7th Warsaw School of Statistical Physics

Poster session

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A stochastic model of mixed-phase cloud micro-physics

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Mixed-phase clouds, i.e., clouds that contain both super-cooled water droplets and ice crystals, are ubiquitous in the atmosphere and play an important role in the climate system. The mixture of liquid and solid water in sub-zero temperatures leads to a condensational instability, in which ice particles tend to grow at the expense of droplet evaporation. Nonetheless, mixed-phase clouds are unexpectedly long-lived. We claim that small-scale turbulence is key to explain the persistence of such systems. Due to limited computational resources, weather simulation on a global scale is limited to coarse grids with a resolution of kilometers at best. On the other hand, a typical turbulent flow inside a cloud will display an intricate structure of eddies down to the scale of centimeters. We propose a Lagrangian stochastic micro-physical scheme to account for sub-grid fluctuations in velocity, temperature and water vapor fields. The impact of our scheme on phase partitioning is tested in a synthetic, turbulent-like flow that mimics an Arctic mixed-phase stratocumulus (AMPS) cloud. Results are confronted with idealized reference simulations that use Eulerian bulk micro-physics based on an assumed (temperature-dependent) phase partitioning function. Our study suggests that accounting for local variability in a turbulent cloud is important for reproducing steady-state mixed-phase conditions.

Coalescence of surfactant-laden droplets

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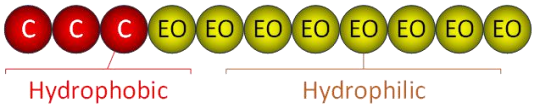
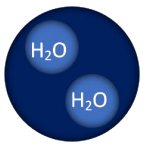
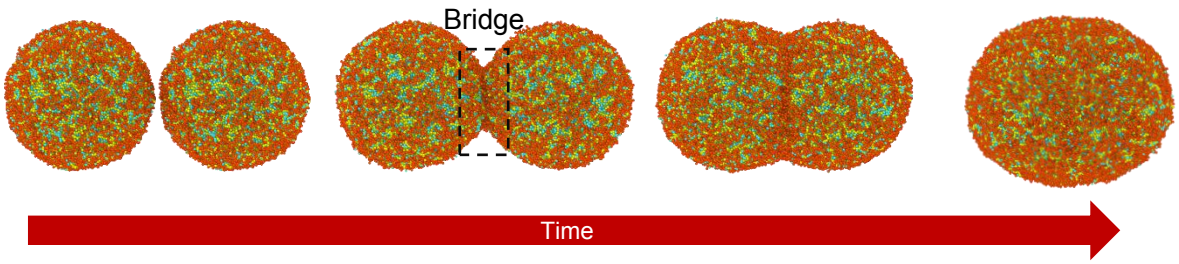
Droplet coalescence is commonly encountered in nature and is also relevant for various technologies, such as inkjet printing. In this poster, we present our results on the coalescence of surfactant-laden water droplets, which have been obtained by means of molecular dynamics simulation of a coarse-grained (CG) force-field. In particular, we will discuss the details of the coalescence mechanism and the bridge growth dynamics.



CG representation of C10E8 surfactant



CG representation of Water



Far from equilibrium transport on TASEP with Pockets

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Nowadays, it is quite unbelievable to think of a world without access to transport. Over the years, transport has enhanced our lives, and we can't imagine thriving in this current world without the capability to transport. However, in real, system of mutually interacting particle occur in environment with a net driving force acts upon them. These systems are in non-equilibrium for all the times and can attain the non-equilibrium steady state. Many physical systems like traffic flow, pedestrian motion, cellular transport, protein synthesis are some intriguing examples of stochastic non-equilibrium system where transport processes occur along complex structure of pathways [1]. In comparison to their equilibrium counterparts, non-equilibrium processes are far more diversified and interesting. Since, the motion of the active species in the above discussed physical and biological transport processes is continuously triggered by the supply of energy, they fall under a special class of non-equilibrium systems known as "driven-diffusive systems".

In last few decades, Totally Asymmetric Simple Exclusion Process (TASEP) is proved to be a paradigmatic lattice-gas model that provides a general framework to study the non-equilibrium transport in these driven-diffusive systems. In this poster, we present the study of a geometric adaptation of a totally asymmetric simple exclusion process with open boundary conditions, where each site of a one-dimensional channel is connected to a sideways space (pocket) on the lateral [2]. The number of particles that may be accommodated in each pocket is determined by its capacity q. The continuum mean-field approximation is deployed for the case $q = 1$ where both lattice and pocket strictly follow the hard-core exclusion principle. In contrast, a probability mass function is utilized along with the mean-field theory to investigate the multiple-capacity case, where the pocket violates the hard-core exclusion principle. The effect of both finite and infinite reservoirs has been studied in the model [3]. The explicit expression for particle density has been calculated, and the evolution of the phase diagram in $\alpha - \beta$ parameter space obtained with respect to q and the attachment-detachment rates. In particular, the topology of the phase diagram is found to be unchanged in the neighbourhood of $q = 1$. Moreover, the competition between lattice and pocket for finite resources and the unequal Langmuir kinetics captures a phenomenon in the form of a back-and-forth transition [4]. We have also investigated the limiting case $q \to \infty$. The theoretically obtained phase boundaries and density profiles are validated through extensive Monte Carlo simulations.

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Colossal Brownian yet non-Gaussian diffusion in a periodic potential: impact of nonequilibrium noise amplitude statistics

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Authors previously studied an overdamped dynamics of nonequilibrium noise driven Brownian particle dwelling in a spatially periodic potential and discovered a novel class of Brownian, yet non-Gaussian diffusion[1]. The mean square displacement of the particle grows linearly with time and the probability density for the particle position is Gaussian, however, the corresponding distribution for the increments is non-Gaussian. The latter property induces the colossal enhancement of diffusion, significantly exceeding the well known effect of giant diffusion. Here we considerably extend the above predictions by investigating the influence of nonequilibrium noise amplitude statistics on the colossal Brownian, yet non-Gaussian diffusion[2]. The tail of amplitude distribution crucially impacts both the magnitude of diffusion amplification as well as Gaussianity of the position and increments statistics. Our results carry profound consequences for diffusive behaviour in nonequilibrium settings such as living cells in which diffusion is a central transport mechanism.

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Universality in dynamical networks undergoing growth and contraction

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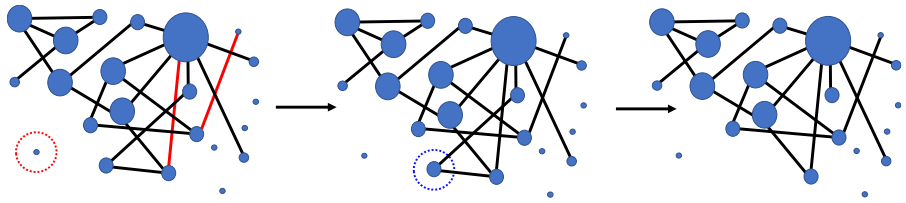
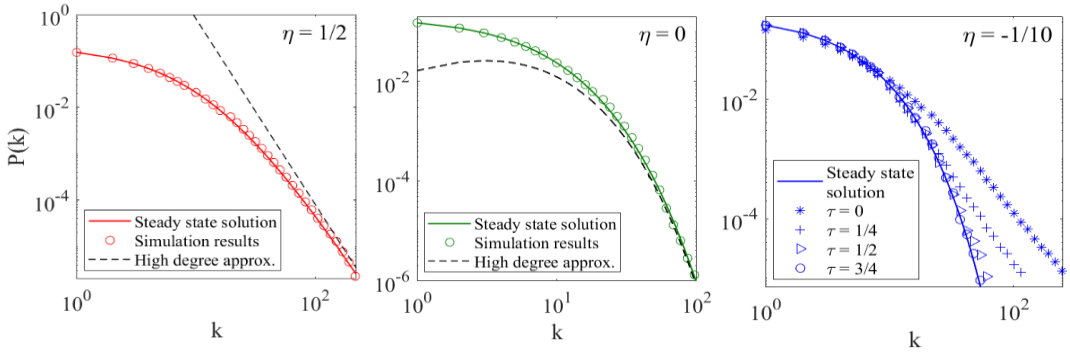


Growth step: with probability $(1+\eta)/2$ add a new node & add m new links, **preferentially**

Contraction step: with probability $(1-\eta)/2$ delete a **random** node

Complex networks and dynamical processes taking place on them play a central role in current research. While models of growing networks were studied extensively, in realistic situations, networks undergo a combination of growth and contraction processes. **We are looking for the dynamical degree distribution of generic networks, $P_t(k)$, while being exposed to all kinds of growth and contraction mechanisms.** For example, we may consider the following model: at each time step one of the following possibilities occur: **(a) growth step:** with probability $(1+\eta)/2$ a new node is added to the network, and m existing nodes are connected **preferentially** (connecting high degree nodes with higher probability). **(b) contraction step**: with probability $(1-\eta)/2$ a **random node** is deleted from the network, together with all its links. The parameter $-1 \le \eta \le 1$ is essentially the rate at which the size of the network, N_t, evolve with time: $N_t = N_0 + \eta t$. This model exhibits a nontrivial phase transition between a power-law (scale free) and an exponential degree distribution that occurs at $\eta = 0$, exactly when the deletion rate balances the growth rate. At the phase transition we get a stretched exponential. This is summarized below:

$$P(k) \underset{k\gg 1}{\sim} \begin{cases} k^{-(2+\frac{1}{\eta})} & \eta > 0 \quad \text{Power law} \\ k^{\frac{m}{2}-\frac{3}{4}} e^{-2\sqrt{k}} & \eta = 0 \quad \text{Stretched exponential} \\ k^{m(1+\eta)+\frac{1}{\eta}} (1-\eta)^{-k} & \eta < 0 \quad \text{Discrete Gamma} \end{cases}$$



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Large deviations of reflected diffusions

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We consider a Markov diffusion $\boldsymbol{X}(t)$ evolving in $\mathbb{R}^d$ according to a stochastic differential equation. For a dynamical observable A_T of the process $\boldsymbol{X}(t)$ having the general form

$$A_T = \frac{1}{T}\int_0^T f(\boldsymbol{X}(t))dt + \frac{1}{T}\int_0^T \boldsymbol{g}(\boldsymbol{X}(t)) \circ d\boldsymbol{X}(t), \tag{1}$$

it is known that in practice the probability density $P(A_T = a)$ often has the asymptotic form

$$P(A_T = a) \approx e^{-TI(a)} \tag{2}$$

for large T. An observable for which the associated probability density has this asymptotic form is said to satisfy a large deviation principle with rate function I. The rate function describes the probability with which both small and large fluctuations of the observable A_T occurs as T becomes large.

Calculating the rate function directly is intractable even for simple systems. As a result, the rate function is often found indirectly via a spectral calculation.

We are interested in the event where the diffusion $\boldsymbol{X}(t)$ evolves in some bounded domain, with the boundaries assumed to be reflective. The proper boundary conditions for the spectral calculation associated with obtaining the large deviation functions in the presence of reflecting boundaries is discussed, and the implications for the effective process (which describes how fluctuations arise in the long-time limit) are explored. Some applications of this work are also discussed. This provides a summary of recent work [1, 2] in which a comprehensive approach to obtaining the appropriate boundary conditions for reflective boundaries was developed for observables having the form (1). Furthermore, this approach can be extended to other boundary types as well.

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Inertial Lévy flights in bounded domains.

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The escape from a given domain is one of the fundamental problems in statistical physics and the theory of stochastic processes. We explore properties of the escape of an inertial particle driven by Lévy noise from a bounded domain, restricted by two absorbing boundaries. The properties of the mean first passage time for the integrated Ornstein-Uhlenbeck process driven by Lévy noise are compared to its Brownian counterpart i.e. randomly accelerated process. Mean first passage time considerations are complemented by analysis of the escape velocity and energy along with their sensitivity to initial conditions.

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MDPD Simulation of Liquid Thread Break-up and Formation of Droplets

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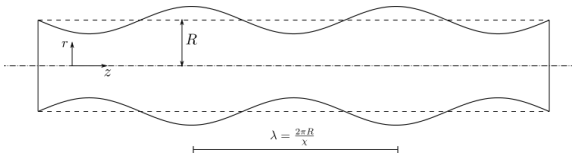
Formation of droplets from the break-up of liquid nano-threads is an interesting phenomena in fluid dynamics that is relevant in many industrial applications, such as: drug manufacturing, inkjet printing, and nanowire fabrication.

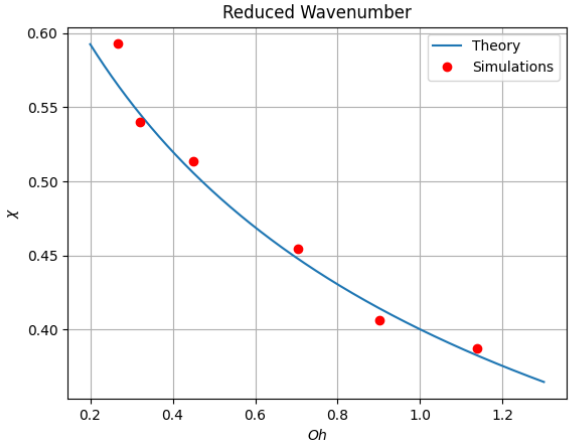
The classical theory, used to describe the break-up of liquid threads, has its origins in the works of Rayleigh and Plateau, who showed through linear stability analysis that a fluid cylinder is unstable for perturbations that have a wavelength superior to its circumference. Moreover, there exists a characteristic wavelength for which the perturbations are the most unstable. The figure below shows a schematic representation of the Rayleigh-Plateau instability problem.



The goal of this work is to assess the validity of the results obtained from linear stability analysis of the continuum fluid dynamics equations at the molecular level, where the thermocapillary waves are responsible for the instability that leads to the break-up of a liquid thread. Because of the spatial scale of interest, we chose a simulation method known as many-body dissipative particle dynamics, which is a coarse-grained molecular method that represents the hydrodynamics of this problem well and is more computationally efficient when compared to traditional molecular dynamics. Different fluids can be simulated by tuning the model parameters. These fluids are studied in terms of their Ohnesorge number $Oh = \mu/\sqrt{\rho\sigma L}$, which is the ratio between viscous forces and inertia and surface tension.

We can calculate the characteristic wavelength that leads to the break-up for different types of fluids by computing the Fourier transform of the density correlation function.

To make the results statistically more relevant, we took the average from 30 trajectories for each fluid simulated and compared it with a theoretical prediction made by Chandraseker. The characteristic wavelengths obtained are presented in the figure below where they show a good agreement.



Ground state energy of the polarized diluted gas of interacting spin $1/2$ fermions by Effective Field Theory

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The effective field theory approach simplifies the perturbative computation of the ground state energy of the diluted gas of fermions allowing in the case of the unpolarized system to easily re-derive the classic results up to the $(k_{\rm F}a_0)^2$ order (where $k_{\rm F}$ is the system's Fermi momentum and a_0 the s-wave scattering length) and (with more labour) to extend it up to the 4-th order in Fermi momentum. The corresponding expansion of the ground state energy of the polarized gas of spin $1/2$ fermions is known analytically or semi-analytically (to the best of our knowledge) only up to the $(k_{\rm F}a_0)^2$ (where $k_{\rm F}$ stands for $k_{{\rm F}\uparrow}$ or $k_{{\rm F}\downarrow}$) order [1], [2]. Here we show that the same effective field theory method allows to easily re-compute also the order $(k_{\rm F}a_0)^2$ correction to this result, and present some results towards extending the computation to the third-order. The obtained results suggest a change of the order of transition to the phase with the spontaneous polarization: with the order $k_{\rm F}a_0$ correction (equivalent to the mean field approximation) it is of the second order, whereas inclusion of the order $(k_{\rm F}a_0)^2$ correction changes it to first-order one.

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Differential diffusion of bouncing grains

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More than two centuries ago, Chladni noticed that salt grains, when deposited on a vibrated metal plate, spontaneously gather into remarkable geometric figures [1]. We now understand that these figures represent the eigenmodes of the vibrating plate: the bouncing grains accumulate along the nodal lines.

The mechanism by which the grains gather, however, remains debated. As the bouncing grains move erratically over the plate, one is tempted to interpret their trajectories as random walks, and their collective motion as diffusion. Here, we suggest the grains gather where diffusivity is low, thus producing Chladni figures by differential diffusion.

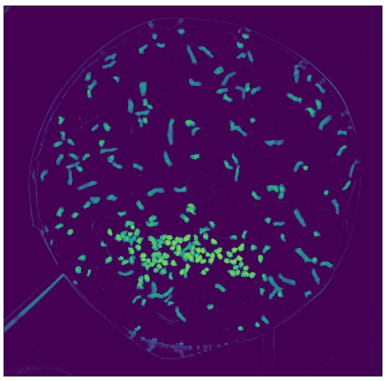
To investigate this hypothesis, we design a series of experiments in which grains bounce on a heterogeneous surface. We observe that the places of lower diffusivity indeed collect a denser population of grains (figure below). At equilibrium, the surface density of grains, ρ, appears to be inversely proportional to the local diffusivity, D:

$$\rho \propto 1/D. \tag{1}$$

This finding accords with the reasoning of Büttiker and Landauer who argued that, when random walkers are submitted to a thermal gradient, they should generate a macroscopic flux [2, 3]. Following these authors, we propose that the flux of bouncing grains reads

$$\mathbf{q} = -\nabla(D\,\rho) \tag{2}$$

which, in equilibrium, yields equation (1). Particles that diffuse according to this law can produce steady states with finite currents, even in closed systems. We pursue these elusive configurations in our experiments.



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Bifurcations in droplet collisions

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Smoluchowski [1] calculated how the collision rate of non-interacting spheres settling due to gravity depends upon the strength of gravity and upon the radii of the spheres. Saffman and Turner [2] argued that the collision rate for non-interacting droplets in turbulence increases as the turbulent strain rate increases. However, these studies ignored the effects of interactions between the droplets. The numerical simulations of droplets settling in a steady straining flow performed by Dhanasekaran et al. [3] show that droplet-droplet interactions result in a complex dependence of the collision rate on the strain rate and on the differential settling speed.

We show that this dependence is explained by a sequence of bifurcations in the collision dynamics. We compute the bifurcation diagram when strain is aligned with gravity, and show that it yields novel insights into the collision dynamics. First, the steady-state collision rate remains non-zero in the limit $\mathrm{Kn} \to 0$, contrary to the common assumption that the collision rate tends to zero in this limit (Kn is a non-dimensional measure of the mean free path of air). Second, the non-monotonic dependence of the collision rate on the non-dimensional differential settling speed is explained by a grazing bifurcation. Third, the bifurcation analysis explains why so-called 'closed trajectories' appear and disappear. Fourth, our analysis predicts strong spatial clustering near certain saddle points, where the strain is balanced by the differential settling.

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Collective dynamics in systems of growing rods

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Recent research shows that in confined populations of growing and dividing rods, such as microcolonies of bacteria, a complex interplay between growth activity, fluctuating inter-particle forces and boundary effects can lead to emergent collective dynamics, including global flow of cellular matter and alignment due to the nematic symmetry of local mechanical interactions. Here, we use a new versatile framework for agent-based simulations to explore these effects in systems with different geometries containing two-dimensional spherocylinders. We observe the emergence of orientational order in rectangular channels and analyse its dependence on both microscopic parameters of the rods and the geometry of the confinement. Further observations of complex orientation patterns in open polygonal domains hint at a link between shear rate anisotropy and orientation.

Self-organized growth of cellular substrates

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Growing colonies of rod-shaped bacteria commonly feature order and alignment of the constituent particles. This is generally thought to be the result of the active stresses generated by growth, mechanical volume exclusion interactions between cells, and shear-flow-induced effects due to confinement. However, how these contributing factors interact to give rise to the observed global alignment patterns remains elusive.

We study, *in-silico*, colonies of growing rod-shaped particles of different aspect ratios confined in channel-like geometries. A spatially resolved analysis of the stress tensor reveals a strong relationship between near-perfect alignment and an inversion of stress anisotropy for particles with large length-to-width ratios. We show that, in quantitative agreement with an asymptotic theory, strong alignment can lead to a decoupling of active and passive stresses parallel and perpendicular to the direction of growth, respectively. Our results illustrate the complexity arising from the inherent coupling between nematic order and active stresses in growing active matter which is influenced by geometric and configurational constraints due to confinement.

Durotaxis motion on brush substrates

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A range of industries require the self-sustained directed motion of nanoscale droplets on different substrates for various purposes [1, 2], for example, in the context of microfabrication [3], coating [4], microfluidics and thermal control [3, 4]. One way of causing such motion is durotaxis, where a gradient stiffness of a substrate is used to enable droplets to move along the direction of the gradient. Using molecular dynamics, we show that the motion of a droplet on a brush substrate depends on the range of stiffness variation compared to the chain length and grafting density of the brush, and the interaction between the brush and the droplet. Our analysis indicates that a brush substrate of a moderate grafting density induces the most efficient droplet motion, while motion efficiency depends only weakly on the stiffness gradient. Finally, a larger size of the droplet favours the durotaxis motion on brush substrates.

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Tubular-body theory for viscous flows

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Cable-like bodies play a key role in many biological fluid systems but are hard to simulate. Asymptotic theories, called slender-body theories, are effective but apply in specific regimes and can be hard to extend beyond leading order.

In this poster I show how to develop an exact slender-body-like theory for the surface traction of cable-like bodies in viscous flow. This theory expresses the traction as a series of solutions to a well-behaved one-dimensional Fredholm integral equation of the second kind. This process can be simply generalised to other systems. We test this theory against known solutions and then use it to look at the swimming of a tightly wound helix exposed to an external torque [1].

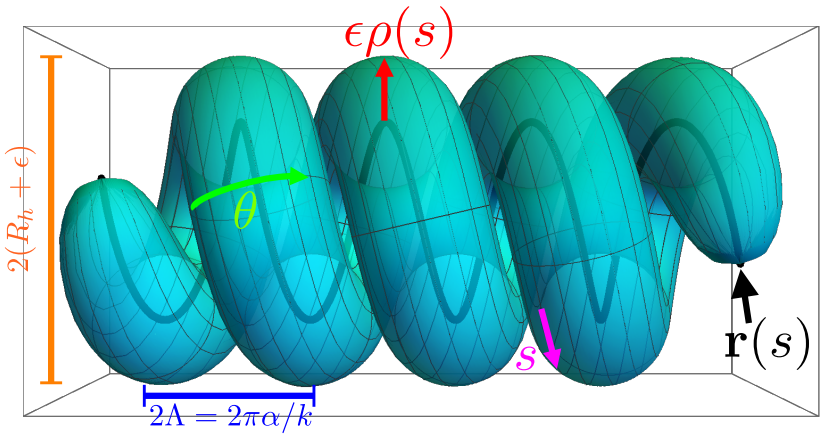

Figure 1: Diagram of of tightly wound helix

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Near-wall dynamics of colloidal dumbbells

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Dynamics of the arbitrarily-shaped colloidal particles in the vicinity of the geometric confinement remains widely unexplored. We provide a numerical tool to simulate the motion of such particles, including their Brownian motion, sedimentation, the wall-particle hydrodynamic and electrostatic interactions. The calculations are feasible given the particle's diffusion matrix and a model for the electrostatic force acting on the body. We took a particular interest in the colloidal dumbbells, which are particles of an axisymmetric bead-like shape, containing two identical spheres. According to the latest experimental results [1], dumbbells of single sphere's size ~ 1 μm surprisingly tend to be oriented at preferred angles with respect to the confining plane. This leads to the discrepancy with theoretical predictions of the most probable parallel-to-wall orientation. We investigate this disagreement numerically and inquire the origins of this unexpected behaviour. We compare our results obtained for numerically calculated exact values of the particle's mobility coefficients with their analytical approximations [2]. With the use of highly accurate tool to obtain the bead-like particle's diffusion matrix, we are capable of simulating the motion of a large ($N \sim 10^2$) number of beads of different sizes in a very short time.

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An Intuitive Understanding of the Spin Excitations of a 1D Antiferromagnet

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Antiferromagnetic Heisenberg spin model is one of the basic models in quantum magnetism. Although in two- and three-dimensional world its ground state has a classical order, in one dimension ("chains") there is no long-range order and the exact form of the ground state is provided by a rather complex Bethe Ansatz [1]. Even more intricate are the low energy magnetic excitations of a spin chain [2] — the notorious spinons, carrying fractional quantum numbers [3]. In this poster we show an alternative approach to the ground state as well as the low-lying excitations of the one-dimensional Heisenberg antiferromagnet, which, although approximate, gives a more physically intuitive picture than the exact Bethe Ansatz solution.

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A front propagation model of leaf growth

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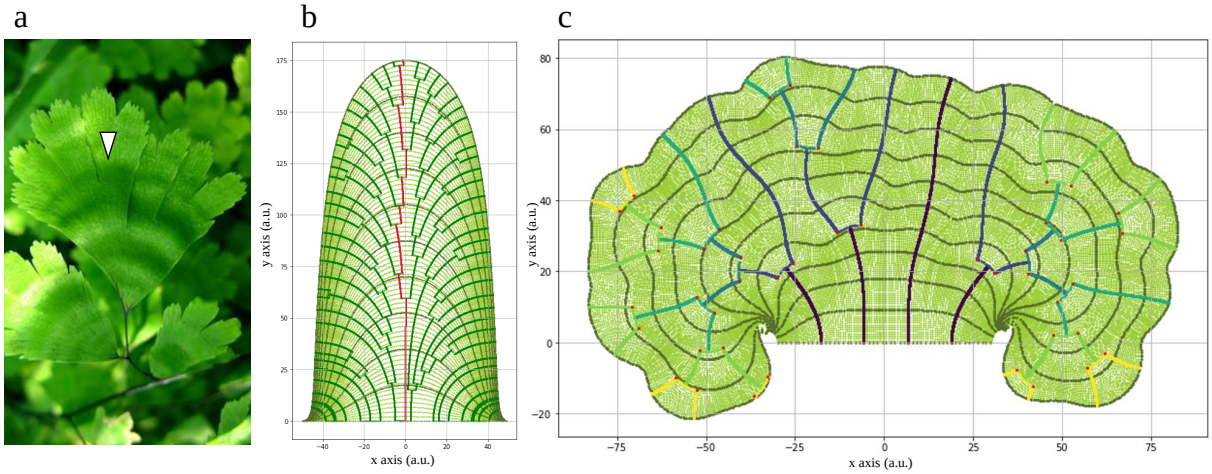
Leaves are photosynthetic organs with a diversity of shapes and complex vascular networks. During morphogenesis, two modes of growth are distinguished, peripheral and global [1]. In order to explain the peripheral development (Fig. (a)), we propose a numerical model of growth by interface propagation describing the dynamics of the vein network as a function of the initial shape of the front and the spacing of the veins.



(a) Leaf of *Adiantum capillari-veneris*. Shows a peripheral mode, and an oscillation of the growth front (arrow). (b) Proposed numerical model of peripheral growth, with growth of a single lobe. Successive growth fronts are emphasized every 50 time steps. The central vein is highlighted in red. (c) Modified model, with interdependence between front and vein growth. The gradient from blue to yellow represents the vein hierarchy. Emphasis every 50 time steps.

In the case of a single lobe growth, we find an unstable central vein, whose position oscillates in the middle of the lobe (Fig. (b)). Its dynamics can be modeled by an iterated function whose geometry explains the instability. On the contrary in nature the central vein presents very stable oscillations [2]. It is therefore necessary to modify the model and introduce a feedback loop. In a second model where the growth of the front is dependent on the position of the veins, we find two lobes by edge effect and an oscillation of the growth front, similar to an optical mode (Fig. (c)). This basic model can be modified to study the global growth.

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Rechargeable self-assembled droplet microswimmers driven by surface phase transitions

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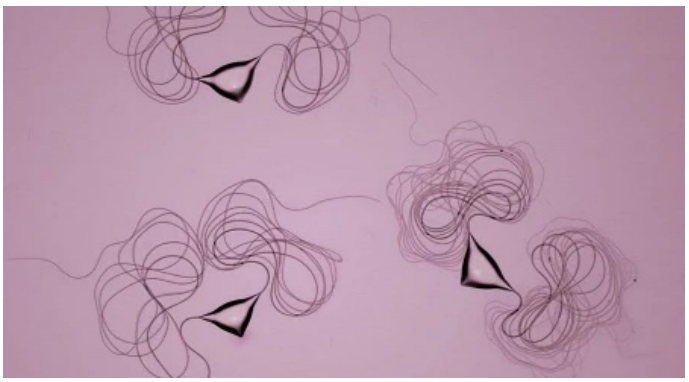
Swimming microorganisms and engineered artificial swimmers use multiple strategies to achieve propulsion in the viscosity-dominated microworld. A number of them use long, filamentous appendages called cilia or flagella. The motion of these slender objects is governed by a complex interplay between the driving forces, the elastic properties of the fibres, and the resistance forces of fluid.

A recently studied artificial system involving an emulsion of microscopic droplets of oil with surfactant in water exhibits swimming induced by the extrusion of elastic fibres by the droplets [1]. The extrusion is controlled by a surface phase transition of the surfactant, and it drives the motion of droplets. The transition is driven by small changes in the temperature of the environment, and can be reversed by switching between cooling and heating the system. The formation of a plastic phase by the surfactant induces shape changes of the droplets, where polyhedral shapes become energetically favourable. Further reconfiguration driven by the phase transition leads to the formation of filamentous structures originating at vertices of the now polygonal droplets. The extruded fibres undergo dynamic buckling and produce complex shapes, but also exert a force and torque on the droplets, resulting in translation and rotation of the droplets. We propose an elastohydrodynamic model for this phenomenon and describe the motion by a combination of theoretical considerations and numerical simulations. Our model serves as the basis for interpretation of experimental data and quantitatively grasps the swimming dynamics.



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Solitonic solutions in one-dimensional superfluid Bose-Fermi mixtures

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In this work we study solitonic solutions in quasi-one-dimensional superfluid mixtures of Bose and Fermi gases at low temperatures. The Fermi gas is studied both for the BCS interaction regime as well as at unitarity, and we allow for a non-zero spin polarization. The Bose gas forms a Bose-Einstein condensate. At this stage of the project, we put particlular emphasis on the solitonic solutions imposed on one of the interacting gases, and we study the response of the entire system to such a condition. The Fermi gas is described with the Bogoliubov-de Gennes equations for the BCS interaction regime and with a more general density functional, namely the Asymmetric Superfluid Local Density Approximation (ASLDA) for the uniatry interaction regime. The Bose-Einstein Condensate is described with the standrad Gross-Pitaevskii equation.

Finite-time dynamical phase transition in non-equilibrium relaxation

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In this poster, we analyse a finite-time dynamical phase transition in the thermal relaxation of a mean-field magnetic model [1]. The phase transition manifests itself as a cusp singularity in the probability distribution of the magnetisation that forms at a critical time. The transition is due to a sudden switch in the dynamics, characterised by a dynamical order parameter. We derive a dynamical Landau theory for the transition that applies to a range of systems with scalar, parity-invariant order parameters. Close to criticalilty, our theory reveals an exact mapping between the dynamical and equilibrium phase transitions of the magnetic model, and implies critical exponents of mean-field type. We argue that interactions between nearby saddle points, neglected at the mean-field level, may lead to critical, spatiotemporal fluctuations of the order parameter, and thus give rise to novel, dynamical critical phenomena.

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Equilibrium properties of the one-dimensional triangle-well fluid

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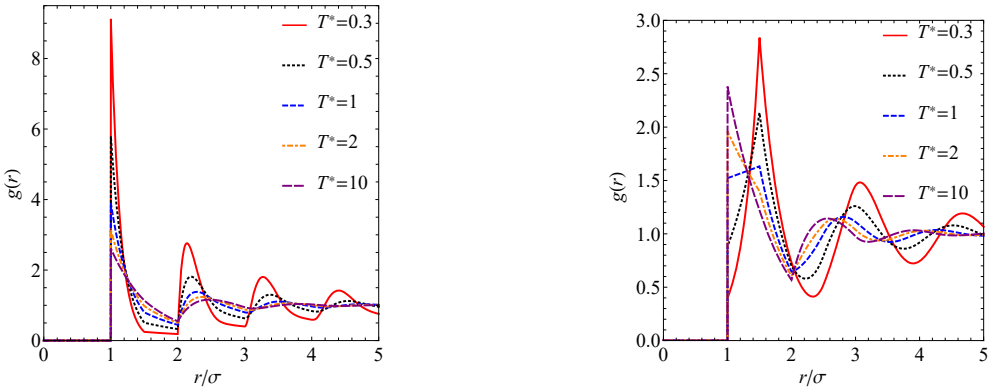
We present a comprehensive study on the thermophysical and structural properties of two prototypical classes of fluids confined in a one-dimensional line, namely the triangle-well and the ramp potentials. Both potentials are finite-ranged and have an impenetrable core of diameter σ plus a continuous linear part between $r = \sigma$ and $r = \lambda$. While the mathematical form of that additional part is analogous in both cases, the physical meaning is not. In the triangle-well potential the tail is attractive and, apart from its own physical interest, the main importance of the potential resides in representing the effective colloid-colloid interaction in the Asakura–Oosawa mixture. On the other hand, the ramp potential is purely repulsive with a softened core between $r = \sigma$ and $r = \lambda$.

The exact statistical-mechanical solution in the isothermal-isobaric ensemble for general nearest-neighbor interactions [1] is applied to the study of equilibrium properties of these two classes of fluids, such as the equation of state, the excess internal energy per particle, the structure factor $S(k)$, the direct correlation function $c(r)$, and the radial distribution function $g(r)$. In the latter case, in contrast to previous studies where $g(r)$ was obtained numerically from $S(k)$ by Fourier inversion [2], a fully analytic representation for $g(r)$ is derived in terms of a finite number of coordination-shell terms for any finite r [3]. As an illustration, the figure below shows $g(r)$ at some representative states for the triangle-well (left) and ramp (right) potentials.



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Optimal Vertical Navigation of Microswimmers in Steady Flow

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Survival of many plankton species depends on the largest biomass migration happening daily on Earth. This migration is known as diel vertical migration, during which planktonic species such as copepods swim towards the surface by dusk to feed form phytoplankton, and return to darker regions by dawn to prevent predation. Therefore, they are expected to have developed efficient swimming strategies, in order to swim up to few hundreds of meters everyday. Some strategies are passive, such as being bottom-heavy that tends to align the swimmer direction upwards. This is efficient for upward migration in quiescent flows, but it is often sensitive to turbulence which upsets the alignment. Since, planktonic swimmers have access to a wide range of hydromechanical information, it is possible for them to exploit this information for efficient navigation in turbulent flows. Here we present an active reorientation mechanism that increases the upwelling region sampling rate of swimmers in steady flows significantly.

Density estimation and fundamental diagrams for crossing flows of pedestrians without a spatial boundary

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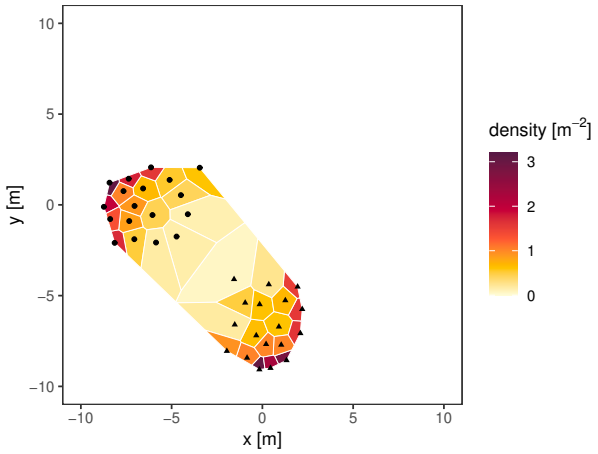
Construction of fundamental diagrams have been an essential tool in the context of crowd motion study to facilitate numerical simulations. There exists various definitions of fundamental diagrams, with the most used one is the variation of pedestrian velocity as a function of crowd velocity. For a crowd without any spatial boundaries, the methods of density estimation is itself a wide area of research.

In our work, we explore several methods of density estimation for the typical scenario of crossing flows. Many real-world situations produce crossing flows, such as streams of pedestrians crossing at a sidewalk intersection, or subway commuters passing each other when entering and exiting a metro car. The density estimation methods for our research consisted of both Lagrangian and Eulerian approaches, as well as voronoi-cell based methods.



For fundamental diagrams, we focus mainly to investigate the velocity-density relationship. In the existing literature, voronoi-cell based density estimation is mostly used [1]. The effectiveness of a method of fundamental diagram in our work was estimated by comparing the results with that obtained by voronoi-cell based method, by finding the set of parameters which minimises ε_i, where

$$\varepsilon_i = \sqrt{\frac{1}{N}\left(\rho_{\text{vc}} - \rho_i\right)^2}. \tag{1}$$

ρ_{vc} is the density estimated by voronoi method, ρ_i is the density obtained by the method for which we intend to minimise ε_i in order to find the correct set of parameters to define the density. We also make an attempt to draw bi-directional fundamental diagrams [2].

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On the energy-momentum relation of the strongly coupled polaron

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We consider the Fröhlich model of a polaron, which describes a quantum particle interacting with a bosonic phonon field via an interaction term that it linear in the field's creation and annihilation operators. At strong coupling, it is expected that the problem is, to leading order, well described by the semiclassical approximation which amounts to treating the field creation and annihilation operators as complex-valued functions. We verify this prediction for the case of the energy-momentum relation of the model. In fact, since the model is translation-invariant, it commutes with the total momentum and the energy momentum relation $E(P)$ is the ground state energy of the Hamiltonian on the subspace where the total momentum of the system is P. A conjecture by L.D. Landau and S.I.Pekar [1] states that $E(P)$ is, for vanishingly small momenta and at large coupling, a parabolic curve with coefficient computed using the semiclassical approximation. This corresponds to the picture of the emergence of a quasi-particle termed the polaron, envisaged as the original particle to which a cloud of phonons is attached during its free motion. We extend this conjecture and predict that the parabolic behavior of $E(P)$ should extend to the entire range of the total momentum where the quasi-particle's kinetic energy is smaller than the corresponding energy of a free phonon, and the quasi-particle is stable until it starts emitting the Cherenkov radiation. At the same time, the coefficient of the parabola should be the semiclassical constant at strong coupling. We prove a weaker version of our conjecture by proving the parabolic behaviour of $E(P)$ with the expected semiclassical constant in the strong coupling limit on an interval with the natural upper boundary, but for momenta large enough such that the particle's kinetic energy is larger than the quantum corrections to the semiclassical asymptotics of the absolute ground state energy. We achieve this for polaron models with an acoustic (superfluid) type dispersion relation for the phonons and for a sufficiently regular interaction. For the physically important case of optical phonons and a charge-dipole-type interaction as in polar crystals, we prove the corresponding upper bound, and the interval of the momenta is smaller but still in the conjectured range.

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Casimir–like interaction of inclusions in lipid bilayer with two order parameters

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We present a simple, exactly solvable model of biological lipid bilayer with two order parameters describing spatial configuration and chemical composition of the membrane. Despite of its simplicity, the system shows quite a rich behavior, including two distinct critical regimes and a Fisher–Widom line. We study the Casimir–like interaction between inclusions on such a membrane. The inclusions are defined as the points where the spatial position of the membrane is fixed; this is mimicking the interaction of biological lipid bilayer with immersed proteins (see the pictures below). Depending on how these inclusions interact with the membrane, three different behaviors of the Casimir–like force are possible. They differ in the strength and the decay lengthscale of the interaction.

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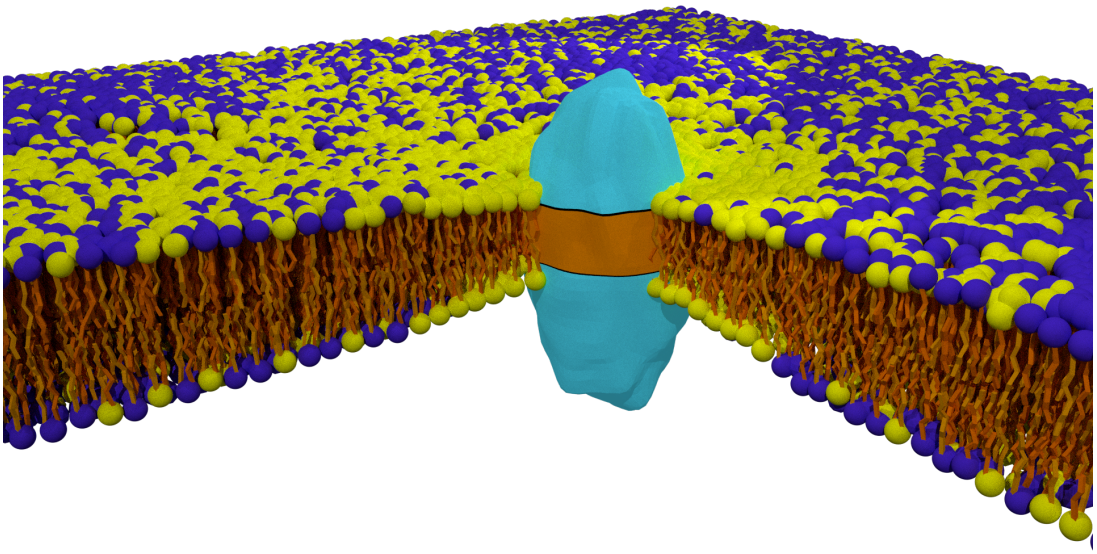

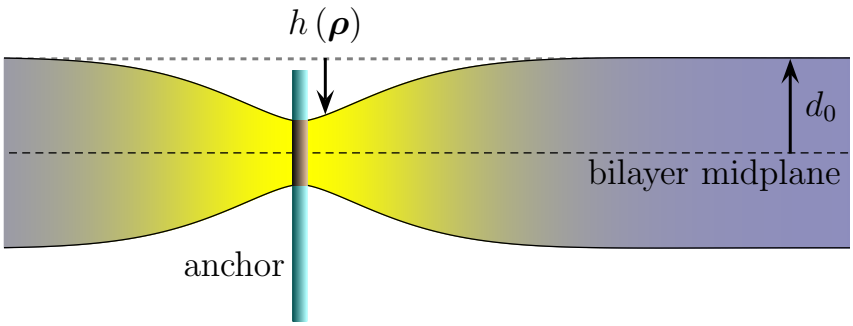

Critical percolation threshold controls Arctic sea ice melt pond evolution

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Arctic sea ice covers a vast area of nearly 15 million square kilometers at its peak annual extent. However, in recent years, it has been rapidly disappearing at a rate underestimated by most climate models. A likely reason for this underestimate are processes on scales smaller than tens of kilometers, which the large-scale models cannot resolve. One such small-scale process that contributes to the disappearance of the Arctic ice are meter-sized melt ponds that form on the ice's surface during summer and absorb significant amounts of solar radiation. During the summer, these ponds evolve in a complicated manner that we do not yet fully understand. In this poster, I will show how the critical point of a connectivity transition — the percolation threshold — controls the melt pond evolution. The ponds evolve by draining through large holes that open over the summer on the ice's surface so that above the percolation threshold, they can drain easily, while below the threshold, their drainage is impaired. In this way, the percolation threshold is an approximate upper bound on the pond coverage fraction. In fact, in a manner typical for critical phenomena, pond drainage is universal. This universality enables us to write an equation for their evolution below the threshold that compares well with field and satellite observations over most of the summer. Our work, thus, might help resolve some of the uncertainty present in the large-scale climate models and help better predict the fate of the Arctic ice.

A stochastic model of mixed-phase cloud micro-physics

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Mixed-phase clouds, i.e., clouds that contain both super-cooled water droplets and ice crystals, are ubiquitous in the atmosphere and play an important role in the climate system. The mixture of liquid and solid water in sub-zero temperatures leads to a condensational instability, in which ice particles tend to grow at the expense of droplet evaporation. Nonetheless, mixed-phase clouds are unexpectedly long-lived. We claim that small-scale turbulence is key to explain the persistence of such systems. Due to limited computational resources, weather simulation on a global scale is limited to coarse grids with a resolution of kilometers at best. On the other hand, a typical turbulent flow inside a cloud will display an intricate structure of eddies down to the scale of centimeters. We propose a Lagrangian stochastic micro-physical scheme to account for sub-grid fluctuations in velocity, temperature and water vapor fields. The impact of our scheme on phase partitioning is tested in a synthetic, turbulent-like flow that mimics an Arctic mixed-phase stratocumulus (AMPS) cloud. Results are confronted with idealized reference simulations that use Eulerian bulk micro-physics based on an assumed (temperature-dependent) phase partitioning function. Our study suggests that accounting for local variability in a turbulent cloud is important for reproducing steady-state mixed-phase conditions.

Coalescence of surfactant-laden droplets

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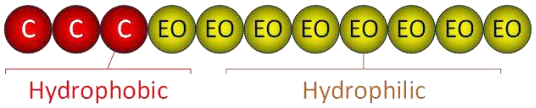
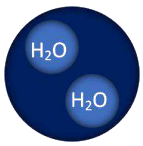
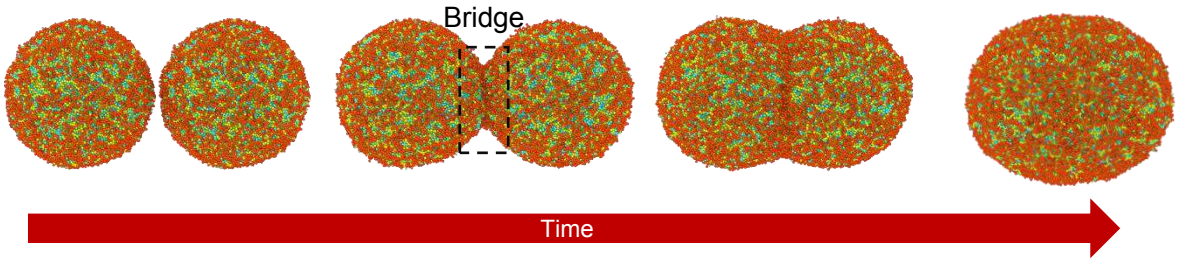
Droplet coalescence is commonly encountered in nature and is also relevant for various technologies, such as inkjet printing. In this poster, we present our results on the coalescence of surfactant-laden water droplets, which have been obtained by means of molecular dynamics simulation of a coarse-grained (CG) force-field. In particular, we will discuss the details of the coalescence mechanism and the bridge growth dynamics.



CG representation of C10E8 surfactant



CG representation of Water



Far from equilibrium transport on TASEP with Pockets

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Nowadays, it is quite unbelievable to think of a world without access to transport. Over the years, transport has enhanced our lives, and we can't imagine thriving in this current world without the capability to transport. However, in real, system of mutually interacting particle occur in environment with a net driving force acts upon them. These systems are in non-equilibrium for all the times and can attain the non-equilibrium steady state. Many physical systems like traffic flow, pedestrian motion, cellular transport, protein synthesis are some intriguing examples of stochastic non-equilibrium system where transport processes occur along complex structure of pathways [1]. In comparison to their equilibrium counterparts, non-equilibrium processes are far more diversified and interesting. Since, the motion of the active species in the above discussed physical and biological transport processes is continuously triggered by the supply of energy, they fall under a special class of non-equilibrium systems known as "driven-diffusive systems".

In last few decades, Totally Asymmetric Simple Exclusion Process (TASEP) is proved to be a paradigmatic lattice-gas model that provides a general framework to study the non-equilibrium transport in these driven-diffusive systems. In this poster, we present the study of a geometric adaptation of a totally asymmetric simple exclusion process with open boundary conditions, where each site of a one-dimensional channel is connected to a sideways space (pocket) on the lateral [2]. The number of particles that may be accommodated in each pocket is determined by its capacity q. The continuum mean-field approximation is deployed for the case $q = 1$ where both lattice and pocket strictly follow the hard-core exclusion principle. In contrast, a probability mass function is utilized along with the mean-field theory to investigate the multiple-capacity case, where the pocket violates the hard-core exclusion principle. The effect of both finite and infinite reservoirs has been studied in the model [3]. The explicit expression for particle density has been calculated, and the evolution of the phase diagram in $\alpha - \beta$ parameter space obtained with respect to q and the attachment-detachment rates. In particular, the topology of the phase diagram is found to be unchanged in the neighbourhood of $q = 1$. Moreover, the competition between lattice and pocket for finite resources and the unequal Langmuir kinetics captures a phenomenon in the form of a back-and-forth transition [4]. We have also investigated the limiting case $q \to \infty$. The theoretically obtained phase boundaries and density profiles are validated through extensive Monte Carlo simulations.

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Colossal Brownian yet non-Gaussian diffusion in a periodic potential: impact of nonequilibrium noise amplitude statistics

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Authors previously studied an overdamped dynamics of nonequilibrium noise driven Brownian particle dwelling in a spatially periodic potential and discovered a novel class of Brownian, yet non-Gaussian diffusion[1]. The mean square displacement of the particle grows linearly with time and the probability density for the particle position is Gaussian, however, the corresponding distribution for the increments is non-Gaussian. The latter property induces the colossal enhancement of diffusion, significantly exceeding the well known effect of giant diffusion. Here we considerably extend the above predictions by investigating the influence of nonequilibrium noise amplitude statistics on the colossal Brownian, yet non-Gaussian diffusion[2]. The tail of amplitude distribution crucially impacts both the magnitude of diffusion amplification as well as Gaussianity of the position and increments statistics. Our results carry profound consequences for diffusive behaviour in nonequilibrium settings such as living cells in which diffusion is a central transport mechanism.

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Universality in dynamical networks undergoing growth and contraction

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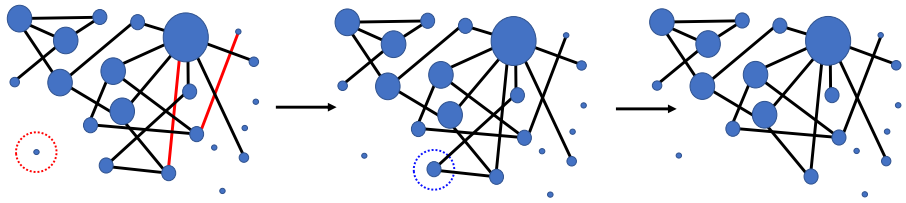
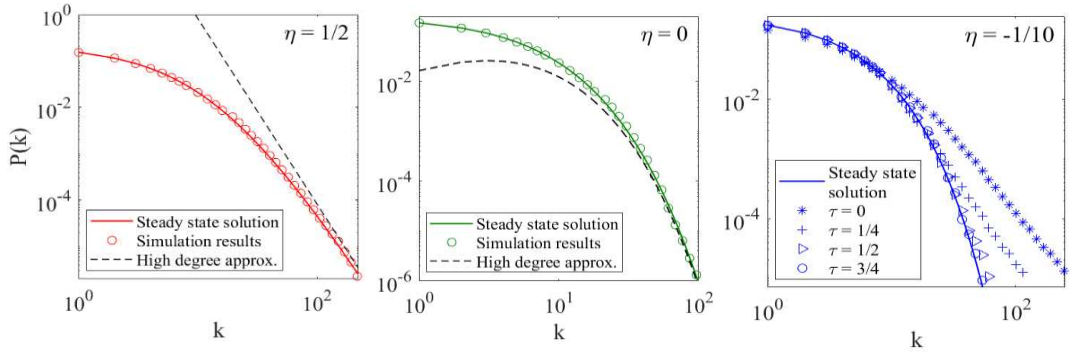


Growth step: with probability $(1+\eta)/2$ add a new node & add m new links, **preferentially**

Contraction step: with probability $(1-\eta)/2$ delete a **random** node

Complex networks and dynamical processes taking place on them play a central role in current research. While models of growing networks were studied extensively, in realistic situations, networks undergo a combination of growth and contraction processes. **We are looking for the dynamical degree distribution of generic networks, $P_t(k)$, while being exposed to all kinds of growth and contraction mechanisms.** For example, we may consider the following model: at each time step one of the following possibilities occur: **(a) growth step:** with probability $(1+\eta)/2$ a new node is added to the network, and m existing nodes are connected **preferentially** (connecting high degree nodes with higher probability). **(b) contraction step**: with probability $(1-\eta)/2$ a **random node** is deleted from the network, together with all its links. The parameter $-1 \le \eta \le 1$ is essentially the rate at which the size of the network, N_t, evolve with time: $N_t = N_0 + \eta t$. This model exhibits a nontrivial phase transition between a power-law (scale free) and an exponential degree distribution that occurs at $\eta = 0$, exactly when the deletion rate balances the growth rate. At the phase transition we get a stretched exponential. This is summarized below:

$$P(k) \underset{k\gg 1}{\sim} \begin{cases} k^{-(2+\frac{1}{\eta})} & \eta > 0 \quad \text{Power law} \\ k^{\frac{m}{2}-\frac{3}{4}} e^{-2\sqrt{k}} & \eta = 0 \quad \text{Stretched exponential} \\ k^{m(1+\eta)+\frac{1}{\eta}} (1-\eta)^{-k} & \eta < 0 \quad \text{Discrete Gamma} \end{cases}$$



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Large deviations of reflected diffusions

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We consider a Markov diffusion $\boldsymbol{X}(t)$ evolving in $\mathbb{R}^d$ according to a stochastic differential equation. For a dynamical observable A_T of the process $\boldsymbol{X}(t)$ having the general form

$$A_T = \frac{1}{T}\int_0^T f(\boldsymbol{X}(t))dt + \frac{1}{T}\int_0^T \boldsymbol{g}(\boldsymbol{X}(t)) \circ d\boldsymbol{X}(t), \tag{1}$$

it is known that in practice the probability density $P(A_T = a)$ often has the asymptotic form

$$P(A_T = a) \approx e^{-TI(a)} \tag{2}$$

for large T. An observable for which the associated probability density has this asymptotic form is said to satisfy a large deviation principle with rate function I. The rate function describes the probability with which both small and large fluctuations of the observable A_T occurs as T becomes large.

Calculating the rate function directly is intractable even for simple systems. As a result, the rate function is often found indirectly via a spectral calculation.

We are interested in the event where the diffusion $\boldsymbol{X}(t)$ evolves in some bounded domain, with the boundaries assumed to be reflective. The proper boundary conditions for the spectral calculation associated with obtaining the large deviation functions in the presence of reflecting boundaries is discussed, and the implications for the effective process (which describes how fluctuations arise in the long-time limit) are explored. Some applications of this work are also discussed. This provides a summary of recent work [1, 2] in which a comprehensive approach to obtaining the appropriate boundary conditions for reflective boundaries was developed for observables having the form (1). Furthermore, this approach can be extended to other boundary types as well.

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Inertial Lévy flights in bounded domains.

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The escape from a given domain is one of the fundamental problems in statistical physics and the theory of stochastic processes. We explore properties of the escape of an inertial particle driven by Lévy noise from a bounded domain, restricted by two absorbing boundaries. The properties of the mean first passage time for the integrated Ornstein-Uhlenbeck process driven by Lévy noise are compared to its Brownian counterpart i.e. randomly accelerated process. Mean first passage time considerations are complemented by analysis of the escape velocity and energy along with their sensitivity to initial conditions.

Acknowledgments: This research was supported by the National Science Center (Poland) grant 2018/31/N/ST2/00598.

MDPD Simulation of Liquid Thread Break-up and Formation of Droplets

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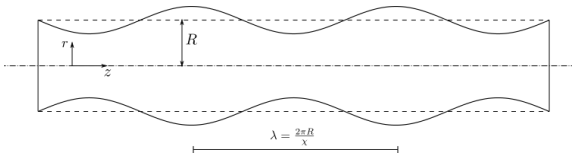
Formation of droplets from the break-up of liquid nano-threads is an interesting phenomena in fluid dynamics that is relevant in many industrial applications, such as: drug manufacturing, inkjet printing, and nanowire fabrication.

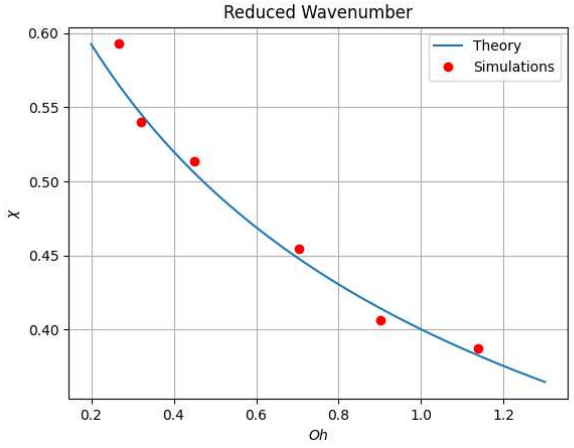
The classical theory, used to describe the break-up of liquid threads, has its origins in the works of Rayleigh and Plateau, who showed through linear stability analysis that a fluid cylinder is unstable for perturbations that have a wavelength superior to its circumference. Moreover, there exists a characteristic wavelength for which the perturbations are the most unstable. The figure below shows a schematic representation of the Rayleigh-Plateau instability problem.



The goal of this work is to assess the validity of the results obtained from linear stability analysis of the continuum fluid dynamics equations at the molecular level, where the thermocapillary waves are responsible for the instability that leads to the break-up of a liquid thread. Because of the spatial scale of interest, we chose a simulation method known as many-body dissipative particle dynamics, which is a coarse-grained molecular method that represents the hydrodynamics of this problem well and is more computationally efficient when compared to traditional molecular dynamics. Different fluids can be simulated by tuning the model parameters. These fluids are studied in terms of their Ohnesorge number $Oh = \mu/\sqrt{\rho\sigma L}$, which is the ratio between viscous forces and inertia and surface tension.

We can calculate the characteristic wavelength that leads to the break-up for different types of fluids by computing the Fourier transform of the density correlation function.

To make the results statistically more relevant, we took the average from 30 trajectories for each fluid simulated and compared it with a theoretical prediction made by Chandraseker. The characteristic wavelengths obtained are presented in the figure below where they show a good agreement.



Bifurcations in droplet collisions

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Smoluchowski [1] calculated how the collision rate of non-interacting spheres settling due to gravity depends upon the strength of gravity and upon the radii of the spheres. Saffman and Turner [2] argued that the collision rate for non-interacting droplets in turbulence increases as the turbulent strain rate increases. However, these studies ignored the effects of interactions between the droplets. The numerical simulations of droplets settling in a steady straining flow performed by Dhanasekaran et al. [3] show that droplet-droplet interactions result in a complex dependence of the collision rate on the strain rate and on the differential settling speed.

We show that this dependence is explained by a sequence of bifurcations in the collision dynamics. We compute the bifurcation diagram when strain is aligned with gravity, and show that it yields novel insights into the collision dynamics. First, the steady-state collision rate remains non-zero in the limit $\mathrm{Kn} \to 0$, contrary to the common assumption that the collision rate tends to zero in this limit (Kn is a non-dimensional measure of the mean free path of air). Second, the non-monotonic dependence of the collision rate on the non-dimensional differential settling speed is explained by a grazing bifurcation. Third, the bifurcation analysis explains why so-called 'closed trajectories' appear and disappear. Fourth, our analysis predicts strong spatial clustering near certain saddle points, where the strain is balanced by the differential settling.

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Collective dynamics in systems of growing rods

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Recent research shows that in confined populations of growing and dividing rods, such as microcolonies of bacteria, a complex interplay between growth activity, fluctuating inter-particle forces and boundary effects can lead to emergent collective dynamics, including global flow of cellular matter and alignment due to the nematic symmetry of local mechanical interactions. Here, we use a new versatile framework for agent-based simulations to explore these effects in systems with different geometries containing two-dimensional spherocylinders. We observe the emergence of orientational order in rectangular channels and analyse its dependence on both microscopic parameters of the rods and the geometry of the confinement. Further observations of complex orientation patterns in open polygonal domains hint at a link between shear rate anisotropy and orientation.

Self-organized growth of cellular substrates

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Growing colonies of rod-shaped bacteria commonly feature order and alignment of the constituent particles. This is generally thought to be the result of the active stresses generated by growth, mechanical volume exclusion interactions between cells, and shear-flow-induced effects due to confinement. However, how these contributing factors interact to give rise to the observed global alignment patterns remains elusive.

We study, *in-silico*, colonies of growing rod-shaped particles of different aspect ratios confined in channel-like geometries. A spatially resolved analysis of the stress tensor reveals a strong relationship between near-perfect alignment and an inversion of stress anisotropy for particles with large length-to-width ratios. We show that, in quantitative agreement with an asymptotic theory, strong alignment can lead to a decoupling of active and passive stresses parallel and perpendicular to the direction of growth, respectively. Our results illustrate the complexity arising from the inherent coupling between nematic order and active stresses in growing active matter which is influenced by geometric and configurational constraints due to confinement.

Durotaxis motion on brush substrates

Russell Kajouri[1], **Piotr Deuar**[1], **Jan Zidek**[2], **Sergei A. Egorov**[3], **Andrey Milchev**[4] **and Panagiotis E. Theodorakis**[1]

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A range of industries require the self-sustained directed motion of nanoscale droplets on different substrates for various purposes [1, 2], for example, in the context of microfabrication [3], coating [4], microfluidics and thermal control [3, 4]. One way of causing such motion is durotaxis, where a gradient stiffness of a substrate is used to enable droplets to move along the direction of the gradient. Using molecular dynamics, we show that the motion of a droplet on a brush substrate depends on the range of stiffness variation compared to the chain length and grafting density of the brush, and the interaction between the brush and the droplet. Our analysis indicates that a brush substrate of a moderate grafting density induces the most efficient droplet motion, while motion efficiency depends only weakly on the stiffness gradient. Finally, a larger size of the droplet favours the durotaxis motion on brush substrates.

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Tubular-body theory for viscous flows

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Cable-like bodies play a key role in many biological fluid systems but are hard to simulate. Asymptotic theories, called slender-body theories, are effective but apply in specific regimes and can be hard to extend beyond leading order.

In this poster I show how to develop an exact slender-body-like theory for the surface traction of cable-like bodies in viscous flow. This theory expresses the traction as a series of solutions to a well-behaved one-dimensional Fredholm integral equation of the second kind. This process can be simply generalised to other systems. We test this theory against known solutions and then use it to look at the swimming of a tightly wound helix exposed to an external torque [1].

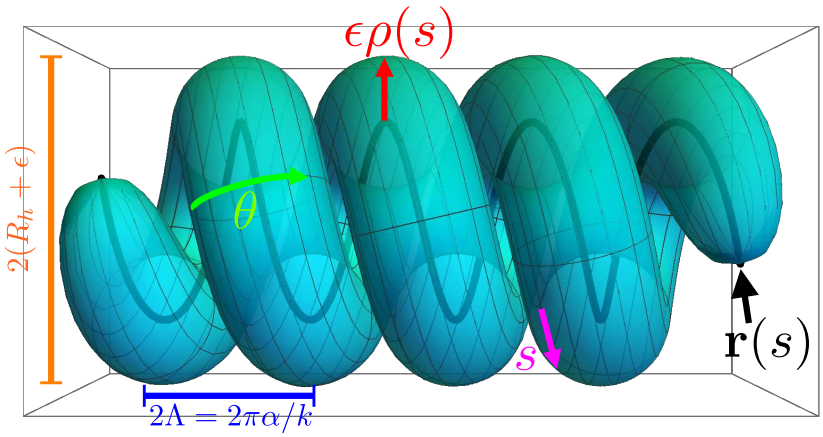

Figure 1: Diagram of of tightly wound helix

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Near-wall dynamics of colloidal dumbbells

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Dynamics of the arbitrarily-shaped colloidal particles in the vicinity of the geometric confinement remains widely unexplored. We provide a numerical tool to simulate the motion of such particles, including their Brownian motion, sedimentation, the wall-particle hydrodynamic and electrostatic interactions. The calculations are feasible given the particle's diffusion matrix and a model for the electrostatic force acting on the body. We took a particular interest in the colloidal dumbbells, which are particles of an axisymmetric bead-like shape, containing two identical spheres. According to the latest experimental results [1], dumbbells of single sphere's size ~ 1 μm surprisingly tend to be oriented at preferred angles with respect to the confining plane. This leads to the discrepancy with theoretical predictions of the most probable parallel-to-wall orientation. We investigate this disagreement numerically and inquire the origins of this unexpected behaviour. We compare our results obtained for numerically calculated exact values of the particle's mobility coefficients with their analytical approximations [2]. With the use of highly accurate tool to obtain the bead-like particle's diffusion matrix, we are capable of simulating the motion of a large ($N \sim 10^2$) number of beads of different sizes in a very short time.

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An Intuitive Understanding of the Spin Excitations of a 1D Antiferromagnet

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Antiferromagnetic Heisenberg spin model is one of the basic models in quantum magnetism. Although in two- and three-dimensional world its ground state has a classical order, in one dimension ("chains") there is no long-range order and the exact form of the ground state is provided by a rather complex Bethe Ansatz [1]. Even more intricate are the low energy magnetic excitations of a spin chain [2] — the notorious spinons, carrying fractional quantum numbers [3]. In this poster we show an alternative approach to the ground state as well as the low-lying excitations of the one-dimensional Heisenberg antiferromagnet, which, although approximate, gives a more physically intuitive picture than the exact Bethe Ansatz solution.

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Rechargeable self-assembled droplet microswimmers driven by surface phase transitions

Maciej Lisicki[1], **Diana Cholakova**[2], **Stoyan K. Smoukov**[3], **Slavka Tcholakova**[2], **E. Emily Lin**[3], **Jianxin Chen**[3,4], **Gabriele De Canio**[5], **Eric Lauga**[5], **and Nikolai Denkov**[2]

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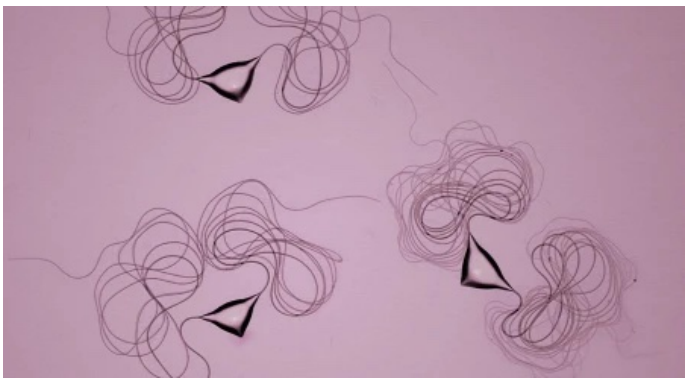
Swimming microorganisms and engineered artificial swimmers use multiple strategies to achieve propulsion in the viscosity-dominated microworld. A number of them use long, filamentous appendages called cilia or flagella. The motion of these slender objects is governed by a complex interplay between the driving forces, the elastic properties of the fibres, and the resistance forces of fluid.

A recently studied artificial system involving an emulsion of microscopic droplets of oil with surfactant in water exhibits swimming induced by the extrusion of elastic fibres by the droplets [1]. The extrusion is controlled by a surface phase transition of the surfactant, and it drives the motion of droplets. The transition is driven by small changes in the temperature of the environment, and can be reversed by switching between cooling and heating the system. The formation of a plastic phase by the surfactant induces shape changes of the droplets, where polyhedral shapes become energetically favourable. Further reconfiguration driven by the phase transition leads to the formation of filamentous structures originating at vertices of the now polygonal droplets. The extruded fibres undergo dynamic buckling and produce complex shapes, but also exert a force and torque on the droplets, resulting in translation and rotation of the droplets. We propose an elastohydrodynamic model for this phenomenon and describe the motion by a combination of theoretical considerations and numerical simulations. Our model serves as the basis for interpretation of experimental data and quantitatively grasps the swimming dynamics.



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Solitonic solutions in one-dimensional superfluid Bose-Fermi mixtures

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In this work we study solitonic solutions in quasi-one-dimensional superfluid mixtures of Bose and Fermi gases at low temperatures. The Fermi gas is studied both for the BCS interaction regime as well as at unitarity, and we allow for a non-zero spin polarization. The Bose gas forms a Bose-Einstein condensate. At this stage of the project, we put particlular emphasis on the solitonic solutions imposed on one of the interacting gases, and we study the response of the entire system to such a condition. The Fermi gas is described with the Bogoliubov-de Gennes equations for the BCS interaction regime and with a more general density functional, namely the Asymmetric Superfluid Local Density Approximation (ASLDA) for the uniatry interaction regime. The Bose-Einstein Condensate is described with the standrad Gross-Pitaevskii equation.

Finite-time dynamical phase transition in non-equilibrium relaxation

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In this poster, we analyse a finite-time dynamical phase transition in the thermal relaxation of a mean-field magnetic model [1]. The phase transition manifests itself as a cusp singularity in the probability distribution of the magnetisation that forms at a critical time. The transition is due to a sudden switch in the dynamics, characterised by a dynamical order parameter. We derive a dynamical Landau theory for the transition that applies to a range of systems with scalar, parity-invariant order parameters. Close to criticalilty, our theory reveals an exact mapping between the dynamical and equilibrium phase transitions of the magnetic model, and implies critical exponents of mean-field type. We argue that interactions between nearby saddle points, neglected at the mean-field level, may lead to critical, spatiotemporal fluctuations of the order parameter, and thus give rise to novel, dynamical critical phenomena.

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Equilibrium properties of the one-dimensional triangle-well fluid

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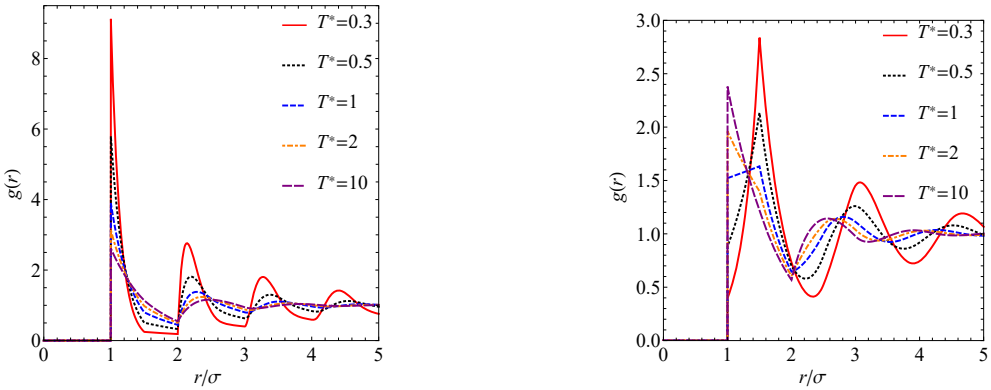
We present a comprehensive study on the thermophysical and structural properties of two prototypical classes of fluids confined in a one-dimensional line, namely the triangle-well and the ramp potentials. Both potentials are finite-ranged and have an impenetrable core of diameter σ plus a continuous linear part between $r = \sigma$ and $r = \lambda$. While the mathematical form of that additional part is analogous in both cases, the physical meaning is not. In the triangle-well potential the tail is attractive and, apart from its own physical interest, the main importance of the potential resides in representing the effective colloid-colloid interaction in the Asakura–Oosawa mixture. On the other hand, the ramp potential is purely repulsive with a softened core between $r = \sigma$ and $r = \lambda$.

The exact statistical-mechanical solution in the isothermal-isobaric ensemble for general nearest-neighbor interactions [1] is applied to the study of equilibrium properties of these two classes of fluids, such as the equation of state, the excess internal energy per particle, the structure factor $S(k)$, the direct correlation function $c(r)$, and the radial distribution function $g(r)$. In the latter case, in contrast to previous studies where $g(r)$ was obtained numerically from $S(k)$ by Fourier inversion [2], a fully analytic representation for $g(r)$ is derived in terms of a finite number of coordination-shell terms for any finite r [3]. As an illustration, the figure below shows $g(r)$ at some representative states for the triangle-well (left) and ramp (right) potentials.



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Optimal Vertical Navigation of Microswimmers in Steady Flow

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Survival of many plankton species depends on the largest biomass migration happening daily on Earth. This migration is known as diel vertical migration, during which planktonic species such as copepods swim towards the surface by dusk to feed form phytoplankton, and return to darker regions by dawn to prevent predation. Therefore, they are expected to have developed efficient swimming strategies, in order to swim up to few hundreds of meters everyday. Some strategies are passive, such as being bottom-heavy that tends to align the swimmer direction upwards. This is efficient for upward migration in quiescent flows, but it is often sensitive to turbulence which upsets the alignment. Since, planktonic swimmers have access to a wide range of hydromechanical information, it is possible for them to exploit this information for efficient navigation in turbulent flows. Here we present an active reorientation mechanism that increases the upwelling region sampling rate of swimmers in steady flows significantly.

Density estimation and fundamental diagrams for crossing flows of pedestrians without a spatial boundary

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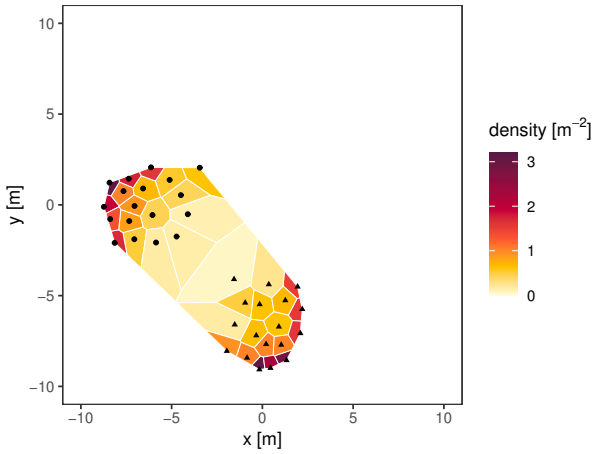
Construction of fundamental diagrams have been an essential tool in the context of crowd motion study to facilitate numerical simulations. There exists various definitions of fundamental diagrams, with the most used one is the variation of pedestrian velocity as a function of crowd velocity. For a crowd without any spatial boundaries, the methods of density estimation is itself a wide area of research.

In our work, we explore several methods of density estimation for the typical scenario of crossing flows. Many real-world situations produce crossing flows, such as streams of pedestrians crossing at a sidewalk intersection, or subway commuters passing each other when entering and exiting a metro car. The density estimation methods for our research consisted of both Lagrangian and Eulerian approaches, as well as voronoi-cell based methods.



For fundamental diagrams, we focus mainly to investigate the velocity-density relationship. In the existing literature, voronoi-cell based density estimation is mostly used [1]. The effectiveness of a method of fundamental diagram in our work was estimated by comparing the results with that obtained by voronoi-cell based method, by finding the set of parameters which minimises ε_i, where

$$\varepsilon_i = \sqrt{\frac{1}{N}\left(\rho_{\text{vc}} - \rho_i\right)^2}. \tag{1}$$

ρ_{vc} is the density estimated by voronoi method, ρ_i is the density obtained by the method for which we intend to minimise ε_i in order to find the correct set of parameters to define the density. We also make an attempt to draw bi-directional fundamental diagrams [2].

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On the energy-momentum relation of the strongly coupled polaron

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We consider the Fröhlich model of a polaron, which describes a quantum particle interacting with a bosonic phonon field via an interaction term that it linear in the field's creation and annihilation operators. At strong coupling, it is expected that the problem is, to leading order, well described by the semiclassical approximation which amounts to treating the field creation and annihilation operators as complex-valued functions. We verify this prediction for the case of the energy-momentum relation of the model. In fact, since the model is translation-invariant, it commutes with the total momentum and the energy momentum relation $E(P)$ is the ground state energy of the Hamiltonian on the subspace where the total momentum of the system is P. A conjecture by L.D. Landau and S.I.Pekar [1] states that $E(P)$ is, for vanishingly small momenta and at large coupling, a parabolic curve with coefficient computed using the semiclassical approximation. This corresponds to the picture of the emergence of a quasi-particle termed the polaron, envisaged as the original particle to which a cloud of phonons is attached during its free motion. We extend this conjecture and predict that the parabolic behavior of $E(P)$ should extend to the entire range of the total momentum where the quasi-particle's kinetic energy is smaller than the corresponding energy of a free phonon, and the quasi-particle is stable until it starts emitting the Cherenkov radiation. At the same time, the coefficient of the parabola should be the semiclassical constant at strong coupling. We prove a weaker version of our conjecture by proving the parabolic behaviour of $E(P)$ with the expected semiclassical constant in the strong coupling limit on an interval with the natural upper boundary, but for momenta large enough such that the particle's kinetic energy is larger than the quantum corrections to the semiclassical asymptotics of the absolute ground state energy. We achieve this for polaron models with an acoustic (superfluid) type dispersion relation for the phonons and for a sufficiently regular interaction. For the physically important case of optical phonons and a charge-dipole-type interaction as in polar crystals, we prove the corresponding upper bound, and the interval of the momenta is smaller but still in the conjectured range.

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Casimir–like interaction of inclusions in lipid bilayer with two order parameters

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We present a simple, exactly solvable model of biological lipid bilayer with two order parameters describing spatial configuration and chemical composition of the membrane. Despite of its simplicity, the system shows quite a rich behavior, including two distinct critical regimes and a Fisher–Widom line. We study the Casimir–like interaction between inclusions on such a membrane. The inclusions are defined as the points where the spatial position of the membrane is fixed; this is mimicking the interaction of biological lipid bilayer with immersed proteins (see the pictures below). Depending on how these inclusions interact with the membrane, three different behaviors of the Casimir–like force are possible. They differ in the strength and the decay lengthscale of the interaction.

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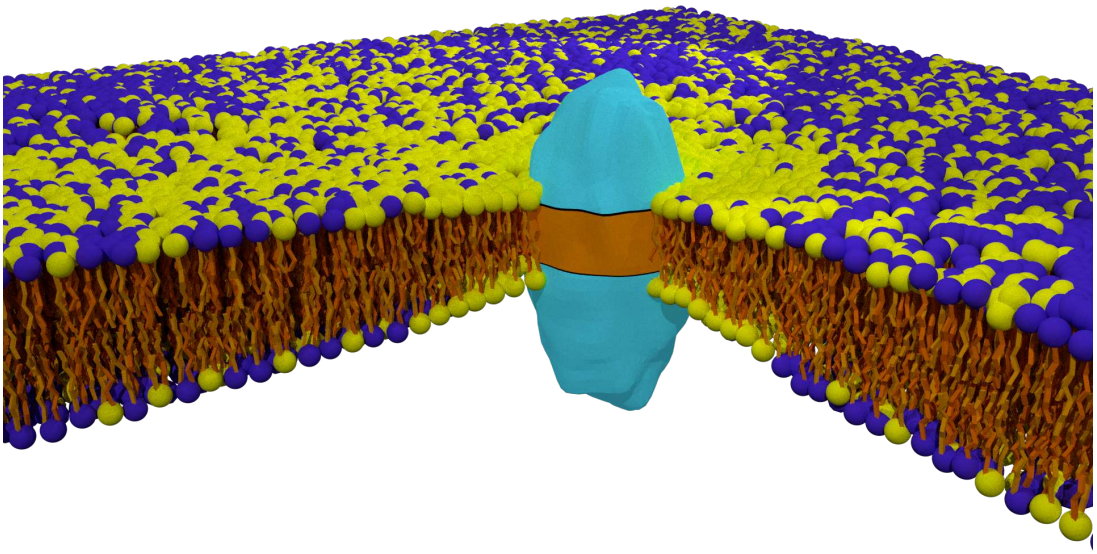

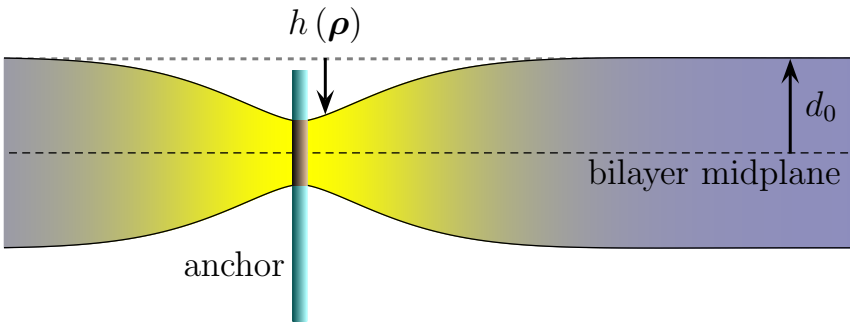

Critical percolation threshold controls Arctic sea ice melt pond evolution

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Arctic sea ice covers a vast area of nearly 15 million square kilometers at its peak annual extent. However, in recent years, it has been rapidly disappearing at a rate underestimated by most climate models. A likely reason for this underestimate are processes on scales smaller than tens of kilometers, which the large-scale models cannot resolve. One such small-scale process that contributes to the disappearance of the Arctic ice are meter-sized melt ponds that form on the ice's surface during summer and absorb significant amounts of solar radiation. During the summer, these ponds evolve in a complicated manner that we do not yet fully understand. In this poster, I will show how the critical point of a connectivity transition — the percolation threshold — controls the melt pond evolution. The ponds evolve by draining through large holes that open over the summer on the ice's surface so that above the percolation threshold, they can drain easily, while below the threshold, their drainage is impaired. In this way, the percolation threshold is an approximate upper bound on the pond coverage fraction. In fact, in a manner typical for critical phenomena, pond drainage is universal. This universality enables us to write an equation for their evolution below the threshold that compares well with field and satellite observations over most of the summer. Our work, thus, might help resolve some of the uncertainty present in the large-scale climate models and help better predict the fate of the Arctic ice.

Thermal Casimir forces in Bose gas in anisotropic optical lattices

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Fluctuation induced (Casimir) forces can be observed not only in QED but also in condensed matter setups. We focus on such forces, both in ideal ($a = 0$) and imperfect ($a > 0$) bosonic gases described by the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}} + \frac{a}{2V} \hat{N}^2$$

in a d-dimensional slab $L^{d-1} \times D$ with peridoc boundary conditions. Both systems exhibit Bose-Einstein Condensation. We consider particles in anisotropic lattices with dispersion [1]

$$\varepsilon_{\mathbf{k}} = t \sum_{i=1}^{d-1} k_i^2 + \tau k_d^2 + \tau' k_d^4,$$

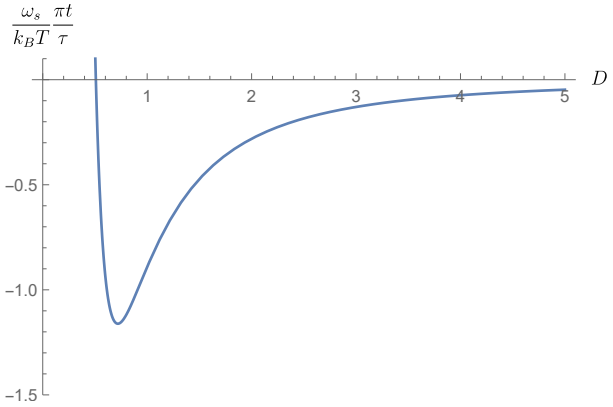
Having obtained the surface contribution ω_s to the grand canonical potential

$$\Omega(T, \mu, L, D) = L^{d-1} D \omega_b(T, \mu) + L^{d-1} \omega_s(T, \mu, D) + \dots$$

we evaluate the Casimir force

$$F_C(T, \mu, D) = -\frac{\partial \omega_s(T, \mu, D)}{\partial D}$$

which turns out to change its sign with growing distance between slab walls D in a critical system of ideal gas with dimensions $d = 4k - 1$. It is attractive for large values of D and repulsive for small values. To our knowledge this is the only system exhibiting such behavior.



Also, such a system displays a "dimensional cross-over" [2], i.e. for $\frac{\beta \tau^2}{8\tau'} = \theta > 0$ it has critical dimensions $d_c^l = 2$ and $d_c^u = 4$. However, as $\theta \to 0$, the critical dimensions shift so that $d_c^l = \frac{5}{2}$ and $d_c^u = \frac{9}{2}$.

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The impact of intersection mixing rules on the network-scale dissolution patterns

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We study flow-induced dissolution of porous rocks using 2D pore network models in which the rock matrix is represented as a series of interconnected pipes with the diameter of each segment increasing in proportion to the local reactant consumption. Most models of this kind assume complete mixing at the pore intersections. As a means to test whether this assumption impacts the evolution of the system, we compare the resulting dissolution patterns with those obtained using streamline routing at the intersections. We observe that the streamline routing affect the patterns particularly strongly at moderate DamkÃűhler numbers, where relatively wide dissolution channels (wormholes) appear spontaneously in the system. Streamline routing is shown to enhance flow focusing, which results in thinner wormholes and shorter breakthrough times. It also affects the velocity distribution in the pores, shifting it towards the larger values.

Stability Conditions for a Single Loop

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The transport networks found in many systems exhibit loops. Coastal river networks, leaf veins, and city streets have loops that are essential to their function. Looping structures within a larger network can arise because of adaptation to fluctuating hydrologic boundary conditions. However, the relationship between fluctuations and loop stability has not been thoroughly tested at the scale of a single loop. We consider a three node loop that it is fed by fluctuating flows at each node, just as a single loop within the channel network of a river delta would need to adapt to flows from (at least) river floods and tides. We then use linear stability analysis to determine conditions where it is stable as a tree or loop.

Consider a network where the discharge in link connecting nodes *i* and *j* is a linear function of pressure differential, scaled by link conductivity k_{ij} and length l_{ij}: $Q_{ij} = \frac{k_{ij}}{l_{ij}} \Delta p_{ij}$. The two fluctuating flows applied to each node can be considered as vectors: $\overrightarrow{Q_a} = [Q_a, Q_a']$, with $\overrightarrow{Q_a} + \overrightarrow{Q_b} + \overrightarrow{Q_c} = 0$ by concentration of fluid mass. The network adapts to these conditions by changing k based on the flows in a link: $\frac{\partial k_{ij}}{\partial t} = a\langle Q_{ij}^2 \rangle^{\gamma} - k_{ij}/\tau$, with a and τ dimensional constants and the angle brackets indicating an average.

Our analysis finds that for $\gamma = 0.5$, a tree is stable with link *ij* having $k_{ij} \approx 0$ if and only if the angle between vectors $\overrightarrow{Q_a}$ and $\overrightarrow{Q_b}$ is less than the angle on the loop at the opposite vertex/node of link *ij*. If all links *ij* have angles between their fluctuation vectors that exceed the loop's angle, then the stabile configuration of the system is a loop with positive conductivities for all links. A larger fluctuation angle relative to the loop angle indicates a larger conductivity for a given link at equilibrium.

If $\gamma > 0.5$, as is the case in many natural systems where larger channels are nonlinearly more efficient, the system is always stable in the tree configuration. However, a loop can also be stable, but the criterion described above must be exceeded by a constant that increases with γ. This reduces the solution space where loops are stable. This work provides a framework to understand the formation and stability of any loop as a geometric function of its morphology (link lengths and node angles) and fluctuations.

A lattice model of vascular network formation

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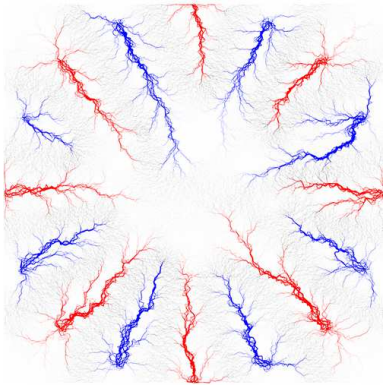
We propose a simple lattice model of vascular network formation involving three main stimuli:

1. Shear stress at the capillary walls: Flowing blood exerts shear stress on the walls of the vessel, causing its widening. As this process is mostly flow-dependent, it results in formation of conductive pathways focusing the blood flow [1].

2. Vascular endothelial growth factor (VEGF): Hypoxic tissues produce VEGF - a protein that leads to the formation of new blood vessels. High gradients of this factor induce the growth of new capillary vessels out of preexisting ones [2].

3. Conducted stimulus: Regulatory signals can be propagated along the vessels, either downstream or upstream, causing the growth of the parent vessel to increase the flow reaching its dependent branches. In this way long loops stretching into furthest regions of the system can be formed, improving the oxygenation [3].

All these factors together result in a transformation of an initial random network of capillaries into a hierarchical system of arterioles and venules. The final result of the evolution is a network with a good balance between oxygen distribution in the system and energy cost of the growth.



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Pinning and its Role in the Directed Motion of Fluids on Solid Substrates

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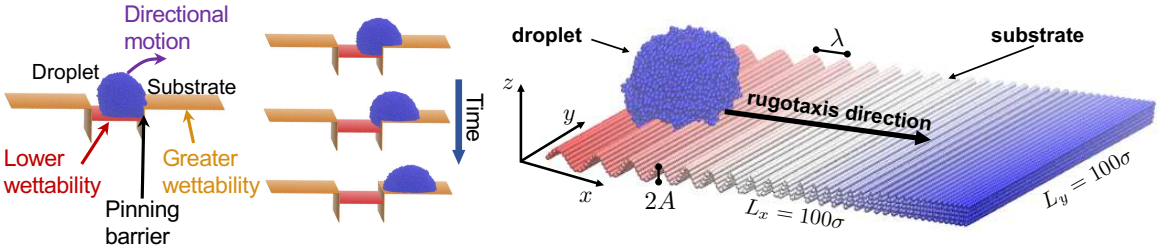
Pinning of liquid droplets on solid substrates is ubiquitous and plays an essential role in many applications, especially in various areas such as microfluidics and biology. Although pinning can often reduce the efficiency of various applications (for example, in the case of rugotaxis), there are situations that this phenomenon can actually offer possibilities for technological exploitation [1]. Here, by means of molecular dynamics simulation of a bead-spring model, we identify the conditions that lead to droplet pinning or depinning and elucidate the effects of key parameters. Moreover, we discuss how pinning can affect rugotaxis, that is, the droplet motion without external energy supply on wavy substrates [2]. Our results have implications for the nanoscale design of substrates in micro- and nanoscale systems and will assist with assessing pinning effects in various applications.



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Anomalous transport in driven periodic systems: distribution of the absolute negative mobility effect

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Absolute negative mobility is one of the most paradoxical forms of anomalous transport behaviour. At the first glance it contradicts the superposition principle and the second law of thermodynamics, however, its fascinating nature bridges nonlinearity and nonequlibrium state in which these fundamental rules are no longer valid. We consider a paradigmatic model of the nonlinear Brownian motion in a driven periodic system which exhibits the absolute negative mobility. So far research on this anomalous transport feature has been limited mostly to the single case studies due to the fact that this model possesses the complex multidimensional parameter space. In contrast, here we harvest GPU supercomputers to analyze the distribution of negative mobility in the parameter space. We consider nearly 10^9 parameter regimes to discuss how the emergence of negative mobility depends on the system parameters as well as provide the optimal ones for which it occurs most frequently.

Ground state energy of the polarized diluted gas of interacting spin $1/2$ fermions by Effective Field Theory

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The effective field theory approach simplifies the perturbative computation of the ground state energy of the diluted gas of fermions allowing in the case of the unpolarized system to easily re-derive the classic results up to the $(k_{\rm F}a_0)^2$ order (where $k_{\rm F}$ is the system's Fermi momentum and a_0 the s-wave scattering length) and (with more labour) to extend it up to the 4-th order in Fermi momentum. The corresponding expansion of the ground state energy of the polarized gas of spin $1/2$ fermions is known analytically or semi-analytically (to the best of our knowledge) only up to the $(k_{\rm F}a_0)^2$ (where $k_{\rm F}$ stands for $k_{{\rm F}\uparrow}$ or $k_{{\rm F}\downarrow}$) order [1], [2]. Here we show that the same effective field theory method allows to easily re-compute also the order $(k_{\rm F}a_0)^2$ correction to this result, and present some results towards extending the computation to the third-order. The obtained results suggest a change of the order of transition to the phase with the spontaneous polarization: with the order $k_{\rm F}a_0$ correction (equivalent to the mean field approximation) it is of the second order, whereas inclusion of the order $(k_{\rm F}a_0)^2$ correction changes it to first-order one.

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Estimations of difference between ground state energies for Hubbard model and its Hartree-Fock approximation

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A lower bound on the difference $E_{\rm gs} - E_{\rm HF}$ of the true ground state energy and the Hartree-Fock approximation to it is derived for a class of Hubbard models. The derivation follows closely the approach used by Bach and Poelchau in [1]. Its main technical tool are the correlation inequalities derived by Graf and Solovej [2]. We extend the results of [1] to several other classes of models. To the first one belong models which are not stricty translationally invariant. The second one form multi-band Hubbard models. To the third one belong Hubbard models with the $SU(N)$ internal symmetry. The common conclusion, pertaining to these three classes of models, is that the Hartree-Fock approximation becomes exact in the limit of vanishing Coulomb interaction U.

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Modeling the growth of Liesegang rings and mineral dendrites

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Liesegang rings and mineral dendrites are two examples of patterns which form in rocks when they are infiltrated by the hydrothermal, manganese-bearing fluids. As these fluids mix with the the oxygenated fluid within the rock pores, manganese oxide precipitates, forming the intricate patterns. Several models of this process have been proposed, which vary in complexity. One model assumes precipitation of manganese oxides directly on the surface of the growing dendrite, which then elongate. Another model involves an initial growth of small nanoparticles of manganese oxide, which then aggregate into larger structures.

We study this process using lattice-Botlzmann method to track the evolving concentrations of all of the species involved in reaction. Next, we analyze the dependence of the morphology of the resulting patterns on the physical parameters characterizing the reaction and growth, such as the concentrations of the initial solutions, reaction rates, nucleation thresholds or surface energy of the dendrites.

Growth dynamics of endothelial cells in the VEGF concentration field

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We analyze the experiments on the capillary plexus formation under in-vitro conditions where both the vascular endothelial growth factor and nutrient concentrations are controlled. The network sprouts from plastic beads coated with a layer of human umbilical vein endothelial cells, transduced for visualization with green fluorescent protein. Using time-lapse images for a detailed representation of system dynamics, we identify sprouting, bifurcation and anastomosis events. We develop a Python code for image analysis and statistics to measure the growing area of the network, its total length, and the maximum extent from the center as it evolves in time. We also quantify the impact of the concentration of the vascular endothelial growth factor on the growth dynamics.

Reconnections after breakthrough

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Usually, modeling of spatial network dynamics includes the elongation of branches, their splitting (to create a ramified network), and events of reconnection between branches (creating closed loops in a network). One can consider the emergence of such network as a result of one phase invading another with a diffusive field driving it (viscous fingering patterns, river or blood vessel networks). In such a case, it was shown that taking into account a finite mobility ratio between the two phases can lead to reconnections [1].

Attraction between branches is even more prominent when one of them reaches boundary of the system (breakthrough). The reconnections after breakthrough were observed in many physical systems (fracture dissolution, viscous fingering, lightnings), as well as in some biological, e.g. a quasi two-dimensional network of canals in the gastrovascular system of jellyfish *A. aurita*. We study this specific case of reconnections numerically and observe the jellyfish in experiments, as they are relatively easy to observe *in vivo* and to clone (due to their specific life-cycle).

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Thermal Casimir forces in Bose gas in anisotropic optical lattices

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Fluctuation induced (Casimir) forces can be observed not only in QED but also in condensed matter setups. We focus on such forces, both in ideal ($a = 0$) and imperfect ($a > 0$) bosonic gases described by the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}} + \frac{a}{2V} \hat{N}^2$$

in a d-dimensional slab $L^{d-1} \times D$ with peridoc boundary conditions. Both systems exhibit Bose-Einstein Condensation. We consider particles in anisotropic lattices with dispersion [1]

$$\varepsilon_{\mathbf{k}} = t \sum_{i=1}^{d-1} k_i^2 + \tau k_d^2 + \tau' k_d^4,$$

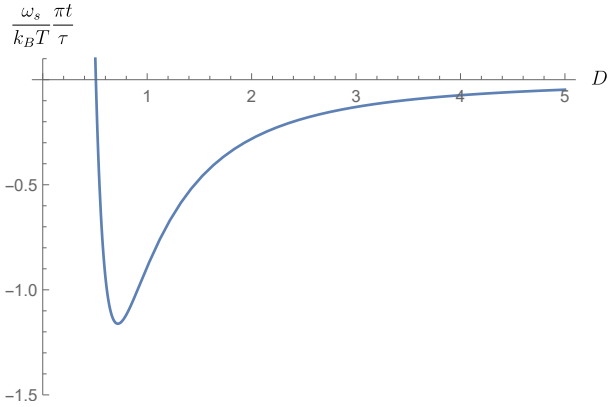
Having obtained the surface contribution ω_s to the grand canonical potential

$$\Omega(T, \mu, L, D) = L^{d-1} D \omega_b(T, \mu) + L^{d-1} \omega_s(T, \mu, D) + \dots$$

we evaluate the Casimir force

$$F_C(T, \mu, D) = -\frac{\partial \omega_s(T, \mu, D)}{\partial D}$$

which turns out to change its sign with growing distance between slab walls D in a critical system of ideal gas with dimensions $d = 4k - 1$. It is attractive for large values of D and repulsive for small values. To our knowledge this is the only system exhibiting such behavior.



Also, such a system displays a "dimensional cross-over" [2], i.e. for $\frac{\beta\tau^2}{8\tau'} = \theta > 0$ it has critical dimensions $d_c^l = 2$ and $d_c^u = 4$. However, as $\theta \to 0$, the critical dimensions shift so that $d_c^l = \frac{5}{2}$ and $d_c^u = \frac{9}{2}$.

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The impact of intersection mixing rules on the network-scale dissolution patterns

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We study flow-induced dissolution of porous rocks using 2D pore network models in which the rock matrix is represented as a series of interconnected pipes with the diameter of each segment increasing in proportion to the local reactant consumption. Most models of this kind assume complete mixing at the pore intersections. As a means to test whether this assumption impacts the evolution of the system, we compare the resulting dissolution patterns with those obtained using streamline routing at the intersections. We observe that the streamline routing affect the patterns particularly strongly at moderate DamkÃűhler numbers, where relatively wide dissolution channels (wormholes) appear spontaneously in the system. Streamline routing is shown to enhance flow focusing, which results in thinner wormholes and shorter breakthrough times. It also affects the velocity distribution in the pores, shifting it towards the larger values.

Stability Conditions for a Single Loop

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The transport networks found in many systems exhibit loops. Coastal river networks, leaf veins, and city streets have loops that are essential to their function. Looping structures within a larger network can arise because of adaptation to fluctuating hydrologic boundary conditions. However, the relationship between fluctuations and loop stability has not been thoroughly tested at the scale of a single loop. We consider a three node loop that it is fed by fluctuating flows at each node, just as a single loop within the channel network of a river delta would need to adapt to flows from (at least) river floods and tides. We then use linear stability analysis to determine conditions where it is stable as a tree or loop.

Consider a network where the discharge in link connecting nodes *i* and *j* is a linear function of pressure differential, scaled by link conductivity k_{ij} and length l_{ij}: $Q_{ij} = \frac{k_{ij}}{l_{ij}} \Delta p_{ij}$. The two fluctuating flows applied to each node can be considered as vectors: $\overrightarrow{Q_a} = [Q_a, Q_a']$, with $\overrightarrow{Q_a} + \overrightarrow{Q_b} + \overrightarrow{Q_c} = 0$ by concentration of fluid mass. The network adapts to these conditions by changing k based on the flows in a link: $\frac{\partial k_{ij}}{\partial t} = a\langle Q_{ij}^2 \rangle^{\gamma} - k_{ij}/\tau$, with a and τ dimensional constants and the angle brackets indicating an average.

Our analysis finds that for $\gamma = 0.5$, a tree is stable with link *ij* having $k_{ij} \approx 0$ if and only if the angle between vectors $\overrightarrow{Q_a}$ and $\overrightarrow{Q_b}$ is less than the angle on the loop at the opposite vertex/node of link *ij*. If all links *ij* have angles between their fluctuation vectors that exceed the loop's angle, then the stabile configuration of the system is a loop with positive conductivities for all links. A larger fluctuation angle relative to the loop angle indicates a larger conductivity for a given link at equilibrium.

If $\gamma > 0.5$, as is the case in many natural systems where larger channels are nonlinearly more efficient, the system is always stable in the tree configuration. However, a loop can also be stable, but the criterion described above must be exceeded by a constant that increases with γ. This reduces the solution space where loops are stable. This work provides a framework to understand the formation and stability of any loop as a geometric function of its morphology (link lengths and node angles) and fluctuations.

A lattice model of vascular network formation

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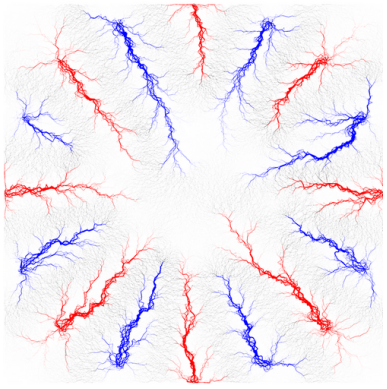
We propose a simple lattice model of vascular network formation involving three main stimuli:

1. Shear stress at the capillary walls: Flowing blood exerts shear stress on the walls of the vessel, causing its widening. As this process is mostly flow-dependent, it results in formation of conductive pathways focusing the blood flow [1].

2. Vascular endothelial growth factor (VEGF): Hypoxic tissues produce VEGF - a protein that leads to the formation of new blood vessels. High gradients of this factor induce the growth of new capillary vessels out of preexisting ones [2].

3. Conducted stimulus: Regulatory signals can be propagated along the vessels, either downstream or upstream, causing the growth of the parent vessel to increase the flow reaching its dependent branches. In this way long loops stretching into furthest regions of the system can be formed, improving the oxygenation [3].

All these factors together result in a transformation of an initial random network of capillaries into a hierarchical system of arterioles and venules. The final result of the evolution is a network with a good balance between oxygen distribution in the system and energy cost of the growth.



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Pinning and its Role in the Directed Motion of Fluids on Solid Substrates

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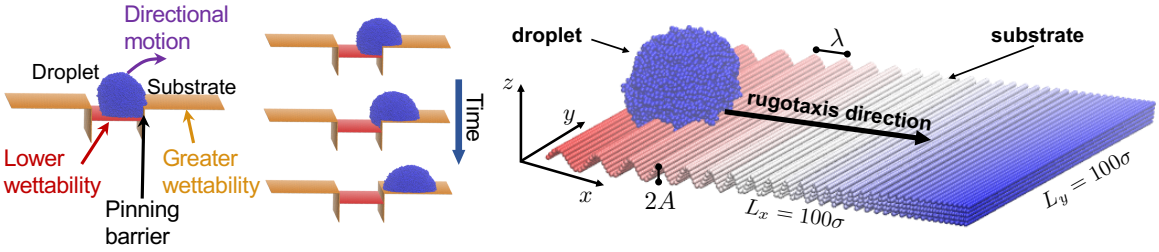
Pinning of liquid droplets on solid substrates is ubiquitous and plays an essential role in many applications, especially in various areas such as microfluidics and biology. Although pinning can often reduce the efficiency of various applications (for example, in the case of rugotaxis), there are situations that this phenomenon can actually offer possibilities for technological exploitation [1]. Here, by means of molecular dynamics simulation of a bead-spring model, we identify the conditions that lead to droplet pinning or depinning and elucidate the effects of key parameters. Moreover, we discuss how pinning can affect rugotaxis, that is, the droplet motion without external energy supply on wavy substrates [2]. Our results have implications for the nanoscale design of substrates in micro- and nanoscale systems and will assist with assessing pinning effects in various applications.



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Anomalous transport in driven periodic systems: distribution of the absolute negative mobility effect

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Absolute negative mobility is one of the most paradoxical forms of anomalous transport behaviour. At the first glance it contradicts the superposition principle and the second law of thermodynamics, however, its fascinating nature bridges nonlinearity and nonequlibrium state in which these fundamental rules are no longer valid. We consider a paradigmatic model of the nonlinear Brownian motion in a driven periodic system which exhibits the absolute negative mobility. So far research on this anomalous transport feature has been limited mostly to the single case studies due to the fact that this model possesses the complex multidimensional parameter space. In contrast, here we harvest GPU supercomputers to analyze the distribution of negative mobility in the parameter space. We consider nearly 10^9 parameter regimes to discuss how the emergence of negative mobility depends on the system parameters as well as provide the optimal ones for which it occurs most frequently.

Estimations of difference between ground state energies for Hubbard model and its Hartree-Fock approximation

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A lower bound on the difference $E_{\rm gs} - E_{\rm HF}$ of the true ground state energy and the Hartree-Fock approximation to it is derived for a class of Hubbard models. The derivation follows closely the approach used by Bach and Poelchau in [1]. Its main technical tool are the correlation inequalities derived by Graf and Solovej [2]. We extend the results of [1] to several other classes of models. To the first one belong models which are not stricty translationally invariant. The second one form multi-band Hubbard models. To the third one belong Hubbard models with the $SU(N)$ internal symmetry. The common conclusion, pertaining to these three classes of models, is that the Hartree-Fock approximation becomes exact in the limit of vanishing Coulomb interaction U.

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Modeling the growth of Liesegang rings and mineral dendrites

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Liesegang rings and mineral dendrites are two examples of patterns which form in rocks when they are infiltrated by the hydrothermal, manganese-bearing fluids. As these fluids mix with the the oxygenated fluid within the rock pores, manganese oxide precipitates, forming the intricate patterns. Several models of this process have been proposed, which vary in complexity. One model assumes precipitation of manganese oxides directly on the surface of the growing dendrite, which then elongate. Another model involves an initial growth of small nanoparticles of manganese oxide, which then aggregate into larger structures.

We study this process using lattice-Botlzmann method to track the evolving concentrations of all of the species involved in reaction. Next, we analyze the dependence of the morphology of the resulting patterns on the physical parameters characterizing the reaction and growth, such as the concentrations of the initial solutions, reaction rates, nucleation thresholds or surface energy of the dendrites.

Growth dynamics of endothelial cells in the VEGF concentration field

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Reconnections after breakthrough

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Attraction between branches is even more prominent when one of them reaches boundary of the system (breakthrough). The reconnections after breakthrough were observed in many physical systems (fracture dissolution, viscous fingering, lightnings), as well as in some biological, e.g. a quasi two-dimensional network of canals in the gastrovascular system of jellyfish *A. aurita*. We study this specific case of reconnections numerically and observe the jellyfish in experiments, as they are relatively easy to observe *in vivo* and to clone (due to their specific life-cycle).

References

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