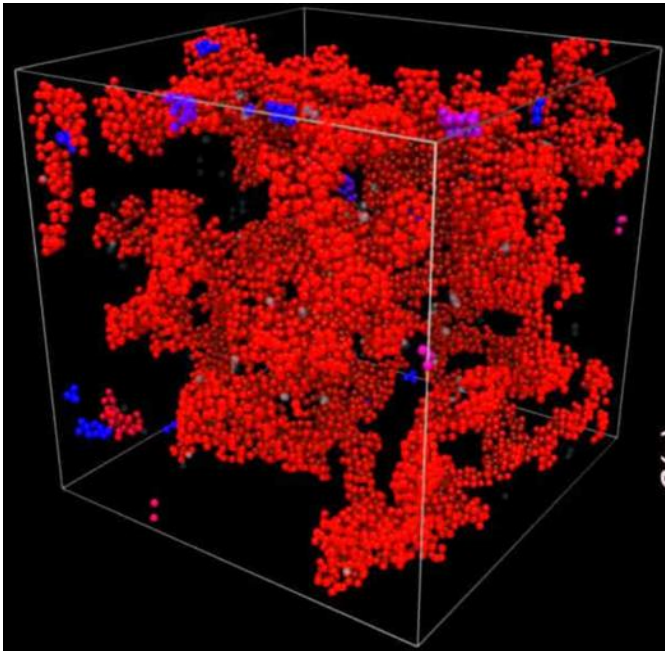
# Boltzmann inversion : measuring forces by watching movies

**Encadrant: Ludovic Berthier (Gulliver)**

**Possibilité de thèse: Oui**

**Financement de thèse:** Candidature à l'EDPIF

**Contact:** ludovic.berthier@espci.fr



Confocal microscopy image of a colloidal gel. The goal is to infer directly from such images the interactions that lead to the formation of this material.

# ACTIVE MATTER & COLLECTIVE EFFECTS

## Résumé

Statistical mechanics traditionally starts from the microscopic details: Given some rules, interactions, equations of motion, one tries to make predictions about 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 microscopic 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**

# Reconfigurable active matter in 3d

## Encadrants:

C. Patrick Royall (Gulliver)

Possibilité de thèse: Oui

Financement: Non

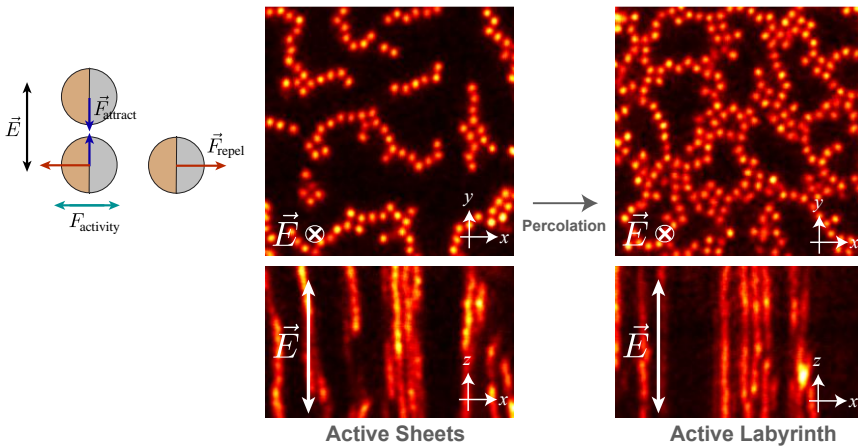


Figure. Active colloids in 3d. (left) The electric field  $E$  provides the activity in the  $xy$  plane. It also induces dipolar interactions, an attraction in  $z$  and repulsion in  $xy$ . (right) Snapshots of new phases of matter using 3d confocal microscopy. Top  $xy$  planes showing sheet phase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

# ACTIVE MATTER & COLLECTIVE EFFECTS

## 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 central role and among these are active micron-sized particles (colloids) [1]. Here the interactions between the particles are well-understood and machine learning methods facilitate long—standing challenges with coordinate tracking. In particular, colloidal particles assemble in to a variety of structures, which can be interpreted with statistical mechanics [2]. However almost all work with active colloids has used 2d systems.

We have developed a 3d active colloidal system of dipolar particles which has already produced two new phases (see Figure) [3]. This project proposes to investigate further 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 [4,5].

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

[2] Royall et al *ArXiv* 2305.02452 (2023), accepted *Rev. Mod. Phys.*

[3] Sakai N and Royall CP, *ArXiv* 2010.03925 (2020).

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

[5] Chao X et al *ArXiv*:2404.12218 (2024).

# Three is a crowd: Many-Body Correlations and Tuning Behaviour in Zebrafish

**Encadrants:**

**C. Patrick Royall (Gulliver)**

**Possibilité de thèse:** Oui

**Financement:** Non

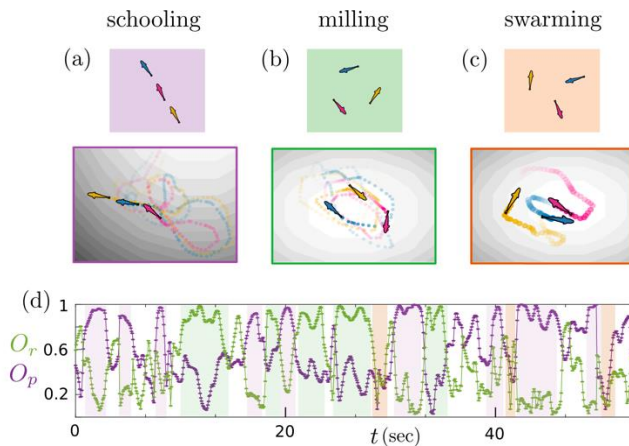


Figure. States in the zebrafish system. (a) Schooling, high polarization  $O_p$ , (b) milling, high  $O_r$  and (c) swarming low  $O_p$  and  $O_r$ . (d) Time-evolution showing multistate system behaviour.



# ACTIVE MATTER & COLLECTIVE EFFECTS

## Résumé

Collective behaviour in biological systems and its connections to phase transitions in physical systems has driven much of the current surge of interest in active matter. From birds to midges to bacteria, a variety of phenomena across a range of lengthscales have been investigated.

While collective behaviour in fish has received some attention, less is known where the fish are tracked in 3d. This project develops our existing work modelling experimental data with simple active matter models, to more sophisticated models which include perception [1,2].

The key aims of this project are as follows:

- We have recently shown there is no fundamental difference in behaviour in groups of 3-50 fish – “three is a crowd” [2]. But how does this change in larger groups? Are the normal order parameters even appropriate to larger groups?
- We have been able to tune the swimming in zebrafish through genetic modification [3]. The swimming behaviour is changed, but can the mutant fish be described within the same modelling framework as the wild type?

[1] Yang Y *et al*, *PLOS Comp. Biol.* 18 e1009394 (2022).

[2] Zampetaki A, et al *Nature Commun* 15 2591 (2024).

[3] Yang Y *et al*, In press, *PLOS Comp. Biol.*, BioRxiv doi.org/10.1101/2024.04.02.587671 (2024).

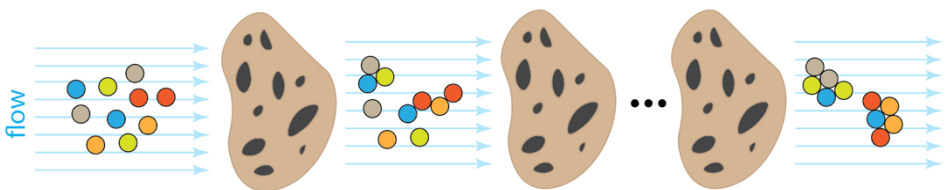
# Material assembler

**Encadrants:**

**Z. Zeravcic (Gulliver)**

**Possibilité de thèse:** Oui

**Financement de thèse:** Non



### Résumé

Biology is a discipline studying life-as-we-know-it: life on earth, based on carbon chemistry. Even though it is the result of millennia of evolution through natural selection, there is no reason to believe that this form of flora and fauna around us is the only possible ``solution'', leading to one of the fundamental obstacles in theoretical biology: how can one establish general theories of life when only one instance of it is available to us? The field of Artificial life — essentially a synthetic approach to biology — is trying to bridge the gap by exploring life-as-it-could-be. The reactions and types of molecules we observe in living systems, however, can constrain and make the exploration and reaching conclusions difficult. We therefore turn to artificial chemistries that study and explore 'chemical' reactions as they could be imagined. In an artificial chemistry, one starts with reactants, i.e., building blocks or 'atoms', that follow certain interaction rules we prescribe. This leads to a combinatorial space of possible structures, i.e., 'molecules', that goes beyond what we know in the chemistry we live in. We then define how the molecules interact leading to the dynamics in this vast combinatorial space.

In this project we want to study how presence of interactions between the building blocks and a porous 2d structure (through which the blocks travel) impact the final assembly observed. We are looking for a candidate with a strong background in statistical physics, programming and an interest for interdisciplinary subjects.

# Emergent computational abilities of chemical reaction networks

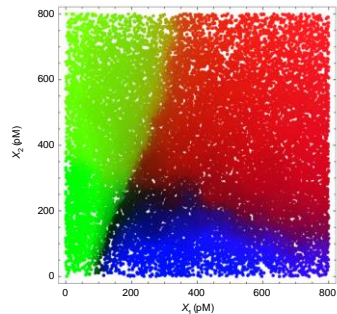
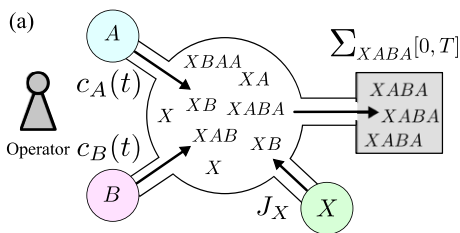
**Encadrant: D. Lacoste (Gulliver)**

**Possibilité de thèse: Oui**

**Financement: Non**

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Left: By introducing template molecules at appropriate times a control in the output of a chemical network can be achieved, with the final composition playing the role of the result of a computation. Figure from I. Kobayashi et al., PRL (2022). Right: classification task performed with enzymatic neural networks [3].

# PROGRAMMABLE MATTER

## Summary

We propose to study strategies to control chemical reaction networks, in order to use them to perform computations, with certain similarities to the computations by biological or artificial neural networks. In these systems, certain properties can be emergent when they arise from the interactions of a large number of components. In the group, we have studied previously two such properties, homochirality [1] and autocatalysis [2] and we have found that their emergence is indeed favored in large chemical networks. We are now interested in new emergent properties, related to the ability to perform some form of computation. Computation should be understood here as the ability of the chemical network to dynamically reach a certain final composition given an initial composition as illustrated in the figure. We are interested in robust computations in the sense small perturbations in the kinetics of chemical reactions should not affect the final composition.

An experimental demonstration of a classification task using molecular chemical networks based on DNA has recently been realized by two members of the lab Y. Rondelez and G. Gines [3]. Inspired by this work, we propose to formalize theoretically and study numerically control strategies of molecular chemical networks based on DNA (or possibly RNA). The control parameters are here template molecules, which can be autocatalytically amplified but are typically in competition with each other. By viewing these templates as weights to be optimized, modern machine learning methods may be used for this problem.

The goal of this internship/thesis is to understand how to best control chemical reaction networks. We ask what are the fundamental limits in the computation power of such networks. These limits may depend on the topology of the chemical network or on thermodynamic constraints [4], because any computation necessarily requires some amount of dissipation. To address these questions, we rely on recent methods of non-equilibrium Statistical Physics, Stochastic Thermodynamics and Machine learning. This theoretical internship will benefit from interactions with experimentalists in the lab and abroad.

[1] Emergence of homochirality in large molecular systems, <sup>†††</sup>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).

[3] Nonlinear decision-making with enzymatic neural networks, S. Okumura et al., Nature, 610, 496 (2022).

[4] Structural constraints limit the regime of optimal flux in autocatalytic reaction networks, A. Despons et al., Commun. Phys. (2024)

# Self-replicating materials

**Encadrants:**

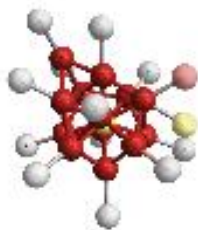
**Z. Zeravcic (Gulliver)**

**Possibilité de thèse:** Oui

**Financement de thèse:** Non



template



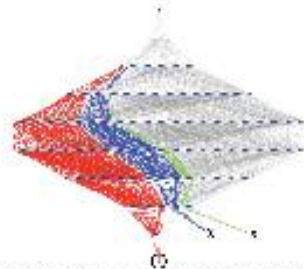
template + attached particles



potential networks of attached particles



examples of detached networks of particles



an example in a potential energy landscape

### Résumé

The next generation of materials is expected to have unprecedented functionalities, like those that already exist in biological systems. To be able to discover and produce novel advanced materials we need new paradigms for their synthesis. Fabrication of materials through the process of self-replication is one such paradigm. In general, the self-replication process starts from a template, i.e., a pre-formed object, which is introduced into a solution of building blocks, all following precise interaction rules. Free building blocks attach to specific places on the template, form bonds between themselves and eventually detach from the template, and fold into a copy of the template. The copy is ready to serve as an independent template, leading to exponential multiplication of the initial object. Over the past decade it has been demonstrated in theory and experiments how very small assemblies of building blocks can self-replicate [1-3]. Going beyond a few building blocks has remained a formidable challenge.

We propose a new way forward, inspired by the structure of biological macro-molecules and by multivalent interactions. The internship will consist in testing replication schemes for an assembly of  $N > 10$  building blocks using coarse-grained computer simulations. We are looking for a candidate with a strong background in statistical physics, programming and an interest for interdisciplinary subjects.

[1] Z. Zeravcic and M. P. Brenner PNAS 111 (2014)

[2] He, X. et al., Nature Materials 16 (2017)

[3] Zhuo, R. et al., PNAS 116 (2019)

**Keywords: self-replication, DNA-coated colloids, self-assembly, template, folding**

# Diffusive transport in complex, near-surface media

**Encadrants:**

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**Possibilité de thèse:** Oui

**Financement:** Non

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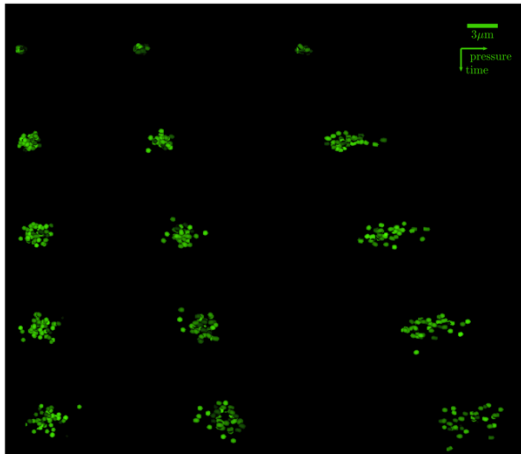


Figure. Near-surface nanoparticle dynamics observed using total internal reflection fluorescence. The columns are time series ( $\Delta t = 12$  ms) for larger and larger mean velocities in a microfluidic flow. Detailed analysis of the dynamics of these particle clouds provide diffusive and advective dynamics.



## Résumé

The dynamics of disordered systems are ubiquitous in condensed matter physics, from glasses to intracellular media. One emblematic example is that of jammed polymer microgel suspensions. Particularly, the surface dynamics of such systems characterized by surface shear stress and slip velocity is the object of much research. In the last decades, these latter quantities were linked under the interpretation of a solvent-rich depletion layer near a smooth wall; often, this wall is one of a channel containing a pressure-driven flow. During this internship, we will study the the complete interfacial transport of jammed microgel suspensions in microfluidic channels. Overall, we will link (i) the microscopic and local diffusive dynamics in the depletion layer, the advective transport there, to (ii) the global dynamics of the gel in the full-channel flow. To study these phenomena, we will use the experimental and surface-sensitive technique total internal reflection fluorescence, while complementary  $\mu$ PIV experiments are planned with collaborators in Lyon. We thus achieve the multi-scale observations needed to link the global/channel and local/near-wall flows. Our study will bring first measurements on the impact of realistic roughness on these common complex flow scenarios, while revealing the fundamental link between the local near-wall dynamics and the macroscopically-measured boundary conditions piloting the entire channel flow.

- [1] A. Vilquin et al., PRL, 130, 038201 (2023)
- [2] G. Guyard et al , Soft Matter, 17, 3765 (2021)
- [3] J Péméja et al. PRFluids, 4, 033301 (2019)

**Keywords: soft matter, hydrodynamics, complex fluids, boundary conditions, diffusion**