Application for a Starting Independent Researcher Grant-part B2
STARTER

Mauro Sbragaglia

Department of Physics, University of 'Tor Vergata', Rome, Italy

DROEMU
DROPLETS AND EMULSIONS: DYNAMICS AND RHEOLOGY

Section 2: The Project Proposal

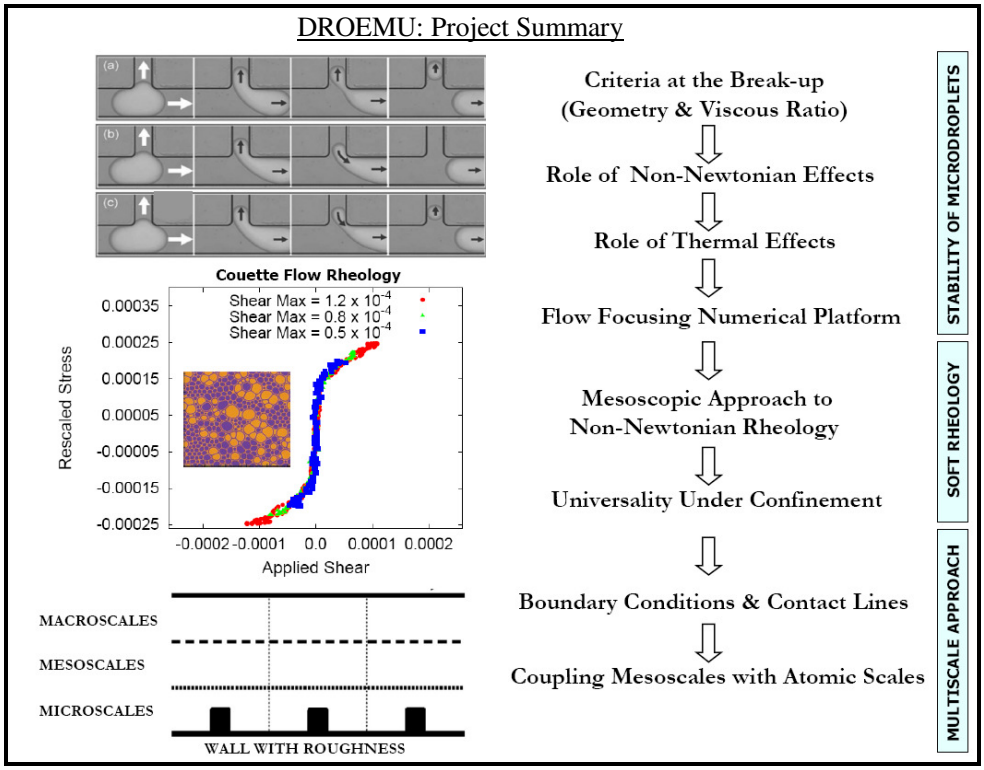
A. STATE OF THE ART AND OBJECTIVES

Understanding the properties of multiphase fluid dynamics in extremely small systems and close to liquid-liquid and liquid-solid interfaces is crucial for many fundamental and applied fields. Some of these problems came out from the very beginning of hydrodynamics, but still occupy a very important place in contemporary science and technology. Micro- and nanofluidics offer unprecedented conditions for controlling droplets [1-6] at all stages of their life, i.e. from the formation up to their storage on the chip. Controlling the production of single droplets is the basic ingredient to upscale the process leading to design and manufacture new smart materials composed of particles or emulsions dispersed in a continuum phase. These particles typically possess structures which are much larger than atomic or molecular scales: probing and understanding the way the structure and dynamics at the mesoscopic scales determines macroscopic physical properties is a challenging open problem [7-12]. A general feature of such systems, well documented yet not really understood, is the strongly nonlinear and nonlocal nature of the flow rule relating stresses and strain rates. Beyond its practical importance for applications, these cooperativity effects have parallels in the behaviour of other glassy, jammed and granular systems, suggesting a possible fundamental universality.

Very often, wetting properties crucially control the patterns of multiphase flows in micro- and nanochannels. As a consequence, there is an exceeding importance of the wall confinement, an aspect that often generates tremendous technical difficulties in the handling of droplets whenever unavoidable physico-chemical constraints have to be taken into account. As a result, beside its theoretical importance, the determination of the phase diagram of confined and unconfined multicomponent systems is of importance in a number of realms: industrial formulation, protein crystallization, bottom-up material assembly from spontaneous ordering of surfactant, polymeric or colloidal systems. Depending on the application, one may want to access only the equilibrium phase diagram or gain additional information concerning the metastable phases that can appear for kinetic reasons. Moreover, the control provided by droplets in micro- and nanofluidic devices can lead to new scientific methods to produce and stabilize monodispersed or polydisperse emulsions and their rheological characterization [7-12]. The problems involved are naturally multiscales and multidisciplinary, touching atomistic scales, mesoscopic collective behaviour and hydrodynamical spatio-temporal evolutions with complex rheology and strong non-equilibrium properties.

The main challenging and ambitious questions I intend to address in my project are: How the stability of micro- and nanodroplets is affected by thermal gradients? Or by boundary corrugation and modulated wettability? Or by complex rheological properties of the dispersed and/or continuous phases? How these effects can be tuned to design new optimal devices for emulsions production? What are the rheological properties of these new soft materials? How confinement in small structures changes the bulk emulsion properties? What is the molecular-hydrodynamical mechanism at the origin of contact line slippage? How to realistically model the fluid-particle interactions on the molecular scale?

The objective of this proposal is to understand and control the dynamics of multiphase flows in micro- and nanostructures, in presence of complex boundary conditions (geometrical roughness, chemical patterning) for the case of single- and multi-droplet dynamics (emulsions), dispersed in Newtonian or non-Newtonian (viscoelastic) fluid matrix. The main tools will be based on the integration of new state-of-the-art numerical schemes based on Lattice Boltzmann Models (hereafter LBM, see box) with theoretical and phenomenological modelling, validated and supported by experiments. This will allow to start, grow and consolidate for the first time in Italy, a group fully dedicated to the development of "in silico micro- and nanofluidics" and on its experimental validation. The project deals with both fundamental and applied problems. The activity will mainly focus on: (i) setting up a unified scientific framework for production, characterization and modeling interfaces and droplets in confined geometries, (ii) investigating complex flow properties at the frontier of research on model emulsions and real nano-composites made of submicron sized polymer particles, (iii) investigating theoretical and numerical fundamental multiscale phenomena connected to contact-line dynamics, emerging slip length and molecular-hydrodynamical couplings.



The Lattice Boltzmann Models (LBM) in a Nutshell

LBM is an optimal form of Boltzmann kinetic equation describing the dynamics of a fictitious ensemble of particles, whose motion and interactions are confined to a regular space-time lattice. Major strengths and advantages with respect to other methods are the capability of handling boundary conditions associated with highly irregular geometries and the efficiency to describe non ideal fluids with phase transitions/phase separation. Moreover, LBM allows for describing hydrodynamical fluctuations on scales of experimental interest. This goes together with a dramatic reduction of the degrees of freedom associated with the velocity space, consequent computational boost and nearly ideal amenability to parallel computing (low communication/computation ratio). Besides the natural realm of macroscopic fluid dynamics, the LBM portfolio of applications keeps expanding across scales of motion, particularly towards micro- and nanofluidics with active thermal dynamics. Realizing the full potential of the method in the latter case, however, still raises many challenges ahead.

Despite the problems are intrinsically related, I split them in three topics for the sake of clearness. I will follow a bottom-up/simple-to-complex trajectory (see inset). Starting from single-droplet dynamics in simple geometrical set-up and increasing complexity in different ways: adding ingredients from the walls (geometrical roughness and/or chemical patterning), adding new control parameters (temperature) and adding new bulk properties (non-Newtonian effects). Then, I will jump from a single- to a multi-agents scenario, studying emulsion rheology. I will develop and present the first numerical scheme based on mesoscopic physics

leading to a non-trivial bulk rheology, as a function of the microscopic parameters entering in the intra-molecular potentials. I will study its constituent equations both in unbounded and bounded structures and I will investigate the statistical hydrodynamical fluctuations of plastic rearrangements inside the flow. Finally, I will close the circle by putting the finger on the intimate multiscale nature of the previous points: studying the molecular-hydrodynamical coupling between polymers and fluids in non-Newtonian systems and by studying the molecular-hydrodynamical couplings close to the contact line between solid-fluid-gas phases.

1. STABILITY OF MICRO- AND NANODROPLETS

Droplets-on-demand, droplet formation and indirect droplet formation from capillary stream break-up are at core of many technologies in biomedicine, mass spectrometry and chemical reaction processing [4]. To actively control the drop interface it is fundamental to understand phenomena occurring at the fluid-fluid or fluid-solid interface. Interface phenomena typically involve the interplay of complex processes such as dynamic contact lines, interface active materials, adhesion, temperature and/or compositional gradients, evaporation, etc. [1-2,7]. The exact mechanics governing such processes, including hydrodynamics controlling wetting, or the macroscopic action of external agents such as surfactants in the evolution of the free interface, is still not fully understood. In an actual experiment all these processes and ingredients occur at the same time and it is next to impossible to separately quantify their relative importance. *The innovative opportunity of the study here proposed, based mainly on quantitative numerical methods, is to allow for a systematic analysis of each of the above effects separately.*

1.1 Criteria at the Break-up (Geometry and Viscous Ratio)

The basic starting point for designing, developing and exploiting micro- and nanofluidic devices is to achieve a precise control over the process of formation of droplets, and characterization or, preferably, understanding of the scaling laws that describe the volume of droplets formed in the devices as a function of the materials (e.g. viscosities, interface tension) and flow parameters (e.g. pressures or rates-of-flow applied to the system). The confinement that naturally accompanies flows in small devices has significant qualitative and quantitative effects on the drop dynamics and break-up [7,13-15]. A setup where one is usually focusing the attention consists of T- and Y-junction channels. Detailed studies [3,13] identified different droplet breaking mechanisms ranging from shear-dominated (like unbounded fluids [5]) to squeezing mechanisms connected to the confined geometry in which the drop is formed. Different scaling laws for the droplet size as a function of the applied shear rates are then identified [3,13-14]. Here I intend to address a series of frontier questions for droplets control in complex geometries. I will:

(i) *study numerically the formation and break-up of confined droplets and systematically prove the existence of geometrical criteria governing the droplet break-up at different viscous ratios and Capillary numbers (i.e. changing the balance between the viscous forces and the surface tension at the interface).*
(ii) *Control the conditions for the existence of break-up mechanisms and study the critical range of Capillary numbers at which the system transits from a squeezing mechanism into a shear-dominated droplet formation, at changing also the junction geometry. I intend to further characterize the criteria built on the notion of a critical finger length that depends on the channel geometry and is independent of the fluid properties and the flow conditions [15], a key basic question in the field.*
(iii) *address the importance of different wetting properties on the channel walls (both induced by geometrical roughness or chemical coating).*

From the experimental side we will use methodologies for the fabrication of devices like T-,Y-junctions, microvalves and microchannels designed for droplet production. Since break-up, migration and coalescence happen on time scales of hundreds of microseconds, we aim to image droplets in microfluidic devices by using high sensitive fast CCD camera covering the range of 5000-100000 frames per second, in order to perform detailed video microscopy of the whole process. Moreover, the coalescence, encapsulation, rotations, storing, and all the other stages of the droplet manipulation will be imaged and processed by means of an environment based on interactive visualization (Interface Data Language from ITT Visual Solutions).

1.2 Role of non-Newtonian Effects

Non-Newtonian components can have significant effects on drop-deformation and break-up and investigation of the corresponding viscoelastic system have been rare. Consequently, there is a lack of understanding of such systems [16-17]. Experiments on systems where either the drop or the matrix phase is viscoelastic, found that the drop elasticity inhibited drop deformation, whereas matrix viscoelasticity enhanced it in simple shear [18]. In Boger fluids, for suitable elasticity ratios (ratio of the relaxation of the drop phase to that of

the matrix phase), the deformation of an elastic drop in an elastic matrix is larger than the Newtonian case [19-20]. More recently, studies based on viscoelasticity models with Oldroyd-B constitutive equations have been performed by using three dimensional front-tracking finite difference method [21]. I intend to go beyond the state-of-the-art by studying:

(iv) *droplet break-up in confined channels for both Newtonian droplets in non-Newtonian fluid matrix and the further more complex case of both non-Newtonian dispersed and continuous phases. The simplest geometry to be considered is the same T-junction described in the previous topic. The numerical method, based on LBM, offers a unique advantage to attack these problems, being able to integrate simultaneously the non-trivial interface dynamics (due to the diffuse interface nature of the method) and the non-Newtonian nature of the bulk phases, by making the relaxation times in LBM dependent on the local shear properties (see methodology). A systematic study in terms of the viscous ratio between the droplet and the ambient viscosity can then be conducted, opening new horizons for droplet control in non-Newtonian environments.*

1.3 Role of Thermal Effects

Temperature gradients and heat exchange may play positive or negative feedback [22], activating droplet breaks-up via surface tension gradients or deteriorating the fluid-fluid mixture due to thermal currents. A systematic analysis of temperature induced instabilities on the transition from squeezing to rate-of-flow controlled mechanisms [3,13-14] has not been performed. I intend to:

(v) *investigate temperature effects in simple T- and Y-junctions, by switching on/off wall temperature during droplet formation and/or break-up, elaborating a new procedure to speed-up and control droplet dynamics. I will control the way capillary forces and thermal gradients can be successfully coupled in numerical simulations based on LBM. The main objective is to systematically investigate the evolution of droplets arriving at T-junctions, depending on their extensions and Capillary numbers and the way this picture changes in terms of thermal activation of the walls. A set of experimental suggestions will be proposed.*

To my knowledge, similar systematic studies have not been performed yet, and may open a new direction in droplet control and manipulation in micro- and nanochannels.

2. SOFT RHEOLOGY

The study of the rheology of flowing soft systems, such as emulsions, foams, gels, slurries, colloidal glasses and related complex fluids, has a larger and larger impact in modern science and engineering [23-29]. Much of the fascination of these systems stems from the fact that they do not fall within any of three basic states of matter, gas-liquid-solid, but live rather on a moving border between them. I have recently developed a new LBM (see inset) able to deal with vanishing small surface tensions without the need to introduce ad-hoc surfactants in the system, thus opening new ways for realistic numerical investigation of concentrated emulsions. In most instances, these materials consist of a disordered collection of droplets with a broad distribution of sizes, randomly mixed and arranged, which do not correspond to the (global) minimum of any thermodynamic function. As a result, they exhibit a number of distinctive features, such as non-Newtonian properties (see inset), long-time relaxation and ageing behaviour, whose quantitative description is calling for profound extensions of non-equilibrium statistical mechanics [30-33].

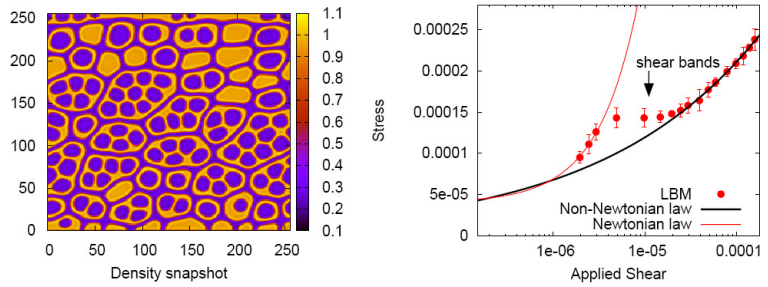


Figure: *Phase separation with competing interactions from LBM. The numerical model is shown to reproduce typical signatures of soft-glassy flows, such as (non-Newtonian) Herschel-Bulkley rheology, shear-banding (right) and complex pattern formation (left) underlying the non linear rheology [88-89]. The control parameters are the ranges of the attractive/repulsive interactions. LBM will serve to attack the problem of the universality in the rheology under confinement.*

2.1 Flow Focusing Numerical Platform

Flow focusing techniques have proven to be powerful and versatile tools to achieve monodisperse drops [6]. A flow focusing device consists of a pressure chamber where one or more focused fluids are injected through

a capillary feed tube whose extremity opens up in a front of a small orifice linking the pressure chamber with the exterior ambient. Despite the wide use of flow focusing techniques, the precise influence of the channel geometry on the droplet formation process remains unexplored, even though it ultimately determines important characteristics: size, polydispersity and formation frequency. I intend to:

(vi) *develop a state-of-the-art numerical platform to simulate a whole realistic flow focusing device, further extending the recent approach proposed in [34] using the LBM. The fully 3d codes will support a large parameter space, spanned by surface wetting, surface tension, viscous ratio, inlet velocity and will go beyond some of the limitations of the already proposed approaches providing accurate modelling of boundary conditions in terms of slip lengths and fully 3d dynamics.*

2.2 Mesoscopic Approach to non-Newtonian Rheology

Disordered packings of small soft units, such as foams, concentrated emulsions and soft pastes show strikingly similar rheological behaviour [35-37], thus prompting renewed interest in formulating models with generic physical mechanisms. This raises the question of the level of coarse-graining necessary to allow maximum physical insight with minimal complexity. To this end, numerical simulations, interplayed with information from experiments on real systems, may play a key and innovative role. All numerical simulations which address hydrodynamical rheological properties of complex emulsions are affected by some degree of modelling. This is because they necessitate of some simplification of the too many and too complex constituents. Nevertheless, the necessity to simplify can be seen as a plus for the "universality" issues. If there is some real common-physics describing the rheology of many soft-materials this must be seen and detectable by exploring the mesoscopic and macroscopic properties of different numerical models. Universality means renormalizability of small scales details. My aim here is to attack this fundamental problem theoretically, numerically and experimentally:

(vii) *The idea is to develop suitable intra-molecular potential models based on efficient LBM and provide an accurate description of their equilibrium properties in terms of free energy functionals for multiphase fluid flows. The main theoretical contribution at this level will result in finally solving a controversy on the lack of free energy functionals for these numerical models (see methods). A systematic physical study in unbounded flows (Kolmogorov flows) will then follow with the idea to assess the universal properties in the rheology at changing the interaction parameters in the numerics.*

2.3 Universality Under Confinement

Important new theoretical and experimental results have been recently published about rheological properties of concentrated emulsions in confined geometries [9-10]. The problem is key for many applied situations and fundamental issues for the understanding of local and global properties of amorphous and glassy systems. In these materials, flow occurs through a succession of global elastic deformations and localized plastic rearrangements associated with a microscopic yield stress. These localized events induce long-range elastic modifications of the stress over the system, thereby creating long-lived fragile zones where flow occurs. Flow in these systems is thus highly cooperative and spatially heterogeneous: a dynamically active region will induce stress fluctuations of its neighbours and thus a locally higher rate of plastic rearrangements. Such non-locality makes the rheology dependent on the boundary conditions and change the bulk properties connecting shear and stress, showing departures from the usual Herschel-Bulkley law [9-10]. I intend to:

(viii) *perform a series of numerical simulations in two different geometries (Couette and Poiseuille flows) at changing the boundary conditions with either chemical patterning or geometrical roughness. This will be done by using the innovative LBM schemes I have recently developed (see inset on page 4) for soft systems. Numerical simulations will allow to study local fluctuations of the fluidity field, the quantity which can be related to the rate of plastic events. Such analysis can strongly benefit from numerical simulations because it is extremely difficult to access experimentally local hydrodynamics.*

(ix) *After further validation of the numerics against experimental measurement of global rheology (see methodology), I intend to use the numerical data to test -and eventually extend- the recent phenomenological approach for the non-local constitutive equation for jammed systems based on a kinetic elastoplastic Boltzmann model [10]. These numerics offer the important flexibility to change the parameters defining the molecular interactions, adding long/short range attractive and/or repulsive forces. At changing these parameters, I will modify the free energies which govern the relation between stress diffusion and plastic events [10], also exploring phases with shear banding and flow-structures coupling in the material.*

On the experimental side the idea is to exploit miniaturization of devices for determining the emulsions rheology at different droplets concentrations approaching the dynamical arrest (jamming). Main advantages rely on the possibility of producing high shear rates under low Reynolds number conditions, visualizing the flow and tuning the flow geometry to enhance particular properties. Microdevices will be made of UV-curable optical glues using soft imprint lithography in clean room conditions. Micron size resolution rheology will be investigated by imaging either emulsion droplets or colloidal probes, dye-labelled, by means of a micron-size resolution Particle Image Velocimetry (micro-PIV) apparatus (see methodology). *We will study model emulsions under pressure driven flows, reconstructing the full velocity profiles along the smallest dimension of the channel with a sub-micrometric resolution.* Local calculation of the stress and shear rate will be performed from the velocity profiles, at a few hundred microns from the channel inlet.

3. MULTISCALE DYNAMICS

Continuity is the most fundamental assumption in macroscopic fluid mechanics which is governed by the Navier-Stokes equations. However, this assumption breaks down as the spatial scale of flows approaches the molecular mean free path [38]. Continuum approaches also fail to describe macroscopic flows where the continuum equations have essential singularities, as in the moving contact-line problem [39-41]. Atomistic descriptions, such as Molecular Dynamics (MD) simulations, are capable of modelling nanofluids and singular flows [42-45]. However, it is unrealistic to use full atomistic simulations to study flows at microscales because of memory and computational time limitations. Moreover, in most cases the breakdown of the continuum description is confined to limited domains, such as fluid-fluid or fluid-solid interfaces. Hence it is desirable to develop hybrid methods that combine continuum fluid dynamics and microscopic descriptions, using the most efficient description in each region of space or to use a continuum description with some ad-hoc introduced parameters to mimic the effect of the small scales on the large ones. *Such methods are known in the literature but they have never been extensively used for the analysis of the complex flows I intend to study. Such work would therefore set the reference guide for future research.*

3.1 Boundary Conditions & Contact Lines

The physics of moving contact lines operates on scales extending from the macroscopic to the molecular ones [46-48]. In between these scales, the strong viscous forces are balanced by surface tension effects [49-51] and a dimensionless measure of this balance is provided by the Capillary number. It is well known that the viscous stress diverges at the contact line [49-51] and to overcome this problem numerous proposals came out [49-53]. A representative example is provided by the slip length at the boundaries, where this small scale parameter is related to the presence of a finite slip [49]. Anyhow, also other mechanisms such as intermolecular forces or diffuse interfaces [52-53] in the immediate vicinity of the contact line can be considered. Once the small scale singularity is cut out, the macroscopic physics emerges as a function of the Capillary number and very interesting behaviours are present close to the wetting transition: when the liquid advances, a critical Capillary number exists above which a stationary contact line cannot be sustained any longer, and liquid deposition may occur on the solid [54-59]. The understanding of this transition is crucial. In fact, the breaking of stationarity can be interpreted as a lost of universality: the hydrodynamical regime does not support anymore a time-independent solution, indicating some singular behaviour in the matching between inner and outer regions. As for this problem, I have developed a sharp interface theory to describe a Couette cell [59] consisting of two fluids sheared one against each other. This analysis has offered the possibility to determine the critical Capillary numbers in terms of all the parameters, especially the viscous ratio, thus extending a similar analysis done in [54-55] . I intend to:

(x) *exploit theoretical calculations based on lubrication approximation and the numerical simulations based on LBM. The aim is to explore the lubrication approximation with a finite viscous ratio between the liquid and the air flow in open geometries such as the one of the Landau-Levich problem [60] in the withdrawing of a plate out of a bath [54]. The novelty I can offer, is also based on a quantitative validation of the LBM code against the analytical results obtained in lubrication approximation. The comparison with LBM results allows us to benchmark the numerical model and to understand the effects of the finite thickness of the interface on global quantities (the critical Capillary number, the viscous ratio) as well as local ones (the interface shape and the velocity profiles). Moreover, after LBM validation, I can use it to go beyond lubrication approximation exploring either variable viscosity ratios or high hydrophobic materials, two cases where lubrication approximation cannot be easily applied. In a second stage, a mixed and inhomogeneous boundary condition will be formulated in the context of lubrication theory with finite viscous ratios and I will look for comparisons with LBM in order to clarify the importance of roughness, contact angle hysteresis and speed dependency of the wetting properties.*

3.2 Coupling Mesoscales with Atomic Scales

Recent, relevant applications in microfluidics are due to non linear effects triggered by non-Newtonian rheology [61]. To describe such non-Newtonian flows in small systems, I intend to explore the idea to couple LBM for the fluid with a Molecular Dynamics (MD) description of millions of single lagrangian structures with internal dynamics (e.g. polymers). The non-trivial problem is to couple the structures back to the fluid and even less trivial is to describe the feedback of millions of such structures at the mesoscopic hydrodynamical level described by the LBM. I intend to:

(xi) *develop a code, able to evolve the point-like polymers described above with a local feedback on the fluid evolution induced by the local conservation of momentum. The code will be first validated in simple mean shear or elongational flow, to be able to gauge the importance of the feedback on the fluid evolution. The goal is to find the proper renormalization of the average feedback such as to be able to describe realistic polymers concentration with only a reasonable number of them. In a second stage, I intend to perform full direct numerical simulations of a normal fluid evolved with LBM, coupled with --millions-- of polymers to simulate the non-linear evolution of non-Newtonian flows in confined structures. The success of this approach would open the way to have a bottom-up description of viscoelastic effects on hydrodynamical fluids in complex geometries. Moreover, having a molecular description of the polymer dynamics, will allow for more realistic modelling of the polymer-wall interactions.*
(xii) *explore also hybrid fluctuating hydrodynamics approach, coupling hydrodynamical fields in the LBM-MD methods with suitable stochastic modelling of small scale noise, mimicking molecular agitation. I will apply such approach to go deeper in the problem of the non-hydrodynamical origin of the slip length, the effect which must cure the singular behaviour of the Navier-Stokes equations close to the contact line. For investigating experimentally these interactions, a suitable tool for studying interfaces and flow at the boundary layers from tens to hundreds of nm is required. The idea is to combine Total Internal Reflection Fluorescence Microscopy (TIRFM) and sub-micrometric piezo-positioning systems.*

B. METHODOLOGY

This project is multidisciplinary, involving theoretical and numerical studies, which are the main skills of the PI. A basic goal is also to extend this work implying experimental studies. The optimal methodology will also depend on the level of description requested to attack each single problem. In what follows I describe the methods I intend to develop.

Methods-Numerics

The methodology stems from innovative numerical tools based on Lattice Boltzmann Models (LBM) [62-65]. There are many advantages of using kinetic description for the study of complex flows in complex geometries: (i) the discretized method is fully local in space, making upscale and parallelization simple and effective, (ii) it supports ideal and non-ideal equation of states, without requiring to solve the strongly non-local Poisson equation as needed for incompressible Navier-Stokes fluids, (iii) at difference from fully continuous approaches, it naturally describes a diffuse physics between different species and phases, without the need to track interface, (iv) it allows for simple and precise way to incorporate non-trivial fluid-solid interactions, (v) at difference from atomistic approaches like Molecular Dynamics (MD), it has access to hydrodynamical scales thanks to the Chapman-Enskog expansion. The LBM method solves a fully discrete kinetic equation for populations designed to reproduce the Navier-Stokes equations in the hydrodynamic limit. The crucial advantage of LBM with respect to all other numerical schemes stems from the fully local nature of interactions, allowing for massive and easy parallelization and scalability even in presence of complex geometrical set up and complex boundary conditions. I already have state-of-the-art fully parallel version of multiphase LBM algorithms using MPI in 2d with different wettability conditions at the boundary and with the possibility to switch on/off geometrical roughness. During the development of the project I intend (i) to finalize the 3d version, (ii) to develop different parallelization schemes (in strips and in cubes, such as to adapt with different massive parallel communication architectures), (iii) to implement thermal fluctuations for multicomponent flows, (iv) to introduce non-Newtonian viscous stress (see below). Typical high resolution studies may vary from billions to hundred millions collocation points, depending on the number of Boltzmann populations needed to reach the desired hydrodynamical accuracy (from a minimum of 9 speeds per lattice node for 2d isothermal flows up to a maximum of 125 speeds for 3d thermal fluids). Besides the mainstream application, namely complex macroscopic flows out of equilibrium, recent work is also hinting at the possibility that LBM may become a method of choice for multiphase fluid flows in micro- and nanofluidics [66-81]. Crucial to the extension of the LBM scheme to non-ideal fluids, is the possibility of en-

coding potential energy interactions at the level of a simple forcing term, acting upon the discrete Boltzmann distributions. Suitable choices of this forcing term have proven capable of triggering a fairly rich non-ideal fluid behaviour, such as phase-transitions and interface formation/propagation without needing to track the shape of the interface, but rather letting it to emerge from the underlying mesoscopic landscape. Quantitative agreement with atomistic Molecular Dynamics results proved LBM to be a robust supra-molecular approach for multiphase confined flows (see inset) [79,82]. A widely used algorithm with inter-particle interactions is the pseudo-potential scheme due to Shan and Chen (SC) [66]. Alternatively, one can also introduce the non-ideal terms directly into the equilibrium distribution in a consistent way with underlying thermodynamics [68-69,83] without a direct link with mesoscopic interactions. A disadvantage of the original SC formulation is that there is usually a single parameter to tune the non ideal effects and one cannot independently change the density ratio and surface tension. As for this point, I have been the first to propose the extension of this model to multirange potentials where one can achieve better realistic control of the interface properties emerging at the hydrodynamical level [70]. Also, I have showed how to extend this model from bulk descriptions to situations where one needs to include interactions with solid walls and model the concept of wetting angles [79]. The situation is also challenging with LBM models for thermal flows. In spite of a number of recent suggestions [84-87], a commonly accepted thermal LBM has not been established yet. Recently, I have been the main contributor in a paper presenting a new approach [87] for thermal lattice kinetic equations incorporating the effects of external/internal force fields via a renormalization of the local fields in the local equilibrium. This provides a general scheme of two-phase hydrodynamics involving the gas-liquid transition in nonuniform temperature profiles. Also, in order to mimic some given bulk non-Newtonian properties the introduction of a shear-rate dependent relaxation time can be used in LBM to reproduce the desired rheological models. Once these rheological models have been provided by an experiment, LBM would serve as a numerical platform where one can perform complex fluids simulations with the desired, eventually complex, geometry. *Even more interestingly and more importantly, recently I have been able to propose an extension of two-species LBM which proves capable of reproducing typical signatures of flowing soft-materials, such as structural arrest, anomalous viscosity, ageing under shear and non linear Herschel Bulkley rheology [88-89] (see inset pag. 4). Despite the study of this model and the use of this LBM multi-species methodology is only at its infancy, I am confident it will become the model of choice, where to test and understand statistical and hydrodynamical properties for elasto-plastic events in a fluid matrix.* One of the most important scientific repercussions of the project will be to upgrade the numerical use of LBM for complex micro- and nanofluidics from a "useful first guess methodology" to a "systematic quantitative tool" to perform "in-silico experiments".

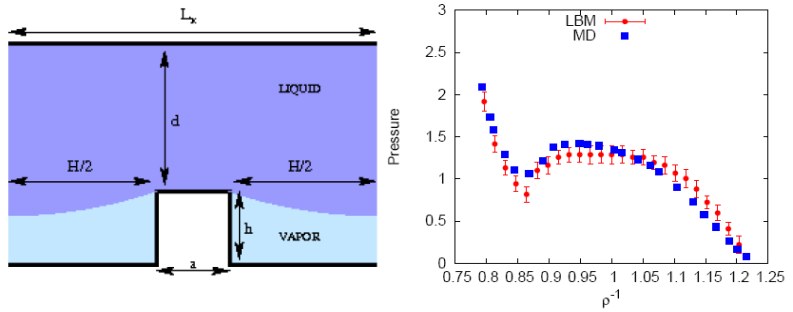


Figure: *LBM simulation of liquid-gas(vapor) coexistence in a nanofluidic channel with controlled roughness [79]. The equilibrium pressure vs. the average density quantitatively matches the atomistic Molecular Dynamics (MD) description (right). Roughness and wetting are control parameters in the LBM. This is the correct starting base to upscale the problem and study out-of-equilibrium multiphase flows in nano- and microfluidics.*

Methods-Analytics

From the theoretical viewpoint, the proposed methodology relies on using and extending the technical tools coming from thin films lubrication theory and multiscale singular expansions. Lubrication approximation [47,90-91] consists of a perturbation expansion (long wavelength expansion) of the laminar equations for thin films. The objective of my analytical investigation in the context of lubrication is to develop a theoretical framework for moving contact lines that incorporates real-life complexities, both macroscopically (geometry & large scale dependence) and microscopically (contact angle hysteresis and roughness). I will further explore the possibility to incorporate a realistic description of the microscopic physics, which is usually and popularly done by introducing slip of the last layers of molecules. This will provide, for example, a natural way to introduce contact angle hysteresis into a continuum theory and also consider explicitly the effect of roughness. Also, most of the existing approaches are limited to liquid films with large viscosity if compared to the air flow and also with small interface bending angles, the latter being a necessary condition for

the lubrication expansion to be valid [90-91]. I plan a systematic investigation to extend lubrication beyond these limitations with the support and benchmark tests coming from numerical simulations supporting both finite angles and finite viscous ratios. The other main analytical tool is connected to the theoretical understanding of the large scale hydrodynamics coming from the LBM [62-65]. To reveal the hydrodynamical content of the numerical model, a multiscale expansion in time and space is needed. Intimately connected with the multiscale expansion of the model is the characterization of its equilibrium free energies. In particular, when interaction forces are constructed directly on the lattice using the SC model for non ideal gases [66-67], a link between the mesoscopic interactions and the large scale interfaces can be established. Recently, I have contributed to define new free energy functionals underlying the equilibrium properties of the SC model for single specie multiphase fluids [67-68], thus providing a significant step in reconciling the most widely used LBM schemes for multiphase fluid flows [66-69]. The objective of this analytical investigation is to further characterize the free energy functionals emerging from the SC model with multirange potentials [70]. This requires a full control of the multiscale analysis with particular emphasis on the corrections induced by the discrete nature of the lattice [71].

Methods-Experiments

Rather to develop locally some experimental facilities ex-novo, we decided to exploit some already established collaboration with the experimental group in Padova, lead by Dr. M. Pierno, who has already agreed to host my group in a collaborative spirit. In Padova, we can access to an experimental platform for microfabrication of microfluidic devices, mass production of chips for single use experiments, optical methodologies for flow visualization and chemical synthesis. The experimental validation activity in Padova can rely on: (i) Microfabrication Laboratory (see below), (ii) custom made Epifluorescence microscope working also in TIRF for micro- and nano-PIV (see below), (iii) custom made Static and dynamic contact angle measuring unit, (iv) Microfluidics Flow Control System (MFCS) from Fluigent, a high precision pneumatic pressure controller designed to handle fluid in microdevices. It allows a stable and pulsation free flow with short response time (100 ms) and a stabilization time as low as 1s. It is also possible to control several independent channels at the same time, (v) National Instruments Labview for Data Acquisition, (vi) ITT Interface Data Language (IDL) software for interactive data visualization.

Microfabrication: MISCHA (MIcrofluidics laboratory for SCientific and technological Applications-Padova) disposes of a class ISO-7 clean room with all accessories for microfabrication. They are using photolithographic technique for the prototyping procedure of microstructures based on NOA (thiolene optical adhesives from Norland Products Inc) and SU-8 (negative epoxy-based photoresist) on the scale of tens of microns. An alternative way to produce micron structured surfaces is the micro Electrical Discharge Machining method. The micro structures can be used directly or as a master for soft-lithography, for example for replica molding process with polydimethylsiloxan (PDMS). The microdevices can be eventually chemically functionalized with coatings to obtain different wetting properties.

Nano-PIV: this technique is dealing with fluorescent tracers which are tens of nm dye particles illuminated by the evanescent wave at the total internal reflection. We plan to improve the spatial resolution of our PIV setup by replacing the prism used for total internal reflection with an optical objective specific for TIRF like an apochromatic 100x 1.49 Numerical Aperture oil immersion. A delicate step is the detection of tracers small compared to the illumination wavelength: this requires a method based on correlation between images of the movie flow and the Point Spread Function (PSF) of the optical system. We also actively collaborates with LILit, Laboratory for Interdisciplinary Lithography at Tasc (Trieste, Italy). The LILit beamline is devoted to the fabrication, by means of X-ray lithography, of structures at micro and nano resolution level, taking advantage of the high brilliance and wide X-ray domain spectrum of ELETTRA.

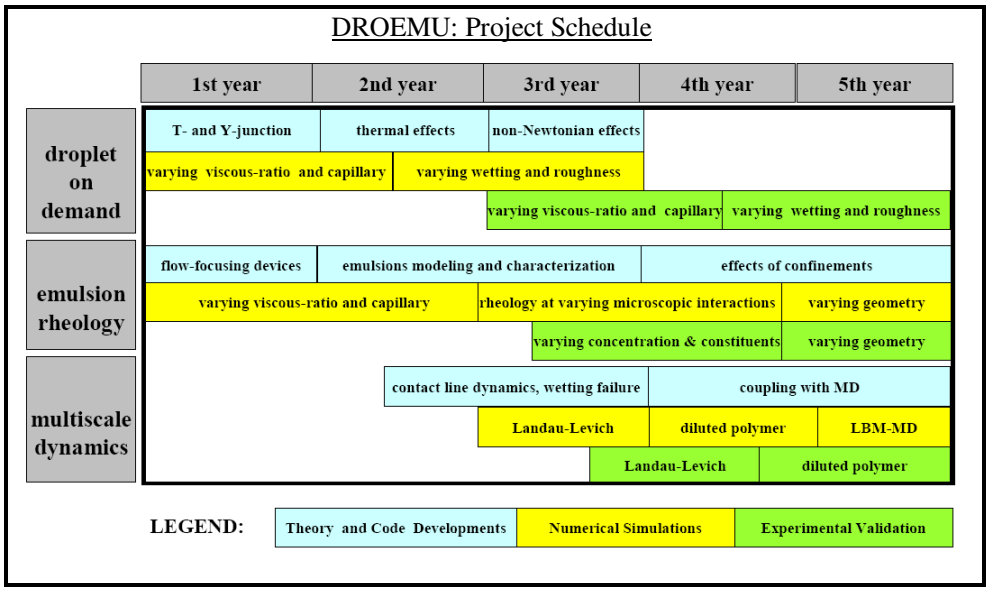
Project Management, Time-Schedule & Benefit/Risks balance

The proposed objectives are divided in three main topics obviously strongly inter-related. Because of that, some steps will be addressed at the same time.

1) I will first develop a fully parallel 2d and 3d code with LBM for multiphase and multicomponent flows with thermal effects in confined geometries. The main risk here concerns with the implementation and quantitative control of the boundary conditions (roughness, chemical coating, temperature). After this first obstacle is overcome, I will address the control of thermal and non-Newtonian effects in LBM numerical simulations with validations in unbounded fluids. I will adapt LBM for T- and Y-junction geometries by exploring droplets break-up at varying Capillary numbers and viscous ratios. I will finally cope with the effects of thermal gradients, thermally actuated walls and non-Newtonian rheology. In the final stage, I transpose the experience on a real lab, providing experimental evidence of the numerical results, defining the limitation of

the numerical approach as a function of the scale separation between the finite interface thickness and the typical scale of the system. The first code-development step is going to take presumably one year after the starting of the project, while the production process will occupy year 2 and year 3 of the project.

2) The study of emulsion rheology will start concurrently with the previous work. In a first step, I plan to develop a versatile LBM code able to reproduce confined geometries (i.e. flow focusing device chamber) where I can perform numerical experiments with the multiphase flows. In a second stage, I will study theoretically and numerically the suitable interaction model to be used in LBM able to capture the correct phenomenology of emulsions. A second step will be fully dedicated to the study of non-trivial rheological properties in presence of confinement. The universality properties of emulsion rheology will also be studied experimentally by my PhD and Post-Doc. The problems I address in this section are at the scientific core of the project, present high-risks and high-gains and it is difficult to think they may be accomplished before 2-3 years from the starting of the project. Some issues depend also on the speed I will be able to accomplish the boundary conditions implementation described in point (1) above. If the requested man power is funded I am anyhow optimistic and I foresee to be able to accomplish the more fundamental part concerning emulsion formation and stability within the first three years and to dedicate the fourth and fifth year to the study of confinement properties and their universal behaviour (varying geometry and concentrations), also experimentally.



3) The goals described in section 3 complete the project and close the scientific loop focusing on important open problems, connected to nano-hydrodynamics and on the multiscale physics. I plan first to validate the numerical code in 2d and 3d studying the classical Landau-Levich transition. Second, I intend to study the effects of roughness on coated surfaces and/or the case of strong hydrophobic surfaces, where the lubrication approximation usually fails. Hybrid LBM-MD descriptions for polymer-fluid interactions and for resolving contact line singularity will occupy the last part of the project. They are much more high-risk and it is not easy to predict how long the project may take to get good solid scientific results. Probably both of them will need some scientific follows-up after the project. The advancements of the project will be scrutinized by the organisation of 3 meetings. The first meeting, will be the subject of a school for PhD students and post-docs, organised soon after the beginning of the project. This is crucial to attract a new generation of young scientists on the themes of the project. The second meeting will be an international workshop or conference, focused on state-of-the-art results on both fundamental and applied problems. It will allow my group to get exposed and synchronized with the most important advancements in the field. The last workshop will be focused on the long range aspect of the project. During the whole project, I will try to enhance and stimulate interactions between different numerical communities in Europe and elsewhere.

European Perspectives

In Europe there are very active groups working on experimental, theoretical or numerical issues connected with this proposal. With some of them I already have/had active interactions and discussions (Prof. D. Lohse and Dr. J. Snoeijer in Enschede; Profs. F. Toschi and J. Harting in Eindhoven; Prof. B. Andreotti in Paris; Prof. J. Yeomans in Oxford; Prof. L. Bocquet in Lyon).

One important aim is to define a common agreement within the numerical and applied communities working in soft matter on what are the "optimal" methods to use for different problems. This can be done only by using the "simulate and validate" principle I will follow in the project

C. RESOURCES

The table represents a balanced budget for the whole 5 years of the project duration. A detailed justification of all costs can be found after the table, including a list of possible other funds already secured or not yet secured, related to basic support that will be provided by the University and by the INFN (Italian Institute of Nuclear Physics). The grant requested to the ERC represents the 78% of the whole project.

	Cost Category	**1st year**	**2nd year**	**3rd year**	**4th year**	**5th year**	**total**
Direct Costs:	*Personnel*						
80% time	PI	38,000	40,000	40,000	40,000	42,000	200,000
10% time (Seniors) 20/30% time (Junior)	Senior/ Junior Staff	21,000	21,000	8,000	12,000	12,000	74,000
12 full-time equivalent (3200 euro per month)	Post docs	76,800	76,800	76,800	115,200	115,200	460,800
Secured on other funds	Students	17,125	17,125	17,125	---	---	51,375
2 PhD Students	Students	17,125	17,125	34,250	17,125	17,125	102,750
long term invitation of senior scientists	Other	14,000	14,000	14,000	10,000	10,000	62,000
	Total Personnel	184,050	186,050	190,175	194,325	196,325	950,925
	Other Direct Costs						
Multi-CPU Server, Storage Facility Fast CCD + TIRF	Equipment	50,000	42,000	10,000	---	---	102,000
Software + Laboratory equipment	Consumables	1,000	1,000	15,000	5,000	5,000	27,000
Missions	Travel	24,000	24,000	24,000	15,000	15,000	102,000
	Publications, etc	1,000	1,000	1,000	1,000	1,000	5,000
School & Workshops	Other	20,000	---	20,000	---	20,000	60,000
	Total Other Direct Costs:	96,000	68,000	70,000	21,000	41,000	296,000
	Tot. Direct Costs	280,050	254,050	260,175	215,325	237,325	1,246,925
Indirect Costs (overheads)	20%	**56,010**	**50,810**	**52,035**	**43,065**	**47,465**	**249,385**
Sub-contracting costs	(No overheads)	---	---	---	---	---	---
Total Costs of project	(by year and total)	336,060	304,860	312,210	258,390	284,790	1,496,310
Requested Grant:	(by year and total)	**259,935**	**226,735**	**247,085**	**206,390**	**230,790**	**1,170,935**

Budget Justification

Personnel
PI and Senior Staff: This project will cover the full time of my research activity, which corresponds to 80% of my work time, being involved also for 20% of my time to teaching activity (see CV). In addition to the PI, to a PhD student hired on other funds and to the initial support (2 years) from two senior local scientists (secured on other funds), an equivalent of 12 full-time post-doc years is requested for the whole duration of the project, plus two PhD fellowships. Last 3 years of Junior staff support (secured on other funds) refer to the experimental activity coordination. A program for long visits of senior scientists in Rome will also be organised.

PhD student in numerical simulations (36 months, secured on other funds): The student will work on the code development for single phase thermal flows in absence of boundaries. His/her initial duty will concern the optimization and parallelization of the numerical algorithms, including benchmarks and validation steps against known results of Navier-Stokes-Fourier dynamics. In particular, he/she will validate the code against known results of stability properties of stationary solutions of multiphase and multicomponent fluid dynamics. These validation steps are already almost accomplished. In the sequel of his/her PhD he/she will help the start-up of the numerical PhD and Post-Doc fellows hired within this project.

PhD student in numerical simulations (36 months): This student will support the code development in the first 3 years of the project, in collaboration with a senior post-doc that will be also hired. In particular, he/she will help in systematic benchmark of different boundary conditions for thermal flows, developing different 3d parallelization structure of the code and following the production run for T- and Y- junctions.

PhD students in experimental validation (36 months): This student will be hired during the last three years of the project, in parallel with another post-doc. They will be fully embedded with the scientific activity in the group of the PI, in order to get involved with the major numerical and theoretical results on droplet-on-demand and emulsion rheology. When needed, they will move to Padova to make the corresponding experimental validation, in collaboration with the local group.

Postdoc in numerical simulations (60 months): Numerical simulations will require a full time equivalent post-doc for the whole duration of the project. For the first 2 years, he/she will be in charge of performing the droplet-on-demand development code, in collaboration with the PhD student. The candidate must have a strong background in parallel codes, multiphase fluid dynamics and droplet formation. In the second half of the project, I will possibly hire a new post-doc with experience on glassy systems to follow the activity on emulsions rheology.

Postdoc in theory and code developments (60 months): A post-doc with theoretical background on complex systems and interest on numerics will complete the team in the first three years of the project. New results are needed to develop a full-fledged description for LBM with thermal fluctuations. In particular, he/she will work on detailed analysis of the Chapman-Enskog expansions, effects induced by the lattice structure and possible computational variants of traditional LBM implementations (e.g. entropic and/or volumetric schemes). In the second half of the project, a post-doc with background on lubrication approximation and multiscale systems will be hired.

Postdoc in experimental validation (24 months): In the last two years of the project, when the validation/support from the experimental activity will become crucial, I intend to hire also a Post-Doc expert of TIRF and nano-PIV techniques, for developing the rheological experimental study in the laboratory of Padova. He/she will be requested to spend a considerable fraction of his/her time in Rome, in close contact with the numerical and theoretical activity.

Other: I intend to organize a long-term visiting program for experts and external collaborators. I allocated 14 Keuro per year for the first three years and 10 Keuro per year for the last two years to this scope.

Equipment

Multi-processor server and High-capacity storage (estimated (50 + 10) Keuro based on a 8 nodes dual Socket with Exacore Intel Xeon X5670 plus 20 terabyte storage facility): I need to buy a new HPC cluster to be used locally for the code development, preliminary code benchmark and for production of data on 2d geometries (when applicable). The total estimated cost of 60 Keuro is split over the first and the third year, to allow for upgrade of the storage facility. The production run for 3d geometries, will, on the other hand, requires ad-hoc applications to infrastructure for supercomputing applications. I regularly apply for -and have already obtained in the past- important grants from different numerical initiatives within the DEISA project (Distributed European Infrastructures for Supercomputing Applications, http://www.deisa.eu/), within CINECA (Italian Consortium of 37 Universities http://www.cineca.it/) and within the CASPUR in Rome (Inter-University Consortium for the Application of Super-Computing for Universities and Research, http://www.caspur.it/). Both data produced in the local computing facility and those coming from supercomputing projects will be needed to be stored locally for post-processing on the high-capacity storage facility.

*Fast CCD (estimated 30 Keuro)***:** We plan to upgrade the measurement facilities by using also a Vision Research Phantom V7.3 refurbished camera, equipped with Full frame 4:3 aspect ratio 14-bit image depth (standard) 800 x 600 active pixel CMOS sensor, 6.688 frames per second full resolution, up to 190.000 fps (standard mode), 500,000 fps (turbo mode) at a reduced resolution adjustable in 32 x 8 pixel increments, Global on-chip shuttering to 2 microseconds, optional 1 microsec (standard mode); fixed 1 microsec (turbo mode) "EDR" Extreme Dynamic Range TM and Auto Exposure control PIV - Particle Image Velocimetry (standard) 4800 ISO/ASA monochrome, 1200 ISO/ASA color sensitivity equivalency, 2 Gigabytes DRAM non-volatile flash memory (Up to 16 Gigabytes), Image control: 10/100MB/1GB Ethernet, Trigger: continuously variable pre/post, rising and falling or switch and with external sync. We plan to buy it in the second year, to be ready for the experimental validation since the third year of the project.

TIRF Objective for NanoPIV (estimated 12 Keuro): The existing micro-PIV set-up has proven capable to image a wide range of flow conditions inside microfluidic devices, in the bulk by epifluorescence microscopy and at the interface with a transparent solid surface by Total Internal Reflection Fluorescence Microscopy (TIRFM). We plan to improve the spatial resolution of our TIRF by replacing the prism with an optical objective specific for TIRF: an apochromatic 100x 1.49 Numerical Aperture (NA) Oil immersion. We plan to buy it in the second year, to be ready for the experimental validation since the third year of the project.

Missions, Schools & Workshops

Costs are needed for team members to participate to conference and for international collaborations, 3.4 Keuro per team member per year the first three years and 2.5 Keuro for the last two years.

Schools & Workshops

A kick-off school and 2 more focused meetings are planned (20Keuro x 3). The school will be organised in the facility of the University of Rome (for free to us), therefore funds are only meant to cover the costs of invited speakers. More funds can be secured also applying to the INFN and to the CNR.

Functioning

Consumable, Software & Publication costs : Software IDL Licenses + Algorithms + Multiprocess Calculus Porting for IDL iTools for interactive image acquisition (10 Keuro the third year of the project). Expenses related to running the experiments (5 Keuro per year, the last 3 years) plus small amount of money needed the first years for starting the different activities (1 Keuro per year). I also allocated a small amount of money to cover the publication of colored figures, if needed.

Bibliographical References

[1] Squires T. & Quake S., Rev. Mod. Phys. 77, 977-1026 (2005)

[2] Tabeling P., Introduction to Microfluidics (Oxford University press, 2005)

[3] Garstecki P., Feuerstman M., Stone H. A. & Whitesides G. M., Lab Chip 6, 437-446 (2006)

[4] Tabeling P., Lab Chip 9, 2428 -2436 (2009)

[5] Stone H. A., Annu. Rev. Fluid Mech. 26, 65102 (1994)

[6] Utada A., Lorenceau E., Link D. R., Kaplan P.D., Stone H. A., & Weitz D. A., Science 308, 537 (2005)

[7] Christopher G. F. & Anna S. L., J. Phys. D: Appl. Phys. 40, R319-R336 (2007)

[8] Pannacci N. et al., Phys. Rev. Lett. 16, 164502 (2008)

[9] Goyon J., Colin A., Ovarlez G., Ajdari A., Bocquet L., Nature 454, 84-87 (2008)

[10] Bocquet L., Colin A. & Ajdari A., Phys. Rev. Lett. 103, 136001 (2009)

[11] Keys A. S., Abate A. R., Glotzer S. C., & Durian D. J. Nature Phys. 3, 260–264 (2007)

[12] Coussot P., Rheometry of pastes, suspensions, and granular materials (Wiley, 2005)

[13] De Menech M., Garstecki P., Jousse F. & Stone H. A., Jour. Fluid Mech. 595, 141-161 (2008)

[14] Thorsen T., Roberts R. W., Arnold F. H. & Quake S. R., Phys. Rev. Lett. 86, 4163-4166 (2001)

[15] Menetrier-Deremble L. & Tabeling P., Phys. Rev. E 74, 035303 (2006)

[16] Flumerfelt R.W., Indust. Engng. Chem. Fund. 11, 312-318 (1972)

[17] Tagvac T., PhD Thesis, Chemical Engineering Department, University of Houston (1972)

[18] Elmendorp J.J. & Maalke R.J., Polymer Eng. and Science 25, 1041-1047 (1985)

[19] Mighri F., Ajji A. & Carreau P.J., Jour. Rheol. 41, 1183-1201 (1997)

[20] Mighri F., Carreau P.J. & Ajji A., Jour. Rheol. 42, 1477-1490 (1998)

[21] Aggarval N. & Sarkar K., Jour. Fluid Mech. 601, 63-84 (2008)

[22] Darhuber A.A. & Troian S.M., Annu. Rev. Fluid Mech. 37, 425-455 (2006)

[23] Larson R.G., The Structure and Rheology of Complex Fluids (Oxford university press, 1999)

[24] Coussot P., Rheometry of Pastes, Suspensions, and Granular Materials (Wiley-Interscience, 2005)

[25] Chaikin P.M. & Lubensky T.C., Principles of Condensed Matter Physics (Cambridge Press, 1995)

[26] Evans D.F. & Wennerstrom H., The Colloidal Domain (Wiley-VCH, New York, 2nd edition, 1999)

[27] De Gennes P.G., Scaling Concepts in Polymer Physics (Cornell University Press, Ithaca, 1979)

[28] Doi M. & Edwards S.F., The Theory of Polymer Dynamics (Oxford University Press, Oxford, 1986)

[29] Weaire D. & Hutzler S., The Physics of Foams (Oxford University Press, 1999)

[30] Russel W.B. et al., Colloidal Dispersion (Cambridge University Press, Cambridge England, 1989)

[31] Poole P.H., Sciortino F., Essmann U. & Stanley H.E., Nature 360, 324 (1992)

[32] Sollich P., Lequeux F., H'ebraud P. & Cates M., Phys. Rev. Lett. 78, 2020 (1997)

[33] Sciortino F., Nature Materials 1, 145 (2002)

[34] Dupin M.M.,Halliday I. & Care C.M., Phys. Rev. E 75, 055701(R) (2006)

[35] Keys A. S., Abate A. R., Glotzer S. C. & Durian, D. J., Nature Phys. 3, 260–264 (2007)

[36] Pouliquen O., Phys. Rev. Lett. 93, 248001 (2004)

[37] Fuchs M. & Cates M., Phys. Rev. Lett. 89, 248304 (2002)

[38] Ho C.M. & Tai Y.C., Annu. Rev. Fluid Mech. 30, 579-612 (1998)

[39] Huh, C. & Scriven, L., J. Colloid Interface Sci. 35, 85-101 (1971)

[40] Dussan V. E. B. & Davis S. H. , J. Fluid Mech. 173, 115-130 (1986)

[41] Koplik J. & Banavar J. R., Annu. Rev. Fluid Mech. 27, 257-292 (1995)

[42] Koplik J. & Banavar J. R. Phys. Fluids 7, 3118-3125 (1995)

[43] Thompson P. A. & Robbins M. O., Phys. Rev. Lett. 63, 766-769 (1989)

[44] Barrat J.L. & Bocquet L., Phys. Rev. Lett. 82, 4671 (1993)

[45] Thompson P. A. & Troian S. M., Nature 389, 360-362 (1997)

[46] DeGennes P.G., Rev. Mod. Phys. 57, 827-863 (1985)

[47] Oron A., Davis S. H., Bankoff G., Rev. Mod. Phys. 69, 931-980 (1997)

[48] Blake T. D., J. Colloid Interface Sci. 299, 1-13 (2006)

[49] Cox R. G., J. Fluid Mech. 168, 169-194 (1986)

[50] Voinov O. V., Fluid Dyn. 11, 714 (1976)

[51] Dussan E. B. V., Rame E. & Garoff S., J. Fluid Mech. 230, 97-116 (1991)

[52] Pismen L. M. & Pomeau Y., Phys. Rev. E 62, 2480-2492 (2000)

[53] Jacqmin D., J. Fluid Mech. 402, 57-88 (2000)

[54] Eggers J.,Phys. Rev. Lett. 93, 094502 (2004); Phys. Fluids 16, 3491 (2004)

[55] Jacqmin D., J. Fluid Mech. 517, 209-228 (2004)

[56] Blake T. D. & Ruschak K. J., Nature 282, 489-491 (1979)

[57] Quere D., C. R. Acad. Sci. Paris II 313, 313-318 (1991)

[58] Simpkins P.G. & Kuck V.J., J. Colloids Interface Sci. 263, 562 (2003)

[59] Sbragaglia M., Sugiyama K. & Biferale L., J. Fluid Mech. 614, 471-493 (2008)

[60] Landau L. D. & Levich B. V., URSS 17, 42 (1942)

[61] Groisman A. & Steinberg V., Nature 405, 53-55 (2000); Nature 405, 905-908 (2001)

[62] Succi S., The lattice Boltzmann Equation (Oxford Science, 2001)

[63] Benzi R., Succi S. & Vergassola M., Phys. Rep. 222, 145 (1992)

[64] Chen S. & Doolen G., Annu. Rev. Fluid Mech. 30, 329-364 (1998)

[65] Wolf-Gladrow D.A., Lattice-Gas Cellular Automata and LBM (Springer, Berlin, 2000)

[66] Shan X. & Chen H., Phys. Rev. E 47, 1815 (1993), Phys. Rev. E 49, 2941 (1994)

[67] Sbragaglia M., Shan X., Chen H. & Succi S., Europhys. Lett. 86, 24005 (2009)

[68] Swift M. R., Osborn W. R. & Yeomans J.M., Phys. Rev. Lett. 75, 830-833 (1995)

[69] Wagner A.J. & Yeomans J.M., Phys. Rev. Lett. 80, 1429 (1998); Phys. Rev. E 4,4366 (1999)

[70] Sbragaglia M. et al., Phys. Rev. E 75, 026702 (2007)

[71] Shan X., Phys. Rev E 77, 066702 (2008)

[72] Lee T. & Liu L., Physical Review E 78, 017702 (2008)

[73] Melchionna S. & Marini Bettolo Marconi U., Europhys. Lett. 81, 34001 (2008)

[74] Li Q. & Wagner A.J., Physical Review E 76, 036701 (2007)

[75] Arcidiacono S., Karlin I. V. & Mantzaras J., Physical Review E 76, 046703 (2007)

[76] Hyvaluoma J. & Harting J., Phys Rev. Lett. 100, 246001 (2008)

[77] Harting J., Kunert C. & Hyvaluoma J., Microlfuids & Nanofluidics 8, 1-10 (2010)

[78] Benzi R., Biferale L., Sbragaglia M., Succi S. and Toschi F., J. Fluid Mech. 548, 257 (2006)

[79] Sbragaglia M., Benzi R., Biferale L., Succi S. & Toschi F., Phys. Rev. Lett. 97, 204503 (2006)

[80] Cercignani C., Theory and Application of the Boltzmann Equation (Scottish Academic Press, 1975)

[81] Ansumali S. & Karlin I.V., Phys. Rev E 66, 026311 (2002)

[82] Cottin-Bizonne C. et al., Nature Materials 2, 237 (2003); Eur. Phys. J. E 15, 427 (2004)

[83] Briant A. J., Wagner A. J. & Yeomans, J. M., Phys. Rev. E 69, 031602 (2004)

[84] Sofonea V., Jour. Comp. Phys. 228, 6107-6118 (2008)

[85] Prasianakis N.I., Karlin I.V., Mantzaras J. & Boulouchos K. B., Phys. Rev. E 79, 066702 (2007)

[86] Watari M., Phys. Rev. E 79, 066706 (2009)

[87] Sbragaglia M., Benzi R., Biferale L., Chen H., Shan X. & Succi S., J. Fluid Mech. 628, 299-309 (2009)

[88] Benzi R., Chibbaro S., Sbragaglia M. & Succi S., Jour. Chem. Phys. 131, 104903 (2009)

[89] Benzi R., Sbragaglia M., Bernaschi M. & Succi S., Europhys. Lett. 91, 14003 (2010)

[90] Snoeijer J.H., Phys. Fluids 18, 021701 (2005)

[91] Snoeijer J.H., Delon G., Fermigier M. & Andreotti B., Phys. Rev. Lett. 96, 174504 (2006)

d. Ethical Issues

ETHICS ISSUES TABLE

	Research on Human Embryo/ Foetus	YES	Page
	Does the proposed research involve human Embryos?		
	Does the proposed research involve human Foetal Tissues/ Cells?		
	Does the proposed research involve human Embryonic Stem Cells (hESCs)?		
	Does the proposed research on human Embryonic Stem Cells involve cells in culture?		
	Does the proposed research on Human Embryonic Stem Cells involve the derivation of cells from Embryos?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

	Research on Humans	YES	Page
	Does the proposed research involve children?		
	Does the proposed research involve patients?		
	Does the proposed research involve persons not able to give consent?		
	Does the proposed research involve adult healthy volunteers?		
	Does the proposed research involve Human genetic material?		
	Does the proposed research involve Human biological samples?		
	Does the proposed research involve Human data collection?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

	Privacy	YES	Page
	Does the proposed research involve processing of genetic information or personal data (e.g. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?		
	Does the proposed research involve tracking the location or observation of people?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

	Research on Animals	YES	Page
	Does the proposed research involve research on animals?		
	Are those animals transgenic small laboratory animals?		
	Are those animals transgenic farm animals?		
	Are those animals non-human primates?		
	Are those animals cloned farm animals?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

	Research Involving non-EU Countries (ICPC Countries)	YES	Page
	Is the proposed research (or parts of it) going to take place in one or more of the ICPC Countries?		
	Is any material used in the research (e.g. personal data, animal and/or human tissue samples, genetic material, live animals, etc) : a) Collected in any of the ICPC countries?		
	b) Exported to any other country (including ICPC and EU Member States)?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

	Dual Use	YES	Page
	Research having direct military use		
	Research having the potential for terrorist abuse		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	