School cum Workshop

Challenges in Multiphase Flows

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Contents

1 School: Lectures

Introduction to hydrodynamics and model H equations

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The lecture first sets out to derive the standard Navier–Stokes equations for a one–component fluid. It is demonstrated that the equations are the logical consequence of (i) the local conservation laws for mass, momentum, and energy, (ii) the concept of local equilibrium, which allows the definition of fields of genuinely thermodynamic character (like pressure, temperature, and entropy, as a function of space and time), plus the application of the first and second law, and (iii) the description of dissipative processes in terms of linear Onsager theory. For a binary fluid, a convection–diffusion equation for the concentration has to be added. Finally, for a system with two–phase coexistence (either a gas–liquid system or an unmixed binary fluid) one needs to take into account interface forces. A particularly straightforward way to do that is via a Ginzburg–Landau type free energy functional, which gives rise to an additional interface stress term in the equations.

Introduction to Lattice Boltzmann

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The lecture will outline how a simple Lattice Boltzmann (LB) algorithm, based upon a linearized Boltzmann equation for an ideal gas, is constructed. The main ingredients are the Maxwell–Boltzmann constraints that allow to find the lattice version of the local equilibrium populations, and the Chapman–Enskog expansion that establishes the link between the update rules of the algorithm and the macroscopic Navier–Stokes equations (NSE). It is thus shown that LB may be used as an NSE solver, with a well–defined and clear underlying theoretical foundation. Time permitting, the lecture will also cover simple extensions of the algorithm, such as bounce–back boundary conditions and external forces.

Lattice Boltzmann simulations of complex fluids

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Landau–like continuum theories have proved very useful in understanding the generic phase behaviour of complex fluids in equilibrium. Coupling these with dynamical equations such as the Navier-Stokes equations or the Beris-Edwards model of liquid crystal hydrodynamics has proved a powerful way to investigate the flows of complex and multiphase fluids. I shall summarise such "free energy" approaches and describe applications to phase ordering, droplet dynamics, flowing liquid crystals and active matter.

Introduction to (Smoothed) Dissipative Particle Dynamics and Smoothed Particle Hydrodynamics

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Dissipative Particle Dynamics (DPD) [1] is a mesoscopic mesh-free particle-based method which reproduces fluctuating Newtonian hydrodynamics. Although having been very successful in modelling complex mesoscopic systems, DPD suffers from the conceptual problem that it has no thermodynamic scale associated with the particles. In addition, in order to specify transport coefficients, one needs to rely on approximate results from kinetic theory or to map and calibrate the model parameters. A corrected version of DPD that does not suffer from this problem is Smoothed Dissipative Particle Dynamics (SDPD) [2,3]. SDPD is a version of the well-known Smoothed Particle Hydrodynamics method (SPH) [4,5] — a mesh-free Lagrangian Navier-Stokes solver — albeit with the proper inclusion and thermodynamic scaling of thermal fluctuations [6]. The SDPD model is entirely embedded in the GENERIC framework [7], therefore it maintains the discrete thermodynamic consistency (1st/2nd Laws of Thermodynamics and Fluctuation-Dissipation Theorem), and in addition allows for a direct specification of the transport coefficients as input parameters. Generalization of SDPD-SPH to more complex viscoelastic flows will be also discussed [8].

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SPH method for violent multi-phase flows with high density ratio

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The weakly compressible SPH (WCSPH) method is known suffering from low computational efficiency, or unnatural voids and unrealistic phase separation when it is applied to simulate highly violent multi-phase flows with high density ratio, such as that between water and air. To remedy these issues, we propose a multi-phase WCSPH method based on a low-dissipation Riemann solver and the transport-velocity formulation. The two-phase Riemann problem is first constructed to handle the pairwise interaction between fluid particles, then modified for the fluid-wall interaction to impose the solid wall boundary condition. Since the method uses the same artificial speed of sound for both heavy and light phases, the computational efficiency increases greatly. Furthermore, due to the transport-velocity formulation employed for the light phase and application of the two-phase Riemann problem, the unnatural voids and unrealistic phase separation are effectively eliminated. The method is validated with several 2- and 3D cases involving violent water-air flows. The results have been compared with existing experimental data, previous numerical and analytical solutions, where the proposed method demonstrates good robustness, improved or comparable accuracy, respectively, comparing to previous methods with same choice of sound speed or those with much less computational efficiency.

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Diffuse interface models for multiphase flows: Mathematical and numerical aspects

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Diffuse interface models are based on describing interfaces by layers of small thickness, whose structure is determined through a non-local mixing energy that captures the balance of molecular forces, where this energy represents the competition for mixing and de-mixing processes. They can be reformulated as a gradient flow problem, in which the free energy, consisting of the double-well potential and the gradient term penalizing the interface between different components, is minimized.

Diffuse phase field models are typically coupled to the fluid equations, i. e., the Navier-Stokes equations. We will give an overview of existing models and their analytical results on existence of suitable solutions [1]. Moreover, we will also review some numerical methods presented in the literature in the last years to approximate the Cahn-Hilliard equation [2-4]. In particular, we will compare the main properties: the order of time accuracy, energy-stability, unique solvability and the linearity or nonlinearity of the resulting systems.

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Developing advanced pore network modelling formulations for two-phase flow and reactive transport

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In this presentation, we will focus on modelling two-phase flow using Pore Network Modelling method. We will show more complex pore-network formulations that have been implemented for a more accurate modelling of transport problems in the presence of the nonwetting phases. This is mainly done by further discretizing the pore space around the non-wetting phases in each pore into smaller components. An implicit numerical scheme is then used to solve the discretised form of the governing equations, and an efficient substitution method is applied to considerably minimize the computational times.

Moreover, the calculated interfaces between wetting-nonwetting phases can serve as locations for adsorption of colloids and particles suspended in the bulk phases. As the amount of interfaces change with time and phase saturations, the capacity of the media for adsorption of colloids and particles will accordingly change.

The methods have been implemented in a computational package called PoreFlow, which enables coupling between various flow types (e.g., single phase, multi-phase, gravity driven) and reactive transport where the size of pores can be changed due to dissolution and precipitations multi-components chemical reactions.

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Level Set methods for multiphase flows

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The lecture is aimed at describing the level-set technique for numerical modelling of interfaces in two-phase flow. In the level-set method the interface is represented by the zero contour (or level-set) of a function defined on the whole domain that the fluid occupies. Usually the level-set function is a signed distance function. The starting point is an interface advected by a known velocity field, which is modeled by a simple advection equation. We will describe how this problem can be solved numerically. In particular we will discuss the need to reinitialise the level-set function. We then proceed to introduce a coupling to the velocity field through surface tension. The model now consists of Navier-Stokes equation coupled to the level-set method. The surface tension introduces a singularity in the Navier-Stokes equation, which is numerically difficult. The most straightforward numerical approach is to regularise the singularity, and to handle the coupled system by a splitting method, which means that in each time-step the velocity-field and the level-set function are advanced separatly. We end the lecture by discussing some of the downsides with the simple approach, and possible ways to avoid them.

Diffuse-interface models: Versatile tools for the solution of moving-boundary problems

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Diffuse-interface models for the description of pattern formation and interface dynamics naturally arise from the continuum description of phase transitions. They can often be obtained from microscopic models with the help of a mean-field approximation. In this view, the interfaces have their natural (physical) thickness, which is usually on the nanometer scale. For a computationally efficient treatment of structures and patterns on larger scales, the interface thickness is often artificially enlarged in simulations. However, this can lead to artefacts since interface dissipation and other interface effects are also reinforced. In order to establish a precise relationship between diffuse-interface and sharp-interface models, a detailed analysis of the equilibrium and kinetics of diffuse interfaces is necessary. In many cases, it is possible to eliminate or at least mitigate undesirable interface effects by judicious choices in the construction of the diffuse-interface model that are not motivated by microscopic physics. As a result, the diffuse-interface model becomes a computationally simple and efficient tool for the quantitative solution of the corresponding moving-boundary problem. This will be illustrated by several examples from the domains of crystallization [1], growth of composites [2], and two-phase flow [3].

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Introduction to Direct Numerical Simulation of multiphase flows using the Front Tracking method

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This lecture will focus on the Direct Numerical Simulation (DNS) of multiphase flows using the Front Tracking (FT) method. This method allows the detailed simulation of dispersed multiphase flows accompanied by mass and heat transport processes which are often encountered in practice. Following the description and numerical implementation of this powerful method the possibilities and limitations of the FT technique will be outlined. Specific attention will be paid to volume conservation and the incorporation of surface tension. Following the explanation of the basic method various illustrative examples will be presented and discussed including the formation and buoyant rise of bubbles in isolation or in dense swarms. Specific attention will be paid to the utilization of the FT method to develop closures for mass, momentum and heat exchange to feed coarse-grained models such as the stochastic Euler-Lagrange model to compute the behavior of large-scale process equipment.

2 Workshop: Talks

Free surface instabilities in complex fluids

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We discuss recent progress in understanding instabilities that arise at the free surface where a flowing viscoelastic fluid meets the outside air. In particular, we discuss so called “edge fracture”, which is often cited as the primary hindrance to obtaining reliable rheological data in shear; and “extensional necking”, often cited as the primary hindrance to obtaining reliable rheological data in extension. For each instability, we derive a fluid-universal criterion for its onset, and discuss the underlying physical mechanism that drives it.

Modelling cell mechanics

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The collective dynamics of cell layers shows many features seen in active nematics. Examples include velocity correlations over several cell lengths, motile topological defects and collective rotation and oscillations in confinement. I shall discuss the extent to which models of active materials can reproduce the cell experiments, comparing continuum, phase field and particle–based approaches.

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Change of two-phase flow parameters due to reactive transport

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Several subsurface applications such as geologic carbon sequestration and hydrocarbon recovery require capillary pressure (P_c) – saturation (S_w) and relative permeability (k_r) – saturation (S_w) relationships to predict reservoir processes. Chemical reactions may cause significant changes in the reservoir at the microscopic (pore scale) level and consequently modify its macroscopic fluid flow and solute transport properties. While capillarity and relative permeability processes have been explored extensively in the literature, few studies have reported changes in these properties as a consequence of mineral dissolution and precipitation reactions. We developed a pore scale model of fluid flow and reactive transport to understand the relationships between multi-phase flow properties and dynamic changes in the porosity of a carbonate rock sample. Simulations were carried for different fluid inject rates, leading to different responses of the rock sample, such as uniform dissolution versus more compact dissolution starting from the injection side. Different inject rates affected the rock pore-size distribution differently by controlling the evolution of the multi-phase flow properties and the shapes of the $P_c(S_w)$ and $k_r(S_w)$ curves. High inject rates caused a uniform dissolution and increased the porosity evenly throughout the sample. However, lower flow rates created larger pores close to the injection location, which caused the pore size distribution of the sample to change non-uniformly from an initially unimodal pore since distribution to a more bimodal distribution. The initial $P_c(S_w)$ curve, i.e., before dissolution, consequently also evolved into a dual-porosity type curve.

Two-phase flow in porous media: Hysteresis and saturation overshoot

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Contrary to claims in the literature, traditional Darcian theory for two-phase flow in porous media is shown to predict the propagation of non-monotone saturation profiles, also known as saturation overshoot [1]. The phenomenon depends sensitively on the constitutive parameters, on initial conditions, and on boundary conditions [2]. Hysteresis in relative permeabilities is required to observe the effect. Two hysteresis models are discussed and compared [3]. The shape of overshoot solutions can change as a function of time or remain fixed and time independent. Fractional flow and pressure-saturation formulations give identical results, if Neuman boundary conditions for pressure are used to emulate flux boundary conditions in homogeneous media [4]. Traveling-wave-like overshoot profiles of fixed width exist in experimentally accessible regions of parameter space. They are compared quantitatively against experiment.

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Direct Numerical Simulation of three-phase flows

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In this presentation several hybrid Direct Numerical Simulation (DNS) techniques for three-phase flow will be discussed. Such flows are frequently encountered in the (chemical) process industries for the production of base chemicals and synthetic fuels. The focus will be on dispersed multiphase flows where simultaneously deformable (bubbles) and non-deformable (particles) dispersed elements are present. Following the explanation of the basic hybrid method various illustrative examples will be presented and discussed including bubble rise induced suspension of (small) solid particles. Finally, areas which need substantial further attention will be discussed.

Hybrid multiscale methods for complex polymeric flows

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In this contribution we present our recent results on modeling of multiscale multiphase flows such as the polymer-solvent mixtures and colloid-polymer systems. Of course, the most accurate description of such complex soft matter systems would be obtained by the molecular dynamics (MD). However, such miscroscale model is computationally inefficient if large scale regions in space and time need to be simulated. We present two approaches how to overcome this restriction and to obtain practically tractable simulation techniques to bridge macroscopic and microscopic models.

Firstly, we present a new *reduced-order hybrid multiscale method* that is based on the combination of the discontinuous Galekin method and molecular dynamics simulations, see [1]. We follow here the framework of the heterogeneous multiscale method [2] that makes use of the scale separation into macro- and micro-levels. On the macro-level the governing equations of the incompressible flow are the continuity and momentum equations. The equations are solved using a high-order accurate discontinuous Galerkin method. The missing information on the macro-level is represented by the unknown stress tensor that is evaluated by means of the molecular dynamics simulations on the micro-level.

The data obtained from the MD simulations underlie relatively large stochastic errors that can be controlled by means of the least-square approximation. Moreover, in order to reduce a large number of computationally expensive MD runs we use the reduced order approach. We split the computations into an off-line phase of expensive training and an on-line phase of fast multiple queries. In the training phase we use the Greedy sampling algorithm as a model reduction technique to replace the unknown nonlinear stress-strain function by a reliable low-dimensional approximation. Numerical experiments confirm the robustness of our newly developed hybrid MD-dG method.

The present research has been supported by the German Science Foundation under the grant TRR 146: Multiscale Simulation Methods for Soft

Matter Systems.

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Multiscale modeling in the context of the digitalization revolution in the process industry: A survey of case studies and the current state of the art, and where to go

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A recent report from the World Economic Forum report on digitalization of the chemical and materials industries [1], describes in detail nothing less than a revolution. In a few decades, we observe the transition from paper to computer, in all aspects of the chemical manufacturing process. The estimated cumulative economic value of the digital transformation is a staggering 310 billion to 550 billion for the period 2016 to 2025.

I will describe in the presentation a few aspects of the industrial transformation, in particular, the role of physics and data-driven modeling of chemical and materials properties.

In a world where massive amounts of data are available, what to do with all those numbers?

I will describe four sets of new algorithms that we need (from the very difficult to perhaps doable): (1) a way to store properties, structure and composition of complex materials, such that the information can easily be indexed and retrieved automatically, (2) a way to read, parse and interpret patents, papers, and for that matter all scientific documentation automatically, (3) a way to calculate quantum and thermodynamic properties by merging physics and data-driven modelling, automatically, and (4), specific to the rheology community: a way to generate system-specific constitutive equations from underlying molecular constituents, automatically.

To illustrate the challenges ahead, I will use case studies from my experience with Culgi, a multiscale modeling and consulting company that I founded some years ago. Case studies include multiphase flow issues from the oil, polymer industries, and personal care industries, and the energy transition.

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The conservative level-set method and contact line dynamics for multiphase flows

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In a standard model for two-phase flow, each phase is governed by the incompressible Navier-Stokes equation, and the interface between the phases is advected with the local velocity. I will discuss how the conservative level set method achieves mass conservation, in contrast to how the standard level-set method can experience severe loss of accuracy. In many applications contact lines are present. A typical contact line is where an interface is in contact with a solid wall. I will discuss how the dynamics of a contact line can be modelled, and in particular how the dynamic behaviour can be included in level set methods in general, and in the conservative level set, in particular.

Mesoscale modelling of near-contact interactions for complex flowing interfaces

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In this talk I will report on recent developments of a novel mesoscale approach for the simulation of soft flowing materials [1], inclusive of near-contact interactions (NCI) between dynamic interfaces, as they occur in high packing-fraction soft flowing crystals.

The method proves capable of predicting the patterns formation of flowing crystals in microfluidic channels[2-3] and capturing non-trivial aspects of their rheology, such as a power-law dependence of the dispersed phase flow rate on the applied pressure gradient and the structural transition between hex-two and hex-one (bamboo) configurations with the associated drop of the flow rate.

It will be also shown that, above a given intensity threshold, near-contact interactions trigger micro-vorticity patterns, which in turn affect the effective near-contact interactions, giving rise to persistent oscillating ripples at the fluid interface.

The agreement with experimental data suggests that NCI can be dramatically upscaled without any major effect on the aforementioned phenomena, this paving the way to the efficient simulation of microfluidic crystals at scales of direct experimental relevance, with no compelling need to resolve the nanoscale details of the near-contact interactions.

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Capillary and electrostatic interactions in multiphase flows

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Colloidal particles adsorb to fluid-fluid interfaces and reduce the interfacial free energy which leads to an efficient interface stabilization. This effect is well known since the pioneering work of Pickering and Ramsden more than a century ago, but only recently scientists started to utilize tunable capillary interactions between adsorbed colloids to self-assemble complex structures for new soft and adaptive materials. We investigate the interplay of particle shape, contact angle, particle surface structure and external fields on the capillary assembly by means of hybrid lattice Boltzmann / molecular dynamics simulations and demonstrate how anisotropy in the geometry and wettability of colloidal particles can be utilized for the direct assembly of well-defined structures.

The second part of the presentation summarizes recent results on electrokinetic effects in multiphase flows. We coupled our lattice Boltzmann solver to a solver for the Nernst-Planck equation. This allows us to resolve the coupled dynamics of several fluid and ion species. I will present first results ranging from floating droplets deforming in electric fields to electrowetting and the formation of ordered nanostructures in fluid mixtures with antagonistic salts.

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Tuning the rheology of emulsions using DNA

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Self-assembly is a promising route for turning collections of functional particles into microstructured bulk materials with useful mechanical properties. When the particles become larger such that their motion is inertia driven, their assembly does not proceed according to a thermodynamic description but must instead be activated by inputting energy. Here I present experiments on DNA-functionalized emulsion droplets, and numerical simulations, to study the response to oscillatory shear driving applied to an athermal assembly in a model system of functionalised particles, linking the emergent rheological behaviour to droplet-droplet binding. For small strain amplitudes and below the jamming volume fraction, we observe an emergent elasticity when the functionalisation is sufficiently strong. At higher volume fractions, where the droplets touch and deform, the elasticity is less dependent on the sticky DNA functionalisation. Under large strain amplitudes we enter a non-linear regime where the material is in a high stress yielded state and the effects of functionalisation on rheology are less prominent. Our results provide insight into the rheology of concentrated suspensions of athermal, attractive particles, and demonstrate that functionalisation enables precision tuning of material rheology. The latter may have applications across soft matter in areas such as replacement food mouthfeel and the elasticity of artificial scaffolds.

Modeling and simulation of particle systems with Newtonian and non-Newtonian matrices

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Particle suspensions are very relevant to understanding many biological and industrial applications. The study of their flow properties is a very important problem for these systems. Although dilute and semidilute cases in Newtonian solvent are well understood, when concentrated systems and / or non-Newtonian matrices are considered, new problems arise. For example, when the concentration of particles is high, they get very close, entering in the so-called lubrication regime. From a computational point of view, this is a very challenging problem because the lubrication forces are divergent. The election of the lubrication model is also important when the solvent is non-Newtonian. In this talk we will explore some novel computational methods for the simulation of dilute and concentrated suspensions in Newtonian [1,2] and non-Newtonian solvents [3,4]. We will compare results from these models with experiments and previous simulations and discuss possible future extensions.

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An integrated multi-resolution meshfree solver for modeling fluid-structure interaction

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We present an integrated multi-resolution meshfree solver for fluid-structure interaction (FSI) problems involving fluid, deformable and rigid bodies. In this solver, the fluid and deformable and rigid bodies are modeled with the SPH (smoothed particle hydrodynamics) method. The SPH solver is further coupled with an open-source multi-body solver. The present solver is able achieve two-way coupling which is characterized by local and global conservation of mass and momentum of the entire complex system. Furthermore, different particle and time-integration resolutions are allowed for fluid and solid bodies to increase computational efficiency. These achievements are due to the unified meshless formulation and a newly developed position-Verlet time integration scheme. Several benchmark tests show that the solver is able to produce efficient and stable simulations and accurate results.

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Challenges of cellular blood flow modelling in health (and disease)

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"Most people are not interested in blood flow as long as it flows well." [1] In fact, there has been a recent increase in modelling of blood flow in disease, such as malaria, sickle cell anemia or cancer. Blood flow modelling becomes particularly challenging at the scale of arterioles and capillaries where the diameters of blood vessels and red blood cells (RBCs) are similar. In these cases, computationally expensive cell–based models are still required to uncover suspension flow effects and predict cell distribution and tissue oxygenation. Deformable RBCs are typically modelled as hyperelastic or viscoelastic capsule–vesicle hybrids that are fully coupled to the ambient fluid flow and allow to capture the cell deformation and dynamics on the micron level. In order to enable more quantitative predictions in larger blood vessel networks (e. g. on the organ level), more efficient reduced models are required. I will give a short overview of existing microscopic blood flow models and ongoing activities to develop effective blood flow models applicable to larger scales.

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[1] Personal opinion of the presenter.

Phase-field simulations of viscous fingering in shear-thinning fluids using the advected-field method

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During viscous fingering, a fluid with a low viscosity is pushed into a fluid with higher viscosity in a Hele-Shaw cell. For Newtonian fluids, this is the classic Saffman-Taylor problem which is well understood: the Saffman-Taylor instability leads to the emergence and growth of fluid fingers. For non-Newtonian fluids, the morphology and dynamics of the fingers depend on the rheological properties of the high-viscosity fluid. We develop a phase-field model for the Hele-Shaw flow of non-Newtonian fluids, which extends a previous model for Newtonian fluids to a wide range of fluids with a shear-dependent viscosity. The model is found to capture the complete crossover from the Newtonian regime at low shear rate to the strongly shear-thinning regime. The width selection of a single steady-state finger is studied in detail for a two-plateau shear-thinning law (Carreau law) in both its weakly and strongly shear-thinning limits, and the results are related to previous analyses. For power law (Ostwald-de Waehle) fluids in the strongly shear-thinning regime, good agreement with experimental data from the literature is obtained.

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Effective rheology of two-phase flow in porous media: Dependence on system size and system disorder

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When two immiscible fluids flow in a porous media the flow does not obey linear Darcy law in the regime where the capillary forces are comparable to the viscous forces. The flow rate was observed experimentally to scale in a quadratic manner with the pressure gradient for two-dimensional Hele-Shaw cells [1] as well as a three- dimensional porous medium [2] constructed with glass bids. The disorder in capillary barriers at pores effectively creates a yield threshold, making the fluids reminiscent of a Bingham viscoplastic fluid [3] in the porous medium, introducing an overall threshold pressure P_t in the system [4]. Due to disorder in capillary barriers, an increasing number of connecting paths appear in the system while increasing the pressure gradient (ΔP), enhancing the increase of overall flow rate Q more faster than the linear dependence. This leads to a quadratic dependence of Q on the excess pressure drop (ΔP-P_t) at the capillary dominated the regime and a linear dependence at a sufficiently high flow rate when all pores open up [4,5]. The disorder in the capillary barriers at the pore the level appears due to two factors: (i) fluctuation in pore sizes and (ii) interface configurations between the two fluids inside a pore. At very high ΔP, when the fluid flows through all possible connecting paths, Q increases linearly with (ΔP-P_t). The present work has a two-fold purpose. The first one is to understand the behavior of the crossover point at beyond which the Darcy like linear flow is observed. When the saturation of the fluid approaches to zero or one, the two- phase flow reduces to single-phase flow governed by a linear Darcy law. Here, we will present a detailed study of the cross-over point with a continuous variation of the above two system disorders. For the second purpose, we will restrict ourselves within the region where the relation of flow-rate with a pressure gradient is non-linear (low capillary number). In this region, P_t is observed with increasing system sizes to understand its behavior in the continuum limit. This involves the problem of upscaling which has been studied earlier in the context of two phase flow. For both the studies, the robustness of the behavior is examined by repeating our numerical simulations for different surface tensions and viscosity ratios.

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Coupling Fluctuating Hydrodynamic and Diffuse Interface modeling for vapor bubble nucleation dynamics

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Vapor bubble nucleation has a major impact in advanced technical applications such as thermal management systems, cavitation, kidney stone removal, microfluidic devices and optical surgery. It is an intrinsically multiscale phenomena since it couples the macroscopic length scales of the bubble with the molecular scale of the liquid-vapor interface. At molecular level the thermal fluctuations are the actual responsible for the phase transition from liquid to vapor, hence nucleation must be understood in a statistical sense.

To cope with this multiscale and stochastic phenomenology, we exploit a mesoscale description that couples a diffuse interface modeling of the two-phase liquid-vapor system together with the Fluctuating Hydrodynamics theory developed by Landau and Lifshitz [1]. This innovative and powerful methodology gives access to the complete bubble dynamics, from its inception up to the long-time macroscopic expansion, with a considerably cheaper computational cost when compared with more traditional techniques such as Molecular Dynamics [2]. We analyze the nucleation dynamics both in homogeneous and heterogeneous conditions showing the effect of multi-bubble interactions during the first stages of vapor formation. The analysis of heterogeneous conditions focuses on the effect of wall wettability and reveals unexpected and non-trivial behaviors.

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Nucleation and growth dynamics of vapor bubbles

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The vapor bubble nucleation represent the *incipit* of the phase transition in metastable liquids. Its complexity is concealed behind its intrinsically multiscale nature, calling for a mesoscale description able to capture both the microscopic and the macroscopic features of the dynamics. Several mathematical models have been proposed to address the key features of bubble dynamics from its formation up to its growth, transport, and deformation inside the mother phase. Most of them focus separately on few of these aspects. Here we present a mesoscopic model based on a phase field description of the two phase (liquid–vapor) system embedded with thermal fluctuations. Recently the Landau and Lifshitz's Fluctuating Hydrodynamic theory (FH) has been generalized to capillary fluids [1]. In the latter model, the deterministic hydrodynamics of the two-phase system is provided by the diffuse interface approach [2], and the stochastic fluxes are determined by the original FH. In the present work we developed a coarse-grained version of this model, by averaging of the three-dimensional equations on spherical shells: the resulting equations depend on the radial distance from the vapor bubble center. For different levels of metastability, *in-silico* experiments give access to the time to be awaited to observe on average the formation of a supercritical vapor bubble, showing good agreement both with the complete three-dimensional model and classical theories [3]. A rough estimate shows that the numerical effort is reduced by four orders of magnitude with respect to brute-force atomistic simulations and by two orders of magnitude with respect to the full three dimensional fluctuating model. The simulations extend up to the very long time scales, allowing for analyzing inertially driven bubble oscillations in confined systems with perfect agreement with available theoretical predictions.

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Optimal motion of triangular magnetocapillary swimmers

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Magnetocapillary swimmers are formed by three or more rigid magnetic particles trapped at a gas/fluid interface. Self-assembly is achieved due to equilibrium between the attractive capillary and the repulsive magnetic forces, while the motion of such a swimmer is induced by a modulation of the magnetic field.

In this contribution the method, the relevant parameters and the dynamics of the swimmer are presented. We combine the pseudopotential lattice Boltzmann method and the discrete element method [1]. The interface and the associated capillary effects are modeled using the approach of Shan and Chen. For creating the swimmer we first investigate the equilibrium properties of a single, two and three particles at the interface to match the parameters of typical experiments [2]. Next, we demonstrate a controlled motion of the swimmer formed by three particles that shows a sharp dependence of the average center-of-mass speed on the frequency of the time-dependent external magnetic field. Finally, we discuss further feasible modes of motion [3].

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Oil droplet and membrane surface hydrodynamic–colloidal interactions

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Membranes offer a superior separation capacity for stable emulsions, which are otherwise difficult to process. However, membrane fouling is always prevalent and requires extensive backwashing and cleaning as part of the operating regime. Oil droplets deform when in close proximity to a membrane, primarily due to permeation drag, which can lead to irreversible deposition on the membrane. Understanding the influence of hydrodynamic stresses and colloidal interactions between droplets and membranes will allow for better engineered membrane surfaces and process conditions. Using a long-wave hydrodynamic description that incorporates wettability via a Derjaguin (disjoining) pressure and electrostatic repulsion via electric double layer (EDL) contributions, we derive a set of equations for the thickness and pressure in the liquid film separating the droplet and the permeable membrane.

Numerical simulations are used to analyse equilibrium states where a zero net force acts on the droplet, to investigate the influence of droplet shape, distance from the membrane, membrane permeability and characteristic parameters of the colloidal interactions on the overall repulsion / attraction towards the membrane surface. A stability phase diagram is constructed in terms of the modified capillary number – accounting for the ratio of the viscous and surface tension forces – and a parameter representing the ratio of the hydrodynamic pressure scale over the electrostatic interaction intensity.

These calculations are used to classify stable (upward deflection, increasing distance from the membrane) vs. unstable drop shapes (downward deflection bringing the droplet closer to the membrane), and investigate conditions leading to irreversible deposition onto the membrane. In particular, the model can describe how membrane properties and emulsion characteristics dictate a 'critical' permeation flux.

3 Workshop: Posters

Some attempts to understand two-fluid models

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We consider the hydrodynamics of a binary fluid. Conventional hydrodynamics assumes strict local equilibrium, which in turn means that the flow velocities of both components must be identical. A two-fluid model goes beyond that picture and allows for a nonzero relative velocity. This is needed for situations where the two components are dynamically very different, and the model aims at a description that is still valid on the time scales of molecular relaxation. A semidilute polymer solution on intermediate time scales is a typical example for such a system. We are here concerned with the simplest possible case, which assumes that (i) there is no dissipation, and (ii) there are no further non-hydrodynamic variables beyond the relative velocity that are taken into consideration. Even for that simple case, the precise form of the equations of motion has been under debate. We here derive the equations unambiguously, using a straightforward generalization of a formalism that is shown to work nicely for a one-component fluid: Firstly, one postulates the form of the mass and momentum conservation equations, where the convection terms result from the molecular picture, and the forcing terms in the momentum equations are unknown. Secondly, one considers the system in the isothermal ensemble, where no further hydrodynamic equations occur, and a conservation law for the free energy must hold. From this latter condition, one finds the forcing terms in an unambiguous fashion, while momentum conservation can then be verified from the result. Finally, for the constant- energy ensemble, one simply has to augment the system by yet another equation of motion for the entropy: The convective derivative of the entropy per unit mass must vanish.

Mathematical treatment of a macroscopic model of viscoelastic phase separation: Well–posedness, numerics and simulations

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We will present our recent results on a macroscopic model of viscoelastic phase separation. Our model is similar to the top-down model from Zhou, Zhang, E in [1], but allows for more nonlinear effects regarding the polymer conformations. Our model couples the Cahn-Hilliard equation for the evolution of the polymer volume fraction to a nonlinear diffusion equation which accounts for the polymer network pressure. Further the model is supplied with the Navier-Stokes-Peterlin model to account for flow and stress effects of the mixture. We will present some rigorous mathematical results on existence, relative energy and weak-strong-uniqueness without going into technical details, [2]. Further, we will discuss the discretization of the continuum model in order to be feasibly computable model which at the same time remains energy dissipative. Therefore, we use a finite element technique in space combined with a Lagrangian characteristic method in time. Together this is the so-called Lagrange-Galerkin finite element method. With the algorithm at hand, we will present some simulations involving relevant examples in two and three space dimensions. Finally, we will give some remarks on multiscale comparison to the mesoscale model in [3].

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Semi-automatic construction of Lattice Boltzmann models

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A crucial step in constructing a Lattice Boltzmann model is the definition of a suitable set of lattice velocities, and the correct assignment of the associated weights. The poster outlines the functioning of a publicly available Python script which has been written to assist researchers in that task. The speed of sound c_s is considered as a parameter, which can, within limits, be chosen at will. Under this premise, the Maxwell-Boltzmann constraint equations are a system of linear equations to determine the weights, and hence amenable to numerical solution by standard linear algebra library routines. By suitable contractions, the tensor equations are mapped to a set of equivalent scalar equations, which simplifies the treatment significantly. Using a singular-value decomposition, the software is able to distinguish between (i) no solution, (ii) one unique solution, and (iii) infinitely many solutions. Case (ii) is analyzed in detail, and the range of permitted c_s values is calculated. The script can treat arbitrary spatial dimensions, and an arbitrarily large degree of isotropy, measured in terms of tensorial velocity moments of the weights. New models that have been found in two and three dimensions are isotropic up to tenth order.

Phase separation in ternary fluid systems

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Phase separation is ubiquitous in nature and industrial applications. Examples range from biological cells and magmas to processes in the chemical industry; and in many relevant scenarios, the system of interest can separate into three distinct fluid compositions. In this work, we use lattice Boltzmann simulation to systematically study the phase diagram of phase separating ternary fluid mixtures and classify the morphologies observed. We investigate how the results are affected by variations in the ratios of surface tensions, mobilities and viscosities. The simulation results are also compared against analytical predictions employing linear stability analysis.

Spreading dynamics of a droplet on a fluid-fluid interface

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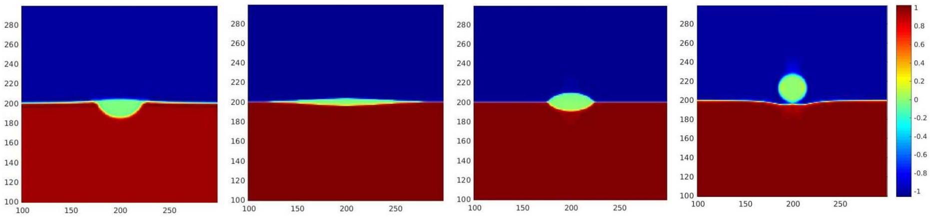
A drop of a liquid forms a lens on a fluid-fluid interface when the spreading coefficient, $S < 0$ [1]. In other words, the spreading coefficient characterises the competition of interfacial tensions between all three fluids and determines both the dynamics and final equilibrium shape of the liquid drop on a fluid–fluid interface. In order to explore this physics and the consequences, we model the hydrodynamics of spreading of a droplet using a continuum theory along with a diffuse interface model [2]. The governing equations are solved simultaneously using the lattice Boltzmann method. The shapes of the drops are validated using Neumann's triangle relation. The spreading dynamics of the drop is characterised by analysing the temporal evolution of the radius and the height of the liquid lens and the contact angle. It was found that each of these quantities follow a power law only at intermediate times, i.e. when the effects of initial conditions have disappeared and the slow convergence to the final state has not started. Then dependence of the power law exponent on the spreading coefficient was investigated as a function of the contact angle. Further, the velocity field around the spreading drop was characterised by defining a topology parameter which quantifies the ratio of vorticity to strain rate. It was found that the flow field can be described using low Reynolds number singularities and the strength of the singularity was obtained as a function of the spreading coefficient. Both these flow characterisations are finally linked to the dependence of the power law exponent on the contact angle of the spreading lens.



(a) (b) (c) (d)

Figure 1: Equilibrium shapes of droplet for different S. (a) $S = -0.1$, (b) $S = 0$, (c) $S = -1$ and (d) $S = -2$.

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Application of a 3D LBM interface tracking model on dam-break flows

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Free surface flows have a pivotal role in many environmental hydraulic problems but, so far, 1D or 2D numerical models, mostly based on the Shallow Water (SW) assumption, have been preferred to 3D counterparts, often unfeasible due to the high computational burden, in order to study their dynamics. Dam-Break (DB) flows are a subset of this kind of phenomena characterized by an impulsive evolution and important scour effects occur due to the high flow velocities; there have been attempts to include movable bed dynamics in SW models [6, 7], but they all rely on the reconstruction of bed velocities from the uniform velocity over depth provided by these model [8].

The need of a correct description of velocity distributions, not natively provided by SW models, and the impressive performance of Lattice Boltzmann Method (LBM) shown by recent works [3, 5] may make 3D computations affordable also for large scale problems but an assessment of LBM models to this kind of phenomena is currently missing.

Fully 3D simulations of DB flows are carried out by means of a interface tracking LBM based model in order to assess its accuracy: numerical outcomes, in terms of water levels and flow velocities, are compared with data from classical experimental benchmarks and previously published SW model, when available [1-2, 4]. Comparison between a free-slip or a no slip approach is also discussed; the former is found to be preferable when underesolved boundary layers are present. Our model proves to describe the phenomena quite well predicting both water depths and velocities, the latter being poorly reproduced by SW even at locations where the assumption of uniform velocity along the water column is met.

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Lattice Boltzmann modeling of coalescence filtration through non-woven fibrous media

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Fibrous porous media have a range of important industrial applications, including separation of water from diesel fuel [1]. The efficiency of the filtration process is critical for the performance and lifetime of engines. However, a comprehensive fundamental understanding of the dynamics of emulsion droplets in fibrous porous media is still lacking. This is due to the complex dependence of the coalescence kinetics on the geometry and surface properties of porous media. In the current work, we focus on wetting and capillarity effects of droplets deposited on two parallel fibers. We present lattice Boltzmann simulations of the wetting behavior of droplets on the fibers and study the spreading and retention of liquid [2]. The results reveal how the morphology of the droplets depends on the drop volume and fiber spacing. Comparison of the simulation data with analytical and experimental results shows good agreement for the steady-state capillary pressure [3].

We further discuss capillary force dependent trapping and detachment of droplets on fibers. The critical capillary number that delineates the boundary between trapping and squeezing is determined through numerical simulation and analysis of barycentric velocity for varying fiber spacing and wettability. The results shed light on the coalescence dynamics and the capture and detachment mechanisms in the loading stage of coalescence filtration. The insights can be used to design filters with optimal quality factor [4].

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The role of advection in the dynamics of self-diffusiophoretic colloids at interfaces

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Active matter is a class of materials composed of units which can transform energy from their surroundings and use it to, e.g., swim in a fluid. Not only do these materials provide insights into the general physics of non-equilibrium statistical mechanics, they are relevant for many research areas, e.g., biology and microrobotics [1]. A paradigm for active matter is a colloid which swims in a fluid due to a self-generated inhomogeneous concentration of solute, in a process called self-diffusiophoresis. Self-diffusiophoretic colloids are typically understood in terms of a slip velocity on their surface [2]. This description is, however, incompatible with the boundary conditions imposed by a fluid-fluid interface. Through Lattice Boltzmann simulations combined with a finite-difference solver for the solute dynamics, we are able to consistently determine the dynamics of a self-diffusiophoretic colloid adsorbed at a fluid-fluid interface. While a Janus colloid with an arbitrary contact angle will eventually be trapped at the interface [3], our preliminary findings are that isotropic colloids can propel indefinitely due to the advection of solute, a mechanism which is typically neglected. The possibility of using active channels as pumps will also be presented.

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The mechanics of cilia beating: Quantifying the relationship between metachronal wavelength and fluid flow rate

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We investigate the relationship between the metachronal wavelength of an array of beating cilia and the resulting fluid flow rate through numerical simulations. Our model is based on a hybrid immersed boundary lattice Boltzmann algorithm [1] written in CUDA so that we can run rapid simulations on a GPU. Our results suggest that varying the metachronal wavelength of the cilia array affects the fluid flow rate by increasing or decreasing the spread of cilia during their active strokes. We quantify this behaviour by constructing an analytical model of the system and deriving an equation for free area within the cilia array that depends on the metachronal wavelength. We show that there is a strong correlation between free area and fluid flow rate that holds for different values of cilia spacing.

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Investigation of slip effect and the entrance/exit effect on water flow through a nanochannel

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Understanding the behaviour of water molecule transport through artificial nanochannels is essential in designing novel nanofluidic devices that could be used especially in nanofiltration processes [1-3]. In this study, the behaviour of the confined water flow through a nanochannel made of two graphene layers was examined by considering the slip and end effects. The water flow rates were measured inside the nanochannels of specified length and various thickness, by using MD simulations (LAMMPS). It was found that the dependence of the water flow rate on the channel thickness and the applied pressure could be described by a third order polynomial. In addition, we modified a flow model based on continuum hydrodynamics by embedding two terms to consider the slip and end effects. The unknown coefficients of two terms added to this equation were estimated through a comparison between the simulation/model values. Our suggested model could be considered to predict the behaviour of the confined water flow inside the nanochannels, by modifying the slip effect and the entrance/exit effect, in which the first term increases the water flow rate, while the second term reduces it. The results of this study could be beneficial in designing multilayer nano-membranes that are used in water purification processes.

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Numerical investigation of cavitation-induced plastic deformation: Coupling the diffuse interface model with plasticity

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The cavitation phenomenon, namely the appearance and collapse of vapor/gas bubbles surrounded by their liquid, has been of great interest in the past decades. In particular, many efforts have been put in the observation of bubbles dynamics and the effects of collapsing bubbles near solid surfaces [1,2]. On the other hand, recent studies have shown the ability of the diffuse interface model to numerically reproduce the dynamics of a collapsing vapor bubble surrounded by its liquid, both in presence and absence of solid boundaries [3,4]. In our study, we present the numerical investigation of a one-way coupled fluid-structure interaction between a collapsing bubble, described by a diffuse interface model, and a solid wall, with an elasto-(visco)plastic behavior. Our aim is to capture the effects of a single bubble collapse on a near wall, and quantify the plastic deformation and indentation in the first stages of cavitation.

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Surface tension between liquids containing antagonistic ions

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The change of the interfacial tension between two liquids due to the addition of dissolved salt has been the subject of many studies in physical chemistry. The salt adds electrostatic forces that typically compete with short-range chemical and long-range van der Waals and entropic interactions. In this work we use a modified Poisson-Boltzmann formalism to examine immiscible electrolytes containing dissolved antagonistic ions. When the ions have preferential solvation to the liquids, the cations and anions partition across the interface, giving rise to an electric field localized at the interface. We solve the nonlinear equation and obtain analytical expressions for the potential profile, ion densities, and surface tension. Our model takes into account the dependence of the Debye lengths in the two liquids on the preferential solvation.

Universal scaling and the characterisation of gelation in associative polymer solutions

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A salient feature of associative polymer solutions is the formation of a thermo-reversible gel. The onset of gelation is governed by the polymer concentration, the solution temperature, the number of stickers per chain, and the strength of association between the stickers. Depending on the solution temperature and concentration, associative polymer solutions undergo a phase transition and get separated into a sol phase (with finite size clusters) and a gel phase (with system spanning infinite size clusters). Several different hypotheses and theories have been proposed in the literature to characterise gelation in associative polymer solutions, but many issues remain unresolved. For instance, the concentration at the inception of gelation is currently unclear. In this work, we carry out multi-particle Brownian dynamics simulations of multi-sticker associative polymer solutions to unambiguously identify the gel point, examine the gel line in temperature-concentration space, and compare simulation results with predictions of scaling theories. We also verify the universality of scaling relations amongst the various parameters that characterise associative polymer solutions, in both theta and good solvents. Simulation predictions of the relaxation time and zero-shear rate viscosity in the pre- and post-gel regimes are compared with previous theories and observations.

Convection during solution mixing: Experiments on a dialysis chamber and models for the effect of convection on the mixing time

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Finding the structure of proteins is critical for the rational design of drugs. To obtain protein structures with X-ray diffraction the crystallisation of proteins is a crucial step. Structural biologists use different crystallisation methods to make different crystal types, all of which typically start by mixing a solution of protein with a solution of precipitant — such as a salt or polyethylene glycol (PEG). Mixing the precipitants with the protein solution induces the supersaturation needed for crystals to form. Mixing is a complex process for volumes above microfluidic standards, that could affect the crystallisation of proteins, but it has not yet been studied extensively by crystallographers. To help bridge this gap, the physics of mixing solutions has been studied for volumes up to one hundred microlitres. The results of dialysis crystallisation experiments were used for the theoretical study on the mixing of crystallisation agents during dialysis crystallisation. The crystallisation experiments were performed with a crystallisation bench [1], which allowed the temperature and chemical composition of the crystallisation solution to be controlled. For volumes larger than a microlitre (lengthscales > 1 mm), convection of the solution and of lysozyme crystals was observed, which accelerated the mixing of the crystallisation solution and the precipitant. This convection, known as natural convection, is caused by gravity acting on a mass density difference. Salt and PEG solutions are only a few percent denser than dilute protein solutions, but this is enough to drive convection. Our theoretical results where validated with experimental data. We showed that natural convection is essential for the prediction of the time at which the final supersaturation in the solution is reached. Crystal growth and nucleation is notoriously sensitive to all aspects of the solution conditions. By proving that convection can radically affect how the supersaturation varies in space and in time during mixing, this model will be useful for any study where crystallisation is started by mixing solutions.

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Long range assembly of Pt nanostructures controlled by peptides: Insights from measurements and molecular simulations

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The hierarchical control of biogenic minerals from the morphology at the nanometer scale to subsequent assembly into macroscopic structures remains a major challenge. Although considerable efforts have been devoted to exploring effects of biomolecules in the biomineralization process, the studies to date are largely limited to atomic/molecular scale crystallization. Here it is shown how molecular dynamics simulation is employed to gain insight of critical effects form biomolecules exerting on the long arrange assembly of biominerals for the example of platinum nanocrystals aligned in 1D and 2D patterns. A Pt(100) specific peptide T7 (Ac-TLTTLTN-CONH2) adopts ST-turn conformations at low concentration in solution that supports the formation of cubic Pt nanocrystals and then spontaneously transforms these structures into β-sheets with increasing concentration.[1] During this molecular assembly process the T7-Pt(100) specific interaction drives cubic Pt nanocrystal into large area and long range linear assembly along the [100] direction. We discuss the analysis of interactions between individual peptides to form long-range ordered structures in atomic-level detail by molecular dynamics simulation and their directional preferences of interaction with Pt nanocubes. The interaction energy with Pt (100) surfaces and facets is larger when peptide strands are parallel to the surface with side chains oriented flat-on to the surface rather than perpendicular. It is also found that docking of the Pt nanoparticles into 1D assemblies typically involves a 1.2 nm thick interlayer of water and a single T7 peptide in quasi ST-turn structure sandwiched between the nanoparticles. The peptide T7 was also found to assist the formation of ultrathin platinum nanoplates assembled from Pt nanocrystals, which demonstrates great oxygen reduction reaction activities compared to current commercial Pt/C electrocatalysts.[2] This 2-D anisotropic assembly scheme is explained by simulation that the peptides tend to adsorb on the nanoplate surface rather than side and thus avoid the 3-D isotropic agglomeration of Pt nanocrystals. The simulation results advance fundamental understanding of biomolecules-nanostructure interface and open vast opportunities for rational design of programmable structures from the atomic scale to the macroscopic scale.

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