University of Ljubljana
Faculty of Mathematics and Physics

MPNS COST Action MP1305 Flowing Matter

COST Workshop on Modelling of Flowing Matter

University of Ljubljana, Faculty of Mathematics and Physics
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http://flowing-matter2015.fmf.uni-lj.si/

Organizers:

MPNS COST Action MP1305 Flowing Matter

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Mission

The aim of this COST Action MP1305 (Flowing matter) workshop is to bring together experts on modelling techniques of complex fluids, complex flows and active fluids, as part of the general idea to bridge ideas and approaches relevant in general flowing matter. The focused number of participants guarantees an open exchange of knowledge, ideas, and opportunities for future research.

Useful links

http://flowing-matter2015.fmf.uni-lj.si/
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Open wifi at the venue (lecture hall F2 and coffee break area):

wifi: **COSTflow**
password: **flow2015**

There is also free wifi provided in Ljubljana city centre:

- WiFreeLjubljana (one hour/day, activation via SMS code):
  http://www.wifreeljubljana.si/en

- Telemach WiFi (activation by a browser click, has to be renewed every 30 min or so).

Abstracts

Invited talks – I

Contributed talks – O

Mesoscopic models for complex and active fluids

Ignacio Pagonabarraga

University of Barcelona, Spain

The wide range of time and length scales that characterize the morphology and dynamics in heterogeneous materials pose a number of computational challenges. The development and use of mesoscopic computational models has opened a fruitful approach to develop approaches that focus on selected relevant scales associated to collective modes in such systems.
In this presentation I will discuss how the use of different mesoscopic models can be exploited to address the emergence of collective dynamics in different types of soft materials.

I2

A TOPOLOGICAL GLASS

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Ring polymers represent one of the last major theoretical challenges facing polymer physics. The essential difficulty lies in the non-local nature of the topological constraint associated with polymers of fixed topology, such as rings (unknots), that cannot cross one-another [1]. A few authors have speculated on the possibility that rings may thread through one-another, forming extremely long-lived entanglements and slowing the dynamics [1-2]. However, these comments have remained at the level of speculation and no convincing evidence has yet been found for such threadings in the melt. Here we report on molecular dynamics and Monte Carlo simulations of ring polymers embedded in a gel [3-4]. We propose a scheme that allows us to identify inter-ring threadings, or penetrations, for the first time. This allows us to monitor their statistical properties and lifetimes. We find evidence of the emergence of a percolating cluster of inter-ring penetrations and argue that, for longer rings, a jammed state that we call a topological glass should arise, even for $T \gg T_g$, the classical glass transition for the polymer itself. In order to further explore this we carry out Monte Carlo simulations on an idealised system in which the rings are assumed to compactify into linear duplex structures. Here we find a clear signature of exponential relaxation, characteristic of such a topological glass. Finally we discuss how this might help us develop a much-needed Universal description of the glass transition.

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[4] D. Michieletto, D. Marenduzzo, E. Orlandini, G. P. Alexander, M. S. Turner. Threading dynamics of ring polymers in a gel. ACS Macro. Lett. 2014, 3:255.

LATTICE BOLTZMANN MODELS BASED ON GAUSS QUADRATURES AND APPLICATIONS

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The theoretical framework of the Lattice Boltzmann models based on Gauss quadratures will be briefly discussed. A particular attention will be given to the implementation of the boundary conditions and the interparticle forces. The capabilities of these models is illustrated by simulation results related to microfluidics phenomena and multiphase fluids.

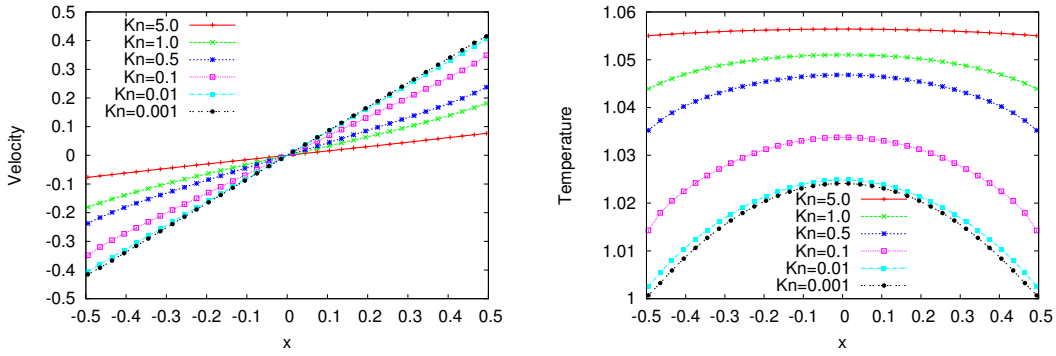

Figure 1: Evidence of velocity slip and temperature jump in $3D$ Couette flow between parallel plates, for various values of the Knudsen number ($u_{walls} = \pm 0.42$, $T_{walls} = 1.0$).

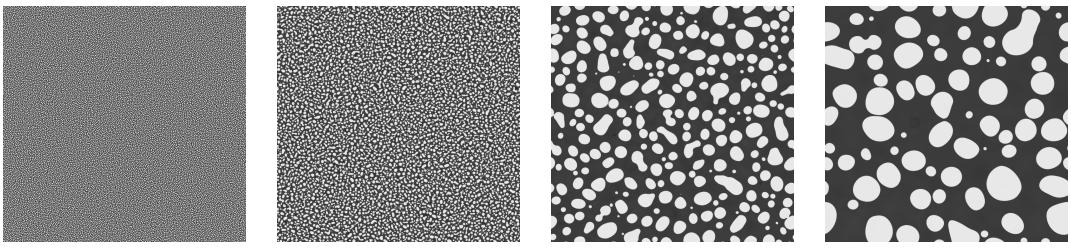

Figure 2: Evolution of the liquid-vapour phase separation. Simulation performed with a nVIDIA Tesla M2090 graphics card on a $2D$ lattice (4096×4095 nodes).

Acknowledgement. This work was supported by Romanian Authority for Scientific Research, CNCS-UEFISCDI projects PN-II-ID-PCE-2011-3-0516 and PN-II-ID-JRP-2011-2.

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[4] T. Biciuşcă, A. Horga, V. Sofonea, submitted to CR Mécanique (2014).

I4

Liquid Crystals at Surfaces and Interfaces: from statics to dynamics

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We address the static and dynamical behavior of liquid crystalline (nematic and cholesteric) phases at surfaces and interfaces.

Using mesoscopic (Landau-de Gennes type) theories for ordered fluids (nematic and cholesteric liquid crystals) and numerical techniques, such as Finite Elements with Adaptive Meshes, to minimize the free energy, we discuss the wetting phase diagram on structured surfaces [1] and the structured interface of cholesterics [2]. The interplay of various length scales leads to surprising results when compared to the results for simple (isotropic) fluids. For example, on structured surfaces, the additional length scale leads to novel phase diagrams, where the stability of the filled and wet phases changes dramatically.

In addition, using the same techniques, we investigate colloidal adsorption at structured surfaces [3] and the colloidal (pair) interactions near surfaces or under confinement [4], unveiling new phenomena in liquid crystal colloids. For example, the topographic modulation of the surface can strongly pin colloidal particles promoting the epitaxial growth of colloidal structures.

Finally, motivated by recent experiments, we use Lattice Boltzmann techniques to address dynamical problems such as pressure driven nematic flows in rectangular microchannels, and the response of nematic droplets at microfibers to time-dependent electric fields.

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[2] N. R. Bernardino, M. C. F. Pereira, N. M. Silvestre, and M. M. Telo da Gama, Soft Matter 10, 9399 (2014).

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Modeling the dynamics inside active gels

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The internal dynamics of active gels, both in artificial (in-vitro) model systems and inside the cytoskeleton of living cells, has been extensively studied by experiments of recent years. These dynamics are probed using tracer particles embedded in the network of biopolymers together with molecular motors, and distinct non-thermal behavior is observed. We present a theoretical model of the dynamics of a trapped active particle, which allows us to quantify the deviations from equilibrium behavior, using both analytic and numerical calculations. We map the different regimes of dynamics in this system, and highlight the different manifestations of activity: breakdown of the virial theorem and equipartition, different elasticity-dependent ”effective temperatures” and distinct non-Gaussian distributions. Our results shed light on puzzling observations in active gel experiments, and provide predictions for future studies.

I6

SHEAR- AND FLOW PROPERTIES OF CLUSTER SOLIDS

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We consider dense systems consisting of ultrasoft, overlapping particles under shear and transport flow, by employing a multiscale simulational approach that combines multi-particle-collision dynamics for the solvent particles with standard molecular dynamics for the solute. We find that the nucleation rates of supercooled liquids can be dramatically accelerated via the shear-induced formation of an intermediate string pattern, which dis-aggregates after the cessation of shear, leading to the emergence of three-dimensional fcc order. Furthermore we expose these cluster crystals to Poiseuille flow and we establish the emergence of a quantized flow pattern, in which both the height and the width of the fluid stream display well-defined plateaus as a function of the applied pressure gradient. The resulting velocity profiles of the solvent closely resemble plug flow. We explain the emergence of the plateaus by successive fluidization of crystalline layers adjacent to the channel walls and discuss the dependence of the discrete flow on the cluster aggregation parameter. Cluster crystals thus emerge as novel systems with applications on nano- and microfluidic devices, allowing the manipulation of flow in a precisely controlled way [1,2].

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MACROSCOPIC BEHAVIOR OF SYSTEMS WITH A DYNAMIC PREFERRED DIRECTION

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We present the derivation of the macroscopic equations for systems with a dynamic preferred direction, which can be axial or polar in nature.

In addition to the usual hydrodynamic variables we introduce the time derivative of the local preferred direction [1] or the macroscopic velocity associated with the motion of the active units [2] as a new variable and discuss their macroscopic consequences [1,2]. Such an approach is expected to be useful for a number of biological systems including, for example, the formation of dynamic macroscopic patterns shown by certain bacteria such as Proteus mirabilis, shoals of fish, flocks of birds and migrating insects.

As a concrete application we set up a macroscopic model of bacterial growth and transport based on a polar dynamic preferred direction – the collective velocity of the bacteria [3]. This collective velocity is subject to the isotropic-nematic transition modeling the density-controlled transformation between immotile and motile bacterial states. The approach can be applied also to other systems spontaneously switching between individual (disordered) and collective (ordered) behavior, and/or collectively responding to density variations, e.g., bird flocks, fish schools etc. We observe a characteristic and robust stop-and-go behavior of the type also observed for the growth of bacteria experimentally [4]. We also discuss our very recent work on the stress tensor critically comparing the results of our model with those of other groups [5].

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I8

Active crystals and the effect of deformability on active motion

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In the first part of the presentation, we consider dense crystallized systems of self-propelled particles. Using a density-field description, namely an extended version of the phase-field-crystal model, which can be motivated from dynamic density functional theory, we study the collective behavior of such dense active ordered structures. As a main result, an onset of collective motion of the whole crystal structure is found at a certain threshold of the active drive. Aspects of linear stability of such structures and the role of hydrodynamic interactions are briefly addressed. In the remaining time, the role of deformability on active motion will be outlined. On the one hand, the deformability of self-propelled particles can promote alignment of the propagation directions of such particles. On the other hand, deformability can destabilize straight active motion. Together with active rotations, deformability of self-propelled particles can lead to the most complex types of motion, evident already when a single such particle is transported by linear shear flow.

DYNAMICS OF POLAR ORDER IN QUINCKE SUSPENSIONS

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Polarization relaxation equation for the dielectric particle in a liquid with a low conductivity [1]

$$\frac{d\vec{p}}{dt} = \vec{\Omega} \times \vec{p} - \frac{1}{\tau}(\vec{p} - \chi\vec{E});\ \vec{\Omega} = \vec{\Omega}_0 + \alpha_r \vec{p} \times \vec{E} \tag{1}$$

predicts different phenomena, which are characteristic for active systems.
Taking into the account the flow created by the rotating particles it is possible to describe the synchronization of the particle rotations in the suspension.The kinetic equation which predits transition to the polar order at $S = 2\alpha n D_r^{-1}\tau^{-1} > 2$ (an external electric field is along z axis, $\vec{n} = \cos\vartheta\vec{e}_x + \sin\vartheta\vec{e}_y$; the parameter α depends on the interaction of particles with substrate) reads (v_0 is the particle rolling velocity on the substrate)

$$\frac{\partial f}{\partial t} + \nabla(v_0\vec{n}f) = D_r\frac{\partial^2 f}{\partial\vartheta^2} - \frac{\partial}{\partial\vartheta}\Big(\frac{\partial}{\partial\vartheta}f(\vec{r},\vartheta,t)2\alpha\int_0^{2\pi}\vec{n}(\vartheta)\cdot\vec{n}(\vartheta')f(\vec{r},\vartheta',t)d\vartheta'\Big)\ . \tag{2}$$

Eq.(2) with the term on the right side $D\nabla^2 f$ accounting for translational diffusion is used for the derivation of the hydrodynamic equations for the slow variables of the system - the concentration of the particles n and the director of the polar order $\vec{h} =< \vec{n} >$. The Toner-Tu equation may be derived from Eq.(2) by keeping in the Fourier series for the distribution function $f = \sum_k f_k \exp(ik\vartheta)$ only terms with $|k| <= 2$, what is valid only near the transition point $S \simeq 2$, when the order parameter is small. In the present work the dynamics of the polar order is studied on the basis of the Eq.(2). It predicts the birth and collision of the soliton-like waves on the background of constant concentration (Fig.1) as seen in experiments [3].

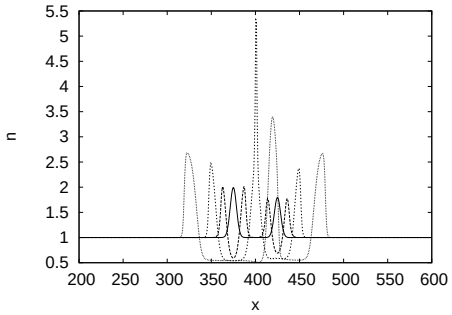

Figure 1: Solid line-two Gaussian peaks($t = 0.002$), dashed line $t = 0.2$, short dashed line $t = 0.4$, dotted line $t = 0.8$. Parameter $S = 2$ for the background,$D/D_r = 0.5$.

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Aggregation of patchy colloids on substrates - A stochastic approach

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Patchy colloids yield directionality of interactions being ideal building blocks for the rational development of self-assembled structures with novel physical properties. Studies of their equilibrium phase diagrams have revealed a myriad of possibilities as, for example, the capability of tuning the density and the temperature of the gas-liquid and sol-gel transitions. However, the kinetics of self-organization and the feasibility of assembling the predicted structures are still poorly understood.
We recently developed a stochastic model to study the irreversible adsorption of patchy colloids on substrates which allows simulating systems with more than one million colloids [1]. Using this model, we compared different mechanisms of mass transport (diffusion and advection) [2], analyzed the influence of the patches spatial arrangement [3], and explored the combination of different types of patches and selective interactions [4]. Our results suggest that the control of experimental conditions and the patch distribution may lead to interesting nonequilibrium interfacial and bulk properties.

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LATTICE BOLTZMANN MODEL FOR BIOPRINTED TISSUE STRUCTURES

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Tissue engineers seek to build living tissue constructs suitable for replacing or repairing damaged tissues. In this effort, computational methods proved useful by revealing dominant mechanisms. Here we develop a finite difference Lattice Boltzmann (LB) model to simulate the evolution of multicellular structures. The model describes a multicellular system in a hydrogel, being suitable to study processes relevant to bioprinting, in which multicellular spheroids or cylinders are delivered in a supportive hydrogel. We simulated post-printing rearrangements of cells, aiming to predict the evolution of certain printed structures. To validate the LB model, we simulated the fusion of multicellular cylinders in a contiguous, hexagonal arrangement. The LB simulation describes the time course of the transversal cross-section of the construct built from multicellular cylinders that are much longer than their diameter. In simulations, fusion leads to a tubular construct, in qualitative agreement with experiments. We also simulate how a defect in a printed tube evolves. In connection with cell sheet engineering, we study the evolution of a planar construct built by printing multicellular cylinders, as well as the spontaneous emergence of a perfusable tissue construct. The agreement with experimental results suggests that the LB model captures certain essential features of in vitro morphogenesis.

This work was supported by the Romanian National Authority for Scientific Research through the CNCS-UEFISCDI project PN-II-ID-PCE-2011-3-0516 / 2011-2015. Our parallel computing code was implemented using the Portable Extensible Toolkit for Scientific Computation (PETSc).

O2

Topology of complex fluids

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In complex fluids, the flow dynamics is coupled to the local state of matter, and more importantly, the coupling is bidirectional. In fluids where the local order supports existence of topological defects, such as in liquid crystals, the defects define the characteristic lengthscale in the system, while the flow drives topological transitions between the defect structures. I will present the geometric and topological properties of defects in nematic liquid crystals and discuss the approaches to their numerical modeling.

Odor landscapes in turbulent environments

Antonio Celani

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The olfactory system of male moths is exquisitely sensitive to pheromones emitted by females and transported in the environment by atmospheric turbulence. Moths respond to minute amounts of pheromones, and their behavior is sensitive to the fine-scale structure of turbulent plumes where pheromone concentration is detectible. The signal of pheromone whiffs is qualitatively known to be intermittent, yet quantitative characterization of its statistical properties is lacking. This challenging fluid dynamics problem is also relevant for entomology, neurobiology, and the technological design of olfactory stimulators aimed at reproducing physiological odor signals in well-controlled laboratory conditions. Here, we develop a Lagrangian approach to the transport of pheromones by turbulent flows and exploit it to predict the statistics of odor detection during olfactory searches. The theory yields explicit probability distributions for the intensity and the duration of pheromone detections, as well as their spacing in time. Predictions are favorably tested by using numerical simulations, laboratory experiments, and field data for the atmospheric surface layer. The resulting signal of odor detections lends itself to implementation with state-of-the-art technologies and quantifies the amount and the type of information that male moths can exploit during olfactory searches.

O4

Open Boundary Molecular Dynamics of Star Polymers

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We present a multiscale method, based on the flux-exchange coupling, which concurrently links atomistic, mesoscopic, and continuum models of liquids [1,2]. Our approach enables the insertion of large molecules into the atomistic domain via a mesoscopic region and it allows for molecular simulations either in the grand-canonical ensemble or under non-equilibrium conditions. The applicability of the method is demonstrated on an open boundary molecular dynamics simulation of a star polymer melt where we open up the molecular system to exchange mass and momentum with its surroundings [3].

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[2] R. Delgado-Buscalioni, K. Kremer, M. Praprotnik, J. Chem. Phys. **131**, 244107, 2009.
[3] R. Delgado-Buscalioni, Jurij Sablić, M. Praprotnik, EPJ ST, submitted.

Effective thermodynamics in systems of self-propelled particles

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Active matter systems are made of interacting units (active particles) which can convert energy from their environment into mechanical work and, in the situations we consider here, locally produce motion. As a result, these self-propelled particles are intrinsically out-of-equilibrium, giving rise to a plethora of interesting collective behaviour (pattern formation, phase separation, large fluctuations, etc.). Self-propelled particles are manifold in biology and can be found at very different length scales. Physicists have recently managed to synthesise non-living active matter at the granular ($\sim$ 1 mm) and colloidal scale ($\sim$ 1 μm) [1]. Artificial active suspensions made of Janus colloids can now be realised in the lab using state of the art techniques [2, 3], opening the possibility of creating new soft materials with novel functionalities. The systematic characterisation of these non-equilibrium systems clearly needs further theoretical work. Here we present our recent results in this direction, and study how the phase behaviour and dynamics of colloidal matter is affected by the competition between self-propulsion and steric effects. In order to do so, we introduce a model of self-propelled disks where particles perform a persistent random walk characterised by a single parameter, the persistence time [4]. We compare the predictions of the model with the experimental results obtained in suspensions of Janus colloids [3].

Purely repulsive hard disks show the emergence, at any finite density, of complex non-equilibrium structures that have a strong impact on the collective dynamics [4]. Using sedimentation experiments one can measure the non-equilibrium equation of state of the active Janus suspensions. We discuss the impact of activity in the equations of state. We found a good agreement between simulations and experiments and show that, despite the non-equilibrium nature of the system, the equation of state of active colloids can be understood as a motility-induced adhesion between the particles. By mapping the active system into the Baxter model of adhesive disks we can associate an effective adhesion to an effective temperature [3]. We further investigate which equilibrium thermodynamic quantities, like temperature, can be extended to characterise active matter. To do that, we extract an effective temperature from the violations of the fluctuation-dissipation theorem. I will discuss the evolution of the effective temperature over a broad range of densities and activities, and discuss whether it is a meaninful thermodynamic concept.

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O6

The immersed boundary method for colloidal fluctuating hydrodynamics at different regimes

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I will present FLUAM [1] a flexible tool to resolve hydrodynamics of immersed objects in the nanoscale and scales above. It consists on an Eulerian-Lagrangian method which resolves fluctuating hydrodynamics in a regular (finite volume) mesh and couples the particles Lagrangian dynamics via the Immersed Boundary (IB) method. FLUAM is extremely efficient. First, it uses a pseudo-spectral approach (linear fluid operators are given in the Fourier space while non-linear or local source terms resolved via Fast Fourier transforms). Second, it runs in Graphical Processors Units (GPU). Third, the particle and local fluid velocity are constrained to the same value, enabling arbitrarily fast inertia forces and physically consistent mass and hydrodynamic particle volume with a minimum resolution (one interpolator per particle). Finally, we have developed FLUAM versions adapted to the physics (and time steps) of different hydrodynamic regimes: compressible, incompressible fluid and diffusive (Stokesian) dynamics.
This last feature is particularly important in the field of "particle" hydrodynamics (polymers, colloids or any other structure) as the computational treatment of each dynamic regime is different enough to divide the whole area in several (almost) independent communities. The fastest hydrodynamic mode is sound or density waves which just need about $\tau \sim 10^{-11}s$ to cross a typical colloidal size in water. Viscous transport of momentum over such distance requires about 10^{-6}s and in about the same time the inertia of a buoyant particle relaxes. Finally, at zero Reynolds number and small Peclet number, colloids diffuse its own size in much longer times of about 10^{-1} s. Here Stokesian diffusion is the leading transport mechanism and there is no inertia.
I will show examples of application of FLUAM in these three different regimes. A full description in a compressible flow of ultrasound manipulation of submicron particles of arbitrary compressibility [2]. Particles in incompressible fluid at moderate and relatively large particle Reynolds number, where the drag force on a blob-resolved particle is found in excellent agreement with that of a real spherical particle [3]. And calculations of the effect of hydrodynamic forces on colloidal clustering and gelation in the Stokesian limit [4], where collective arrangements require very long time to relax. Here hydrodynamics might play some role, although this question is still not completely understood.

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[2] F. Balboa Usabiaga, R Delgado-Buscalioni, Phys. Rev. E **88**, 063304 (2013)
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[4] S Delong, F Balboa Usabiaga, R Delgado-Buscalioni, BE Griffith, A Donev J. Chem. Phys. **140**, 134110 (2014)

Liquid-Liquid Critical Point in Water and Methanol and the Hydrophobic Effect in a Core-Softened Fluid Model

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A core-softened fluid is used as an efficient and simple model to describe water. The model treats water molecules as spherical particles interacting by an isotropic potential with two characteristic lengths to account for the anomalous properties of water due to hydrogen bonding. As next a simple model is constructed to study the phase diagram and thermodynamic properties of methanol, which is described as a dimer of an apolar sphere mimicking the methyl group and a sphere with core-softened potential as the hydroxyl group. Performing Monte Carlo simulations and integral equations, the models were found to predict the density anomaly and correctly reproduce trends in the coefficients of thermal expansions, isothermal compressibility and heat capacity for water. Both models predict a second critical point between two liquid phases of different densities, as postulated in the case of real water. From the experimentally determined hydrogen bond strength and length in methanol and water, we propose where the second critical point of methanol should be. Hydration of non-polar solutes was studied, as well. Modelling non-polar solutes as Lennard-Jones particles of different sizes and interaction strengths, the model describes the experimentally observed hydrophobic effect. Calculated thermodynamics of solvation quantitatively agree with experimental data for noble gases and small hydrocarbons hydration.

O8

A stochastic model for particle agglomeration in parcel-tracking approaches

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A large variety of industrial and academic systems involve suspensions where the formation of larger bodies through collision and adhesion of two smaller bodies can occur. Depending on the context, this phenomenon is referred to as agglomeration, coagulation, flocculation or aggregation. As underlined in recent reviews (see for instance [1]), agglomeration phenomena involve bodies of different nature (for instance solid particles, colloidal particles, biological organisms) and have applications in various fields (among which filtration technologies, water treatment facilities or papermaking industry).

The aim of this study is to describe a stochastic model for the agglomeration of particles suspended in a fluid. The main feature of the proposed algorithm is to track parcels of particles instead of tracking all particles. This allows to significantly reduce the computational cost compared to finer particle-tracking approaches (for example [2, 3]) while remaining tractable for industrial applications. For that purpose, the model is based on O'Rourke model for bubble coalescence [4] - which is based on the notion of collision kernels (used in PBE approaches) - with an extension to account for particle adhesion (using the DLVO theory) and agglomerate morphology.

Numerical results obtained with this approach showed good agreement with theoretical predictions from PBE solutions in various situations. In addition, the comparison to experimental data on nanoparticle agglomeration highlights the impact of particle morphology (porosity or fractal dimension) on the results. However, these results also show the need for further fine experimental and numerical studies of agglomerate morphology.

References

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SEDIMENTATION OF LARGE PARTICLES IN TURBULENT ENVIRONMENTS

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Particle sedimentation is encountered in a wide number of applications and environmental flows. It is a process that usually involves a high number of particles settling in different environments. The suspending fluid can either be quiescent or turbulent, therefore involving eddies of different sizes. Owing to the range of spatial and temporal scales generally involved, the interaction between the fluid and solid phases is highly complex and the understanding of the problem is still incomplete.

In most of the numerical studies, small and heavy particles are considered. Wang and Maxey [1] studied the settling of heavy particles in homogeneous isotropic turbulence. The authors showed that heavy particles smaller than the Kolmogorov lengthscale are often swept into regions of downdrafts (the so called preferential sweeping) and in doing so, the particles mean settling velocity is increased respect to the still fluid case. On the other hand, Good et al. [2] studied the settling of particles slightly larger than the Kolmogorov lengthscale both experimentally and numerically. They found a reduction in mean settling velocity respect to the still fluid case.

In the present study we perform direct numerical simulations to investigate the sedimentation of rigid spherical particles larger than the Kolmogorov lengthscale. The Immersed Boundary method originally developed by Breugem [3] is used to account for the presence of the solid phase. In order to generate and sustain an isotropic and homogeneous turbulent flow field a random forcing is added to the right hand side of the Navier Stokes equations. With this forcing we obtain a Reynolds number based on the Taylor microscale of 90 and a Kolmogorov lengthscale which is approximately 1/12 of particle diameter. The solid to fluid density ratio is set equal to 1.02 while two solid volume fractions ϕ of 0.5% and 1% are considered. The same simulations are also performed in still fluid to single out the effect of turbulence. We find a reduction in mean settling velocity respect to quiescent cases. The overall drag is increased both by the non-linear finite Reynolds number behavior and by unsteady effects, which are negligible in quiescent cases.

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O10

Designing stimulus-sensitive colloidal walkers

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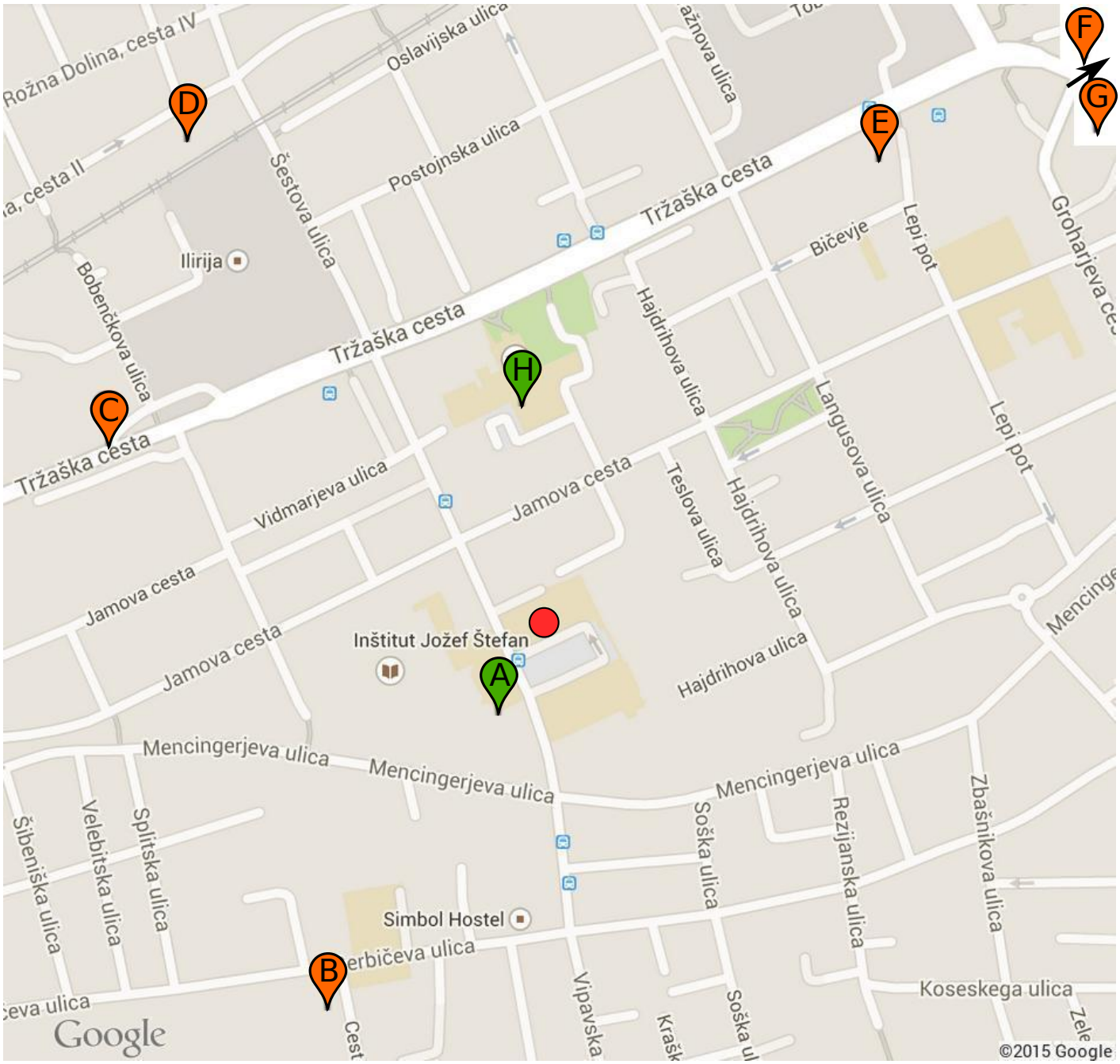
Colloidal particles with DNA “legs” that can bind reversibly to receptors on a surface can be made to ‘walk’ if there is a gradient in receptor concentration. We use a combination of theory and Monte Carlo simulations to explore how controllable parameters, e.g. coating density and binding strength, affect the dynamics of such colloids. We find that competition between thermodynamic and kinetic trends imply that there is an optimal value for both, the binding strength and the number of “legs” for which transport is fastest. Using available thermodynamic data on DNA binding, we indicate how directionally reversible, temperature-controlled transport of colloidal walkers can be achieved. Present results should make it possible to design a chromatographic technique that can be used to separate colloids with different DNA functionalization.

Nearby restaurants



- Venue
- A IJS canteen
- B Hombre (Mexican food)
- C Za pumpo
- D Rožna hiša
- E Mirje (Italian food)
- F Foculus (Pizzeria)
- G Gostilna Pod lipo
- H FE/FRI canteen

More info:

Programme of the "COST workshop on Modelling of Flowing Matter"

16-18 February, Ljubljana, Slovenia

Invited talks - I 45mins

Contributed talks - O 30mins

Monday 16th Feb - Day 1

Starting hour	Ending hour	Speaker	
9:00	9:15		*welcome & registration*
9:15	10:00	I1 - Pagonabaraga	Mesoscopic models for complex and active fluids
10:00	10:30	O1 - Cristea	Lattice Boltzmann model for bioprinted tissue structures
10:30	11:00		*coffee break*
11:00	11:45	I2 - Turner	A topological glass
11:45	12:30	I3 - Sofonea	Lattice Boltzmann models based on Gauss quadratures and applications
12:30	14:00		*lunch*
14:00	15:00		Informal discussions
15:00	15:45	I4 - Telo da Gama	Liquid crystals at surfaces and interfaces: from statics to dynamics
15:45	16:15	O2 - Čopar	Topology of complex fluids
16:15	16:45		*coffee break*
16:45	17:30	I5 - Gov	Modeling the dynamics inside active gels
17:30	18:00	O3 - Celani	Odor landscapes in turbulent environments

Tuesday 17th Feb - Day 2

Starting hour	Ending hour	Speaker	
9:15	10:00	I6 - Likos	Shear- and flow properties of cluster solids
10:00	10:30	O4 - Praprotnik	Open boundary molecular dynamics of star polymers
10:30	11:00		*coffee break*
11:00	11:45	I7 - Brand	Macroscopic behavior of systems with a dynamic preferred direction
11:45	12:15	O5 - Levis	Effective thermodynamics in systems of self-propelled particles
12:15	14:00		*lunch*
14:00	15:00		Informal discussions
15:00	15:45	I8 - Menzel	Active crystals and the effect of deformability on active motion
15:45	16:15	O6 - Delgado - Buscalioni	The immersed boundary method for colloidal fluctuating hydrodynamics at different regimes
16:15	16:45		*coffee break*
16:45	18:00	M1	M1 - Organised discussion on methods in flowing matter
19:00			*get together (in the city centre)*

Wednesday 18th - Day 3

Starting hour	Ending hour	Speaker	
9:15	10:00	I9 - Cebers	Dynamics of polar order in Quincke suspensions
10:00	10:30	O7 - Urbič	Liquid-liquid critical point in water and methanol and the hydrophobic effect in a core-softened fluid model
10:30	11:00	O8 - Henry	A stochastic model for particle agglomeration in parcel-tracking approaches
11:00	11:30		*coffee break*
11:30	12:15	I10 - Araujo	Aggregation of patchy colloids on substrates - a stochastic approach
12:15	12:45	O9 - Fornari	Sedimentation of large particles in turbulent environments
12:45	13:15	O10 - Dobnikar	Designing stimulus-sensitive colloidal walkers