Simulation of deformable objects transported in fluid flow

by

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Cover: Visualisation of nucleated capsules in shear flow at $Re = 0.1$, $Ca = 0.5$.

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Simulation of deformable objects transported in fluid flow

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Abstract
Deformable particles suspended in a viscous fluid can be found in many industrial and biological applications. In this thesis, two different numerical tools have been developed to simulate suspensions of capsules, thin membranes enclosing a second fluid and a rigid nucleus so to work as model for "Eukaryotic" cells, and flexible slender bodies known as filaments/fibres. Both tools use a semi-implicit fluid flow solver with different approaches for the deformable structure. The capsule membrane is modelled as a thin hyperelastic material and the elasticity equations are solved with an accurate spectral representation of the capsule shape as a truncated number of spherical harmonics. The filaments are considered as one dimensional inextensible slender bodies obeying Euler-Bernoulli beam equations which is solved by a two-step method using finite difference discretisation. The immersed boundary method is exploited to couple the fluid and solid motion using different versions for the two different objects considered. The nucleus inside the capsules is modelled either as a second stiffer capsule or as a rigid particle. In order to avoid membrane-membrane, membrane-wall and membrane-nucleus overlapping, a short range repulsive force is implemented in terms of a potential function of the distance between the approaching objects. For the short range interactions between the filaments, both lubrication correction and collision forces are considered and it is found that the inclusion of the lubrication correction has significant effect on the rheology in shear flow. Both codes are validated against the numerical and experimental data in the literature. We study the capsule behaviour in a simple shear flow created by with two walls moving in opposite directions. The membrane obeys the Neo-Hookean constitutive equations and, in the simulations with a rigid nucleus, its radius is fixed to half the capsule initial radius. The filaments, on the other hand, are studied in 4 different flow configurations: shear flow, channel flow, settling in quiescent fluid and homogeneous isotropic turbulence. The results indicate that for single capsule, the nucleus reduces the membrane deformation significantly and changes the deformed shaped when there is negligible bending resistance of the membrane. The rheological properties of nucleated capsule suspensions result from the competition between the capsule deformation and their orientation angle and similarly to the case of single capsules, the nucleus reduces the mean deformation. By increasing the capsule volume fraction, the relative viscosity increases and capsules become more oriented in the mean flow direction. Filament suspensions in shear flow exhibit shear thinning behaviour with respect to deformability; inertia has a significant effect on the rheological properties of the suspensions as documented here. For
the case of settling fibres, we document the formation of columnar structures with higher settling velocity known as streamers, which are more pronounced at higher volume fractions and for flexible fibres. For a single filament in homogeneous isotropic turbulence, two distinct regimes for the filament motion are identified with a sharp transition from one to another at a critical bending stiffness. In turbulent channel flow, we demonstrate how finite-size filaments cause considerable drag reduction, of the order of 30% for volume fractions of the order of 1.5%, and that the main averaged quantities are almost independent of the filament flexibility for the bending rigidities studied here.

**Key words:** deformable objects, nucleated capsules, filament suspensions, streamers, drag reduction
Numerisk simulering av transport av deformabla kroppar i strömmande medier

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Sammanfattning
Vi använder den så kallade ”immersed boundary” metoden för att koppla vätskans och den fasta kroppens rörelsen. Kärnan inuti kapslarna modelleras antingen som en annan styvare kapsel eller som en styv partikel. För att undvika olika överlappningar av membraner och membrankärnor är en repulsiv kraft med kort räckvidd implementerad. Denna kraft är en funktion av avståndet mellan de närliggande föremålen. För korta interaktioner mellan filamen
ten tar vi hänsyn till både lubrication correction och kollisionskräftarna. Vi har konstaterat att införandet av smörgjärningar kan haber en signifikant effekt på reologin i skjutflöde. Båda koderna har validerats mot de existerande numeriska och experimentella data i litteraturen.
Resultaten av våra studier indikerar att för en entstaka kapsel reducerar kärnan signifikant deformationen av membranet samt ändrar den deformationsformen om membranet har ett försömbart böjningsmotstånd.
De reologiska egenskaperna hos kapselsuspensioner med kärnor är resultatet av konurrensen mellan kapseldeformationen och deras orienteringsvinkel. På ett liknande sätt som fallet med enkla kapslar, minskar kärnan den genomsnittliga
deformationen. Med ökande kapselvolymfraktionen ökar den relativa viskositeten och kapslarna blir mer orienterade i medellödesriktningen. Suspensioner av filament i skjuvflöde uppvisar en skjuvningsförtunnningseffekt med ökande filament deformabilitet. Som är dokumenterat i denna avhandling tröghet har en signifikant inverkan på de reologiska egenskaperna hos suspensionerna. I fallet med sedimentierande fiber visar vi bildandet av kolumnstrukturer med högre sedimenteringhastighet. Förekomsten av dessa kolumnstrukturer, så kallade streamers, är mer uttalad vid högre volymfraktioner och för flexibla fiber. För ett enskilt filament i ett homogent och isotropiskt turbulent flöde identiferas två distinkta regimer för filamentrörelsen med en skarp övergång från den ena till den andra vid en kritisk böjstyrhastighet. För ett turbulent kanalflöde visar vi hur filament med finit storlek orsakar en avsevärd motståndshöjning, i storleksordningen 30% för volymfraktioner av storleksordningen 1.5%. Vi också visar att medelvärdet av flödets karakteristiska storheter är nästan oberoende av filamentets flexibilitet för de parametervärden vi har studerat här.

Nyckelord: deformbara partiklar, kapselsuspensioner med kärnor, suspensioner av filament, streamers, motståndshöjning
Preface

This PhD thesis deals with the numerical study of elastic objects in fluid flows. An introduction on the equations and numerical methods is presented in the first part. The second part contains six articles. The papers are adjusted to comply with the present thesis format for consistency, but their contents have not been altered as compared with their original counterparts.


**Paper 2.** A. Alizad Banaei, A. Shahmardi and L. Brandt, 2019. *Suspensions of nucleated capsules at finite inertia.* To be submitted.


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Division of work between authors
The main advisor for the project is Prof. Luca Brandt.

Paper 1. The code has been developed by Arash Alizad Banaei (AAB). Simulations and data analysis are performed by AAB. The paper is written by AAB with feedback from Jean Christophe Loiseau, Iman Lashgari and Luca Brandt (LB).

Paper 2. The code has been developed by AAB. Simulations are performed by AAB and Armin Shahmardi. Data analysis is performed by AAB. The paper is written by AAB with feedback from LB.

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Paper 5. The code has been developed by AAB. Simulations and data analysis are performed by MER. The paper is written by MER with feedback from Andrea Mazzino and LB.

Paper 6. The code has been developed by AAB. Simulations and data analysis are performed by MER and Stefano Olivieri. The paper is written by MER and Stefano Olivieri with feedback from Andrea Mazzino and LB.
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Part I

Overview
Chapter 1

Introduction

This thesis deals with the interactions between deformable objects and the flow of a viscous fluid. In this work, we have studied these complex interactions by means of numerical simulations, focusing on capsules formed by close thin membranes, with and without nucleus, and long flexible filaments. The objective is to understand how the object dynamics is affected by the gradients in the flow and the modifications of the macroscopic transport properties in the presence of a significant number of suspended object. In particular, we have tried to related these global properties to the deformation and motion of the different deformable objects. This work is of more fundamental nature, although interactions between deformable objects and fluid flows are ubiquitous in nature and applications. In this first chapter we report some applications and report main findings from previous studies. The following chapters will present the details of the mathematical and numerical models adopted, and summarise the main findings from the papers in the appendix as well as from more recent work about turbulent channel flow laden with finite-size elastic filaments.

1.1. Deformable cells and capsules

Liquid droplets being enclosed by an elastic membrane known as *capsules* can be found in many industrial and biological applications such as blood cells, drug delivery, pharmaceutical, cosmetic, and food industries for the controlled release of active principles, aromas, or flavours (Barthes-Biesel 2016). Individual behaviour of capsules in fluid flow and the bulk properties of the capsule suspensions is affected by the capsule size, shape, deformability and volume fraction as well as rheological properties of the suspending liquid and flow conditions. Several numerical and experimental works have been devoted to study effect of above-mentioned parameters on the flow behaviour and capsule dynamics. The dynamics of capsules might be more complicated when there is a nucleus inside the capsules such as Malaria infected blood cells (see Fig.1.1) and Eukaryotic cells since the nucleus affects the capsule stresses and its deformed shape.
1. Introduction

Figure 1.1: Surface rendered views of Malaria infected red blood cells at different stages of parasite development. The bottom row illustrates the growth of parasite inside the infected red blood cell at various times. Scale bar is 5 µm. The figure is adopted from the paper by (Waldecker et al. 2017).

1.1.1. Single capsule

Many early experimental studies have addressed the interaction between tiny deformable particles and an external flow. Several interesting types of motion have been discovered such as tumbling and tank-treading in shear flow (Goldsmith & Marlow 1972; Fischer 1977), the zipper flow pattern (Gaehtgens et al. 1979) or parachute cell shapes (Skalak & Branemark 1969). More recent studies focused on cells that exhibit very large deformations at high shear rates, which can cause breaking (Chang & Olbricht 1993), just to mention few examples. Most of these studies are of experimental nature. Such investigations can however be quite expensive since they require dedicated facilities not easy to fabricate. In addition, experimenting measuring the exact deformation and stresses can be rather complicated. Developing robust and reliable numerical platforms is thus of increasing importance in order to perform high-fidelity simulations beside laboratory experiments.

Many cells, including red blood cells, can be modelled as capsules. Capsules consist of a droplet enclosed by a thin membrane: the membrane area can vary while the enclosed volume is constant. Nowadays, several numerical studies on the deformation of a capsule in shear flow have been reported in literature. At certain shear rates, the capsule reaches a steady shape while its membrane
1.1. Deformable cells and capsules

exhibits a rotation known as tank-treading motion (Huang et al. 2012). This tank-treading motion disappears when the viscosity or shear rate of the external fluid becomes low enough and instead a flipping or tumbling motion similar to that of a rigid body appears (Schmid-Schönbein & Wells 1969; Fischer et al. 1978). Membranes can also undergo buckling or folding for high elastic moduli or at low and high shear rates in absence of bending rigidity (Walter et al. 2001; Huang et al. 2012). A solution to this problem is proposed by introducing a stress on undeformed membrane, the so-called pre-stressed capsule (Lac & Barthès-Biesel 2005). As regards the motion of non-spherical capsules in shear flow, different types of motion occur when changing the fluid viscosity, the membrane elasticity, the geometry of the problem or the applied shear rate. In (Skotheim & Secomb 2007), a phase diagram is presented for biconcave shaped capsule in which the transition from tank-treading to tumbling motion is identified when decreasing the shear rate.

For eukaryotic cells, the overall mechanical properties of a cell are not only determined by its membrane but also by other cell organelle such as the cell nucleus (Rodriguez et al. 2013). Typically, the nucleus is stiffer than the surrounding cytoplasm which results in lower deformation when subject to the external stimuli (Caille et al. 2002; Guilak & Mow 2000). To model and predict the cell behaviour, the mechanical properties of the nucleus need to be quantified. To this end, both experimental tests and numerical simulations have been performed by (Caille et al. 2002). The elastic modulus of the nucleus in round and spread cells was found to be around 5000 N/m², roughly ten times larger than for the cytoplasm. As further example, the nucleus of bovine cells is nine times stiffer than the cytoplasm (Maniotis et al. 1997), yet small deformations of the nucleus may occur when a cell is subjected to flow (Galbraith et al. 1998). Though the cell membrane can exhibit large deformation on a substrate when highly compressed, stretched or flattened (Guilak 1995; Caille et al. 1998; Ingber 1990), the nucleus may be assumed as a rigid particle for an intermediate range of the applied forces (external shear). Dynamics of spherical and non-spherical nucleated capsules in shear flow were studied numerically by (Luo et al. 2015; Luo and Bai 2016). The nucleus was modeled as a capsule and it was found that the inner capsule can significantly change the outer capsule dynamics by defining inner capsule size as an important parameter on dynamics of outer capsule.

1.1.2. Capsule suspensions

Studying rheological properties of capsule suspensions have great importance in medical applications. As an example, blood is typically considered as capsule suspension with non-Newtonian behaviour by the presence of red blood cells and the rheological properties are highly correlated by the membrane elasticity and cell-cell interactions (Reasor et al. 2013). Furthermore, it is found that the relative viscosity and normal stresses of capsule suspensions depend both on deformation and orientation angle of the capsules (Matsunaga et al. 2016). An expression for the relative viscosity of capsule suspensions was derived by
1. Introduction

(Barthes-Biesel and Chhim 1981) in case of small capillary numbers observing shear thinning behaviour for the suspensions. (Bagchi and Kalluri 2010) studied rheology of dilute capsule suspensions considering viscosity difference between inside and outside of the capsules. They observed shear thinning behaviour and a non-monotonic variation of the relative viscosity by viscosity ratio. Effect of flow inertia on rheology of semi-dilute capsule suspensions was studied by (Krüger et al. 2014) indicating that for low capillary numbers there is monotonic increase in viscosity by flow inertia while for larger capillary numbers there is an increase in viscosity followed by a reduction by further increasing the flow inertia. (Bagchi and Kalluri 2011) studied effect of swinging and tumbling motion of initially oblate capsules on the rheological properties of dilute suspensions showing that unlike spherical capsule suspensions, the rheological properties are time dependent while time averaged rheological properties are qualitatively similar to spherical capsule suspensions.

Rheology of dense biconcave capsule suspensions was studied by (Gross et al. 2014) by varying volume fraction up to 90%. They observed very large viscosity and first normal stress difference at high volume fractions while the suspensions keep their shear thinning behaviour and Herschel-Bulkley curves were fitted to their data. Rheology and microstructure of dense capsule suspensions was studied by (Clausen et al. 2011). They found that the first normal stress difference undergoes a sign change at relatively small deformations. (Reasor et al. 2013) studied rheology of dense suspensions of red blood cells and it was found that the viscosity is dependent on orientation and bending modulus of the cells and normal stress tensor indicated that there is a transition from compressive to tensile states in the flow direction by increasing the shear rate. They mentioned effect of bending stiffness and initial shape of capsule has considerable effect on first normal stress difference. A multiscale study on blood flow was performed by (Fedosov et al. 2014) by means of numerical simulations. They studied rheology of red blood cell suspensions in tubes with different diameters observing a large increase in relative viscosity by decreasing the tube diameter. (Winkler et al. 2014) investigated rheology of polymeric semi-dilute soft colloid, vesicle, capsule and cell suspensions where in the case of cell suspensions, there is much more viscosity for aggregating cell suspension than Non-aggregating one. A novel coupled lattice-Boltzmann and finite element method was proposed by (MacMECCAN et al. 2009) for simulation of deformable particles to increase the efficiency of simulations of suspensions at high volume fractions. They performed simulations on initially spherical and biconcave capsule suspensions at 40% volume fraction and obtained significantly less viscosity for initially spherical capsule suspensions while both suspensions have shear thinning behaviour. An extensive study on rheology of dense capsule suspensions was done by (Matsunaga et al. 2016) for initially spherical capsules with volume fraction up to 40%. They found that unlike rigid spheres, for deformable capsules the relative viscosity increases almost linearly with volume fraction even at high volume fractions. It was found that deformation of capsule increases by increasing the volume fraction while orientation angle with respect
1.2. Flexible filaments/fibres

Flexible filaments/fibres can be found in many industrial and biological applications such as papermaking, composite materials, drag reduction in turbulent flows and swimming of microorganisms (Lundell et al. 2011; Lindström & Uesaka 2008; Bagheri et al. 2012). There are several studies on flexible filaments in different flow configurations to investigate their dynamics as well as the bulk behaviour in case of suspensions.

1.2.1. Laminar flows

The study of the rheology of filament suspensions is essential in many industrial applications. The rheological properties of the filament suspensions may be affected by fibre aspect ratio, flexibility and flow inertia. Numerical simulations have been used to address fibre suspensions only quite recently; in these studies the effects of deformability are accounted for by modeling the fibres as chains of connected spheres or cylinders (Joung et al. 2001; Wu & Aidun 2010b). In this thesis, the rheology of semi-dilute and concentrated suspensions of flexible filaments is studied by assuming fibres as continuously deformable objects. The rheology of rigid fibre suspensions has been extensively studied in the past both experimentally and numerically. Typically fibre suspensions are characterized by their number density, $nL^3$ where $n = \frac{n_f}{V}$ is the number of fibres per unit volume and $L$ their length. Three regimes are usually identified (Wu & Aidun 2010b): dilute, semi-dilute and concentrated suspensions (see Fig. 1.2). In the dilute limit, $nL^3 < 1$, fibre-fibre interactions are negligible and fibres move independently from each other. In the semi-dilute regime, $1 < nL^3 < \frac{d}{2}$ with $d$ the fibre diameter, fibre-fibre interactions start to affect the global dynamics and in the concentrated regime, $nL^3 > \frac{d}{2}$, interactions between fibres are dominant. By further increasing the volume fraction, fibre rotations are hindered by the adjacent fibres and the system transitions to an organised state (Butler & Snook 2018).

(Blakeney 1966) measured the effect of the solid volume fraction on the suspension viscosity in the dilute regime, with concentrations up to 1%. It was
found that the relative viscosity rapidly grows for volume fractions above the critical value of 0.42%, then slightly decreases for volume fractions between 0.5% and 0.6% followed by a second rapid increase for volume fractions above 0.6%. (Bibbó 1987) first experimentally investigated the rheology of semi-concentrated rigid fibres suspensions in both Newtonian and Non-Newtonian solvents, and observed that the relative viscosity is only a function of the volume fraction and independent of the fibre aspect ratio for large enough values of the imposed shear rate for a Newtonian suspending fluid. Similar experiments were performed more recently by (Chaouche & Koch 2001) and (Djalili-Moghaddam & Toll 2006). The former authors found a nearly Newtonian behaviour in semidilute suspensions, while shear-thinning was observed in more concentrated regimes; also, this Non-Newtonian behaviour was found to increase with the fibre concentration and to decrease with the solvent viscosity. (Djalili-Moghaddam & Toll 2006) observed a strong dependency of the suspension viscosity on the fibre aspect ratio for volume fractions above 5% due to the presence of friction forces at fibre-fibre interactions. Numerical simulations of fibre suspensions have been performed only quite recently. (Yamane et al. 1994) were the first to study dilute suspensions of non-Brownian fibres under shear flow by exploiting analytical solutions for rigid slender bodies: they considered short range interactions between fibres due to lubrication forces but neglected long range interactions. These authors concluded that the relative viscosity of the suspension is only slightly altered by fibre-fibre interactions in this dilute regime. (Mackaplow & Shaqfeh 1996) considered fibres as line distributions of Stokeslets and used slender body theory to determine the fibre-fibre interactions; they observed that the suspension viscosity can be well predicted analytically considering simple two-body interactions for dilute and semidilute concentrations. (Lindström & Uesaka 2008) performed numerical simulations of rigid fibre suspensions to study fibre agglomeration in the presence of friction forces. These authors observed that the apparent viscosity increases non-linearly with the friction coefficient and fibres tend to flocculate even in the semidilute regime. The role of the fibre curvature on the effective viscosity of suspensions of rigid fibres was studied by (Joung et al. 2002) who showed that this results in a large increase of the
1.2. Flexible filaments/fibres

Suspension viscosity already for small curvatures. While most of the previous studies on rigid fibre suspensions consistently report an increase of the suspension viscosity with the volume fraction, different results have been reported in the past on the effect of the fibre flexibility on the global suspension rheology. One of the first study on flexible fibres was the experimental investigation by (Kitano & Kataoka 1981). These authors considered vinylon fibres immersed in a polymeric liquid and observed an increase of the suspension viscosity and of the first normal stress difference with the volume fraction and fibre aspect ratio. Although these authors mentioned that the fibre deformability may affect the rheological properties of the suspension, its effect was not discussed explicitly. This was done more recently by (Keshtkar et al. 2009) who investigated fibres suspensions with different flexibilities and high aspect ratios in Silicon oil. These authors found that the viscosity of the suspensions increases when the fibre is deformable. (Yamamoto & Matsuoka 1993) proposed a numerical method to simulate flexible fibres by modeling the fibres as chains of rigid spheres joined by springs, which allow each element to stretch, bend and twist. (Joung et al. 2001) used this method and found an increase of the suspension viscosity with the fibre elasticity. A similar procedure was adopted by (Schmid et al. 2000) who modeled the flexible fibres as chain of rods connected by hinges. Using this method, (Switzer III & Klingenberg 2003) studied flexible fibre suspensions and found that the viscosity of the suspension is strongly influenced by the fibre equilibrium shape, by the inter-fibre friction, and by the fibre stiffness. In particular, they reported a decrease of the relative viscosity with the ratio of the shear rate to the elastic modulus of the fibres. Finally, the rod-chain model was also used by (Wu & Aidun 2010a,b) who found again an increase of the suspension viscosity with the fibres flexibility, in contrast with the computational results by (Switzer III & Klingenberg 2003) who employed the same rod-chain model for fibres with aspect ratio of 75 and the experimental results by (Sepehr et al. 2004) who studied suspensions of fibres with aspect ratio 20 in viscoelastic fluids. Note that, suspensions of other deformable object, such as particles of viscoleastic material and capsules (thin elastic membranes enclosing a second liquid) also exhibit a suspension viscosity decreasing with elasticity and deformation (Matsunaga et al. 2016; Rosti & Brandt 2018). In particular, (Rosti et al. 2018b) and (Rosti & Brandt 2018) show that the effective suspension viscosity can be well predicted by empirical fits obtained for rigid particle suspensions if the deformability is taken into account as a reduced effective volume fraction. Sedimentation of fibre suspensions is present in many industrial processes and biological flows. In paper making procedure, sedimentation of flexible fibres and their flocculation in the pulp suspension significantly influences the final structure of the paper (Provatias et al. 1996). The efficiency of the treatment of the pulp and paper mill wastewater also often depends on the sedimentation speed of the residue fibres (Kamali & Khodaparast 2015). Settling and deposition of airborne particles, with arbitrary flexible shapes, near the surface of products creates contamination concerns in industrial clean rooms (Cooper 1986). Carbon nanotubes are used in different
industrial applications as reinforcing fibres particularly due to their flexibility (Cheng et al. 2013). Settling of flexible carbon nanotubes plays an important role in the dispersion process in suspensions used in industrial processes (Jiang et al. 2003). Near the sea floor, settling is an important mechanism of transportation of microorganisms and organic material which commonly have slender flexible body shapes (Gooday & Turley 1990). The settling behaviour of flexible fibre suspensions is determined by intriguing interactions between viscous, gravitational, elastic and long-range hydrodynamic forces that depend on the fibre structure, aspect ratio, flexibility, density and the volume fraction of the suspension. The effects of these factors on settling of fibres have been explored in several computational and experimental studies in the past. Settling speed of single a single rigid fibre in Stokes flow was theoretically derived by Batchelor (Batchelor 1970) and Mackaplow & Shaqfeh (Mackaplow & Shaqfeh 1998) using a slender body approximation, showing that unlike spheres in Stokes flow, an isolated fibre can have a motion perpendicular to the gravity direction while maintaining its initial orientation. Bending and re-orientation of flexible fibres make their settling more complicated compared to rigid fibres. The slender body theory analysis of Xu & Nadim (Xu & Nadim 1994) suggested that an isolated fibre, with a small elasticity, settling in a viscous fluid experiences a torque that makes it re-orient to the direction perpendicular to the gravity while it maintains a stable U shape. In numerical simulations of settling of semi-flexible fibres by Llopis & Pagonabarraga (Llopis et al. 2007), the re-orienting torque and the bending amplitude (defined as the maximum distance between two points in the filament in the direction of gravity) both increased with increasing the filament flexibility, implying that more flexible fibres adjust to the direction perpendicular to the gravity faster. Li et al (Li et al. 2013) showed analytically and numerically that the horizontal drift of settling fibres remains finite for flexible fibres as opposed to rigid fibres, and decreases with increasing fibre deformations. These results however were observed for filaments with sufficiently small flexibility. At higher filament flexibility, fibres settling along their long axis became unstable to buckling (Li et al. 2013), and fibres settling with their long axis perpendicular to the gravity direction can take shapes with more than one minima, with their bending amplitude saturating at high fibre flexibilities (Llopis et al. 2007). The instabilities of flexible fibres to buckling has also been addressed in shear flows (Tornberg & Shelley 2004; Wiens & Stockie 2015) and cellular flows (Young & Shelley 2007).

1.2.2. Turbulent flows

There are several studies on interaction of flexible filaments with turbulent flows as they appear from several applications ranging from biological applications (Fish & Lauder 2006; Bagheri et al. 2012; McKinney & DeLaurier 1981; Boragno et al. 2012) to energy harvesting (McKinney & DeLaurier 1981; Boragno et al. 2012; Li et al. 2016). The study of (Zhu & Peskin 2003) enabled a huge step forward in understanding the coupling between laminar flows and structure elasticity. This breakthrough was possible thanks to the combined choice of a
simple flow configuration (a soap film used as a laminar two-dimensional flow tunnel (Couder et al. 1989; Martin & Wu 1995; Kellay et al. 1995; Lȇcis et al. 2014)) and a simple elastic structure (a flexible fibre of given rigidity and inertia). Even in this apparently simple configuration the coupling between fluid and structure gives rise to a nontrivial and rich phenomenology. Once this has been described and the underlying mechanisms understood, new open questions arise about the dynamics of a fibre freely-moving in a three-dimensional turbulent environment: how does a flexible fibre interact with a turbulent flow? Under which conditions will flapping motion appear? How many states of flapping are possible? Can the amplitude/frequency of the resulting flapping states be controlled? Can the fibre be used to reveal the two-point statistics of turbulence? Answering these questions is one of the main objectives of this thesis. The findings will therefore also indicate how to exploit the motion of a flexible fibre in turbulence to obtain a proxy of two-point statistics of turbulence.

One of the interesting problems in fluid mechanics is drag reduction in turbulent flows which can be achieved with fibres. (Vaseleski & Metzner 1974) studied drag reduction in smooth tubes over a range of flow rates, tube sizes, fibre concentrations, and fibre aspect ratio. They observed considerable drag reduction in particular with Nylon fibres up to 70%. Drag reduction in turbulent flow of fibre suspensions with polymeric solutions was studied by (Lee et al. 1974). They found that by combining fibres and polymer solutions which are both known to exhibit drag reduction in turbulent flows, very large drag reductions can be achieved up to 95%. Regarding the numerical works, (Paschkewitz et al. 2004) performed direct numerical simulations on turbulent channel flow of rigid fibres suspended in a Newtonian fluid. Drag reductions up to 26% was observed which occurs in semi-dilute regime. The fibres are found to alter the turbulent statistics: The Reynolds stresses and velocity fluctuations in the wall-normal and spanwise directions, and streamwise vorticity is reduced while streamwise fluctuations are increased. (Gillissen et al. 2008) studied turbulent drag reduction with rigid polymer additives referred as fibres. They neglect fibre-fibre interactions in their model however they showed a good agreement with the experimental data.

In this thesis new numerical tools have been developed to simulate capsules and flexible slender bodies known as filaments/fibres in different flow configurations. Both the capsules and the filaments are considered as continuously deformable objects solving continuum elasticity equations with efficient numerical methods. In chapter 2 the governing equations and physical assumptions are explained followed by chapter 3 where the numerical methods are described. In chapters 4 and 5 a summary of the results are presented and finally in chapter 6 the main conclusions for the different works are discussed and possible future works in each field are introduced.
In this section the governing equations for fluid flow and motion of different deformable objects are introduced. Since the objects are suspended in fluid flow, the hydrodynamic forces acting on the bodies need to be related to their deformation to get their configuration in the flow. This is possible by analysing the equations of elasticity. First we start with the flow equations followed by different flow configurations that are considered in this thesis. Then the elasticity equations for membranes and slender bodies are discussed.

2.1. Fluid flow

2.1.1. Fluid flow equations

The dynamics of an incompressible Newtonian fluid flow with constant density is governed by continuity and Navier-stokes equations,

\begin{equation}
\nabla \cdot \mathbf{u}^* = 0,
\rho \left( \frac{\partial \mathbf{u}^*}{\partial t} + \mathbf{u}^* \cdot \nabla \mathbf{u}^* \right) = -\nabla p^* + \nabla \cdot [\mu (\nabla \mathbf{u}^* + (\nabla \mathbf{u}^* )^T )] + \mathbf{f},
\end{equation}

where \( \rho \) is the fluid density, \( \mathbf{u}^* \) the velocity field, \( p^* \) the pressure, \( \mu \) the dynamic viscosity of the fluid and \( \mathbf{f} \) a volume force. Equation 2.1 can be made non-dimensional by choosing a reference velocity scale \( U \), a reference length scale \( L \) and a reference viscosity \( \mu_o \). Based on the length and velocity scales, one can define \( \frac{L}{U} \) as time scale and \( \rho U^2 \) as pressure scale. Finally the equations in non-dimensional form read as

\begin{equation}
\nabla \cdot \mathbf{u} = 0,
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla \cdot [\mu^* (\nabla \mathbf{u} + (\nabla \mathbf{u} )^T )] + \mathbf{f},
\end{equation}

where \( Re = \frac{\rho U L}{\mu} \) is the Reynolds number and \( \mu^* = \frac{\mu}{\mu_o} \) the viscosity ratio. Depending on the case of study, different velocity and length scales can be chosen and in the case of gravity driven flows, the Reynolds number may be replaced by Galileo number which will be discussed later.
2.2. Mechanics of hyperelastic membranes

2.1. Flow configurations

2.1.2.1. Shear flow

This classic configuration is used to define rheological properties of suspensions and dynamics of a nucleated capsule under an imposed shear rate. In the case of shear flow, a 3-dimensional channel is considered with top and bottom walls moving in the opposite directions with velocity $U$ imposing a shear rate $\dot{\gamma} = \frac{U}{H}$ where $H$ is channel half height. At the walls no slip boundary condition is imposed for velocities and zero gradient for the pressure. In the directions perpendicular to the wall normal direction periodic boundary condition is imposed.

2.1.2.2. Channel flow

This configuration is used to study drag reduction in turbulent flows of filament suspensions. For the case of 3-dimensional channel flow, the fluid is flowing through two stationary walls in with an imposed external pressure. The mean velocity $U$ is kept constant by varying the pressure gradient. No-slip boundary condition is considered at walls for the velocity and zero gradient for the pressure. In the other directions the periodic boundary condition is imposed.

2.1.2.3. 3-periodic flow

In a 3-periodic flow, the domain of study is a cube without walls and periodic boundary condition is imposed in all three dimensions. This kind of boundary condition is appropriate for flows driven by the gravity (see section 5.2) or homogeneous isotropic turbulence (HIT) (see section 5.3).

2.2. Mechanics of hyperelastic membranes

2.2.1. Consideration of reference frames

In order to study dynamics of a deformable membrane, two sets of reference frames are needed. One fixed Cartesian frame that is used to quantify the kinematic properties of the membrane and another moving curvilinear frame in which the deformation of the body is defined. The membrane is assumed to be very thin and its deformation can be assumed to be two-dimensional. Figure 2.1 represents the two coordinates: the Cartesian coordinate $(x_1, x_2, x_3)$ with the base vectors $(e_1, e_2, e_3)$ and the curvilinear system $\xi_1, \xi_2$ with the covariant base vectors $(a_1, a_2, a_3)$ following the surface deformation.

2.2.2. Governing equations

The aim of this section is to relate the membrane deformation to the external load acting on the membrane. For this purpose, we start with vector analysis: the base vectors of the local covariant coordinate system are defined as

$$a_1 = \frac{\partial x}{\partial \xi^1}, \quad a_2 = \frac{\partial x}{\partial \xi^2}, \quad a_3 = \frac{a_1 \times a_2}{|a_1 \times a_2|}, \quad (2.3)$$
2. Governing equations

Figure 2.1: Schematic of a deformed body and Cartesian and curvilinear base vectors

where $\theta$ and $\phi$ are latitudinal and longitudinal angles on the cell surface representing the local curvilinear base. The contravariant base vector can be represented by $(a^1, a^2, a^3)$ which reads:

$$a^\alpha . a_\beta = \delta_\beta^\alpha,$$

(2.4)

where $\delta_\beta^\alpha$ is the Kronecker delta. Any arbitrary vector, such as $U$ can be written in each of the coordinates:

$$U = u^i a_i = u_i a^i = U_{x_i} e_i,$$

(2.5)

where $x_i$ stands for Cartesian components. The metric tensors are defined as:

$$a_{\alpha\beta} = a_{\alpha} . a_{\beta}, a^{\alpha\beta} = a^{\alpha} . a^\beta.$$

(2.6)

The basis vectors and metric tensors in the undeformed (reference) state are hereafter denoted by capital letters. The invariants of the transformation $I_1$ and $I_2$ are defined as

$$I_1 = A^{\alpha\beta} a_{\alpha\beta} - 2, \quad I_2 = |A^{\alpha\beta}| |a_{\alpha\beta}| - 1.$$  
(2.7)

Equivalently, they can also be determined from the principal stretching ratios $\lambda_1$ and $\lambda_2$ as

$$I_1 = \lambda_1^2 + \lambda_2^2 - 2,$$

$$I_2 = \lambda_1^2 \lambda_2^2 - 1 = J_s^2 - 1.$$  
(2.8)

The ratio of the deformed to the undeformed surface area is defined by the Jacobian $J_s = \lambda_1 \lambda_2$. The two dimensional Cauchy stress tensor, $T$, is obtained from the strain energy function $W_s$ per unit area of the undeformed state.

$$T = \frac{1}{J_s} F^{\gamma} \frac{\partial W_s}{\partial e} \cdot F^\gamma,$$

(2.9)
where $F = a_i \otimes A^i$ is the deformation gradient tensor and $e = (F^T \cdot F - I)/2$ is the Green-Lagrange strain tensor. Equation (2.9) can be further expressed component-wise as

$$T^{\alpha \beta} = \frac{2}{J_s} \frac{\partial W_s}{\partial \{ A^{\alpha \beta} \}} + 2J_s \frac{\partial W_s}{\partial \{ a^{\alpha \beta} \}}.$$  \hspace{1cm} (2.10)

The external load $q$ causing deformation of the membrane can be related to the Cauchy stress tensor by an equilibrium equation

$$\nabla_s \cdot T + q = 0,$$ \hspace{1cm} (2.11)

with $\nabla_s$, the surface divergence operator. In curvilinear coordinates, the load vector is written as $q = q^\beta a_\beta + q^n n$. The force balance in equation (2.11) is further decomposed into tangential and normal components,

$$\frac{\partial T^{\alpha \beta}}{\partial \xi^\alpha} + \Gamma^\alpha_{\alpha \lambda} T^{\lambda \beta} + \Gamma^\beta_{\alpha \lambda} T^{\alpha \lambda} + q^\beta = 0, \quad \beta = 1, 2$$ \hspace{1cm} (2.12)

$$T^{\alpha \beta} b_{\alpha \beta} + q^n = 0,$$

where $\Gamma^\alpha_{\alpha \lambda}$ and $\Gamma^\beta_{\alpha \lambda}$ are the Christoffel symbols defined as

$$\Gamma^\beta_{\alpha \lambda} = a_{\alpha \lambda \beta} \cdot a_\beta.$$ \hspace{1cm} (2.13)

### 2.2.3. Constitutive equations

As mentioned in section 2.2.2, The Cauchy stress is derived from the strain energy. The strain energy depends both on membrane material and its deformation. The way which the strain energy is related to the membrane deformation is called constitutive law and the corresponding equation is constitutive equation. The constitutive equation depends on the membrane material. In the following, three types of constitutive equations will be introduced.

#### 2.2.3.1. Linear Hookean law

For a simple Hookean material the elastic force has linear dependence on the deformation. In the limit of small deformations, all other constitutive laws reduce to the Hookean model (Pozrikidis 2010). The strain energy for a Hookean membrane is defined as (Pozrikidis 2010)

$$W_s^H = G_s \left[ tr(e^2) + \frac{\nu_s}{1 - \nu_s} (tr e)^2 \right],$$ \hspace{1cm} (2.14)

where $e$ is the two-dimensional linearised Green-Lagrange strain tensor, $G_s$ the surface shear modulus and $\nu_s$ the surface Poisson ratio. The area dilation modulus $K_s$ is defined as

$$K_s^H = G_s \frac{1 + \nu_s}{1 - \nu_s},$$ \hspace{1cm} (2.15)
showing that in order to have area-incompressible membrane the Poisson ratio should be equal to 1.

2.2.3.2. Neo-Hookean law

For the materials so called hyperelastic materials which may exhibit large deformations, the elastic force doesn’t have linear dependence on the deformation. There are different constitutive laws for hyperelastic materials. In this thesis the neo-Hookean law (Rivlin 1948) is considered for all cases reads as

\[ W_{NH}^{s} = \frac{G_{NH}^{s}}{2} \left[ \lambda_{1}^{2} + \lambda_{2}^{2} - 3 + \frac{1}{\lambda_{1} \lambda_{2}} \right]. \] (2.16)

The area dilation modulus is shown to be \( K_{NH}^{s} = 3G_{NH}^{s} \).

2.2.3.3. Skalak law

Another constitutive law which is appropriate for simulation of blood cells is Skalak law (Skalak & Branemark 1969) with the constitutive equation

\[ W_{SK}^{s} = \frac{G_{SK}^{s}}{4} \left[ (\lambda_{1}^{4} + \lambda_{2}^{4} - 2\lambda_{1}^{2} - 2\lambda_{2}^{2} + 2) + C(\lambda_{1}^{2}\lambda_{2}^{2} - 1)^{2} \right], \] (2.17)

where \( C \) is a constant determining area dilation. The area dilation modulus is \( K_{SK}^{s} = G_{SK}^{s}(1 + 2C) \). For the cases with \( C \gg 1 \) the membrane becomes area-incompressible like red blood cells (Pozrikidis 2010) but this law is capable of modeling the membranes which their shear and area dilation moduli are the same order of magnitude like alginate membranes (Pozrikidis 2010; Carin et al. 2003).

As mentioned before, all constitutive laws should reduce to linear Hookean law. The equivalence between the laws requires

\[ G_{s} = G_{NH}^{s}, \quad \nu_{s} = \frac{1}{2} \] (2.18)

for neo-Hookean model and

\[ G_{s} = G_{SK}^{s}, \quad \nu_{s} = \frac{C}{1 + C} \] (2.19)

for Skalak model. It is important to mention that the neo-Hookean material is strain-softening while the Skalak material is strain-hardening (Pozrikidis 2010; Barthes-Biesel et al. 2002)

2.2.4. Consideration of membrane bending stiffness

In the case of noninfinitesimal membrane thickness or a preferred configuration of an interfacial molecular network, bending moments accompanied by transverse shear tensions play an important role on cell deformation (Pozrikidis 2001).
Bending stiffness can be incorporated into the model using a linear isotropic model for the bending moment (Pozrikidis 2010, 2001):

\[ M_\beta = -E_B (b_\beta^a - B_\beta^a), \]

where \( E_B \) is the bending modulus and \( b_\beta^a = a_{a,\beta} \cdot n \) is the second fundamental form of the surface (\( B_\beta^a \) corresponds to that of the reference configuration). According to the local torque balance, including bending moments on the membrane, the transverse shear vector \( \mathbf{Q} \) and in-plane stress tensor \( \mathbf{T} \) can be obtained

\[ M_\alpha^\beta = Q_\beta^\alpha = 0, \]

\[ \varepsilon_\alpha^\beta \left( T_\alpha^\beta - b_\gamma^\beta M_\gamma^\beta \right) = 0, \]

where \( \varepsilon_\alpha^\beta \) represents the covariant derivative and \( \varepsilon \) is the two-dimensional Levi-Civita tensor. The left hand side of equation (2.21) identifies the antisymmetric part of the in-plane stress tensor, which is always zero as proved in Zhao et al. (2010). Including the transverse shear stress \( Q \), the local stress equilibrium, including bending finally gives

\[ \partial T_\alpha^\beta / \partial x^\alpha + \Gamma_\alpha^\lambda^\beta T_\lambda^\alpha + \Gamma_\alpha^\beta^\gamma T_\alpha^\gamma - b_\alpha^\beta Q^\alpha + q^\beta = 0, \quad \beta = 1, 2 \]

\[ T_\alpha^\beta b_\alpha^\beta - Q_\alpha^\alpha + q^n = 0. \]

Equations 2.3 to 2.22 can be made non-dimensional by choosing a reference velocity \( U \), a reference length \( L \) and a reference density \( \rho \). All the equations remain in the same form as their dimensional form. Only in equations 2.14 to 2.17 the shear modulus \( G_s \) will be replaced with inverse Weber number \( \left( W e^{-1} = \frac{G_s}{\rho U^2 L} \right) \).

2.3. Dynamics of flexible slender bodies

In this section dynamics of slender bodies will be reviewed. Slender bodies can be defined as objects with their length much larger than other dimensions. Slender bodies are usually called Fibres/Filaments. The cross section of slender bodies can have different shapes with varying surface area but in this thesis the cross section is assumed to be circular with constant surface area.

2.3.1. Models for flexible slender bodies

There are different ways for modelling of flexible slender bodies. One common way is to consider the fibres as interconnected rigid objects. In this model the flexible fibre is composed of several rigid objects connected to each other by joints. The rigid objects can extend, bend and twist around the joints. The Newton’s second law is directly solved for each joint to obtain its new configuration under external forces. This model has been used by (Yamamoto & Matsuoka 1993) for fibres as interconnected spheres and by (Wu & Aidun 2010a; Lindström & Uesaka 2008) for fibres as interconnected rigid rods.
Governing equations

There is another method for the simulation of flexible fibres by assuming them as a continuous flexible object. By consideration of their slenderness, the equation of elasticity will reduce to mono-dimensional equations which can be used for definition of their dynamics. This model has been used by (Huang et al. 2007; Pinelli et al. 2016; Rosti et al. 2018a). In this thesis the continuous approach has been considered and the related equations will be introduced in the following sections.

2.3.2. Euler Bernoulli equations

By assumption of the filaments as continuously flexible one-dimensional objects, the well known Euler-Bernoulli equations can be derived for motion of the filaments suspended in a fluid read as

\[
\rho \frac{\partial^2 X}{\partial t^2} = \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) - \gamma^* \frac{\partial^4 X}{\partial s^4} + \rho g - F + F^c, \tag{2.23}
\]

where \( \rho = (\rho_f - \rho) A_f \) is the linear density difference, \( \rho_f \) the filaments linear density and \( A_f \) their cross-section. \( X \) is the filament position, \( s \) the curvilinear coordinate along the filaments, \( T \) the tension, \( \gamma^* = EI \) the bending rigidity with \( E \) the elastic modulus of the filament and \( I \) the second moment of area around filament axis, \( g \) the gravitational acceleration, \( F \) the hydrodynamic force per unit length, and \( F^c \) other linear forces. In general the filaments can both extend and bend but usually their extensional resistance is very large and they can be assumed as inextensible but can only bend (Huang et al. 2007; Pinelli et al. 2016). The constraint of inextensibility reads as

\[
\frac{\partial X}{\partial s} \frac{\partial X}{\partial s} = 1, \tag{2.24}
\]

Equations 2.23 and 2.24 can be made non-dimensional by choosing filament length as reference length, a reference velocity \( U \), and \( \rho_l \) as reference density. Equation 2.24 remains unchanged and equation 2.23 gets its non-dimensional form

\[
\frac{\partial^2 X}{\partial t^2} = \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) - \gamma^* \frac{\partial^4 X}{\partial s^4} + Fr g - F + F^c, \tag{2.25}
\]

where \( \gamma = \frac{\gamma^* L^2}{\rho_s} \) is the non-dimensional bending stiffness, \( Fr = \frac{gL}{U^2} \) the Froude number and \( g = |\mathbf{g}| \). In the case of neutrally buoyant filaments \( \rho_l = 0 \) and cannot be used as reference density hence the linear density of the surrounding fluid \( \rho A_f \) is used as reference density where \( A_f \) is cross sectional area of the filaments. In this case the equation 2.23 in non-dimensional form reads as

\[
0 = \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) - \gamma^* \frac{\partial^4 X}{\partial s^4} - F + F^c, \tag{2.26}
\]
2.3. Dynamics of flexible slender bodies

where \( \gamma = \frac{\alpha^2}{\rho A_f^2 L_t} \) is the non-dimensional bending stiffness. Since (LHS) of equation 2.26 is zero, special numerical treatment is necessary for the numerical solution which will be discussed in the next chapter therefore it is better to write equation 2.26 in the form

\[
\frac{\partial^2 X}{\partial t^2} = \frac{\partial^2 X_f}{\partial t^2} + \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) - \gamma \frac{\partial^4 X}{\partial s^4} = F + F^c ,
\]

where the first term on the RHS is the fluid particle acceleration which is identical to the (LHS) for neutrally buoyant filaments.

There can be three types of boundary conditions at the two ends of the filaments. If the end is free the boundary conditions are zero force, moment and tension

\[
\frac{\partial^2 X}{\partial s^2} = 0, \quad \frac{\partial^3 X}{\partial s^3} = 0, \quad T = 0. \quad (2.28)
\]

When one end is fixed at a point, two types of boundary conditions are possible. One is *hinged* boundary condition with zero moment

\[
X = X_0, \quad \frac{\partial^2 X}{\partial s^2} = 0. \quad \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) \bigg|_{X=X_0} = -Fr \frac{g}{g} + F \quad (2.29)
\]

The other is *clamped* or build-in supported boundary condition

\[
X = X_0, \quad \frac{\partial X}{\partial s} = n_c \quad \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) \bigg|_{X=X_0} = -Fr \frac{g}{g} + \gamma \frac{\partial^4 X}{\partial s^4} + F, \quad (2.30)
\]

where \( n_c \) is a unit vector normal to the surface which the filaments are clamped. Note that for the neutrally buoyant filaments the gravitational term is zero.

Equations 2.25 and 2.24 have to be solved together for the position and tension. In order to avoid non-linearity in the numerical solution, (Huang et al. 2007) derived an equation for the tension by taking derivative of equation 2.25 and inner multiplication by \( \frac{\partial X}{\partial s} \) which reads as

\[
\frac{\partial X}{\partial s} \cdot \frac{\partial^2}{\partial s^2} \left( T \frac{\partial X}{\partial s} \right) = \frac{1}{2} \frac{\partial^2}{\partial t^2} \left( \frac{\partial X}{\partial s} \cdot \frac{\partial X}{\partial s} \right) - \frac{\partial^2 X}{\partial t \partial s} \frac{\partial X}{\partial t \partial s} - \frac{\partial^2 X}{\partial s^2} \frac{\partial X}{\partial s} \left( F^a + F^b + F^c - F \right), \quad (2.31)
\]

where \( F^a = \frac{\partial^2 X}{\partial t^2} \) is the acceleration of the fluid particle at the filament location for neutrally buoyant filaments (it is zero for inertial filaments) and \( F^b = -\gamma \frac{\partial^4 X}{\partial s^4} \) the bending force. Note that the first term in (RHS) of Equation 2.31 is theoretically zero but it should be kept for reducing numerical errors.
(Huang et al. 2007). Equation 2.31 is solved in combination with Euler-Bernoulli equations to get position and tension for the filaments.
Chapter 3

Numerical methods

As discussed in the previous chapter, the problems are governed by the non-linear sets of equations which should be solved numerically with efficient methods. Since the objects interact with the fluid flow, motion of the fluid and the solid should be coupled properly. Furthermore, the short range interactions between the objects should be considered which might be computationally expensive. In this chapter the numerical methods for solution of the equations are discussed followed by introducing Immersed boundary method for coupling between fluid and solid motion and description of computational procedure. Finally the interactions between the different objects are discussed with an efficient numerical treatment.

3.1. Numerical solution of the Navier-Stokes equations

3.1.1. Choice of schemes and discretisation

The fluid equations are solved with finite volume method (Versteeg & Malalasekera 2007). All equations are discretised on a uniform staggered grid to avoid checkerboard solution. The time integration relies on the classical projection method (Chorin 1968). This method is a three-step procedure: first, a predicted velocity field \( \hat{u} \) is computed as

\[
\frac{\hat{u} - u^n}{\Delta t} = \text{RHS}(u, p),
\]

(3.1)

where \( \text{RHS}(u, p) \) is the right-hand side of the discretised Navier-Stokes equations and excluding any body forces and \( \Delta t \) the time step. This predicted velocity is used for computation of fluid-solid interaction forces for the filaments which will be discussed later. Then any body forces can be added to the right hand side of the Navier-Stokes equations

\[
\tilde{u} = \hat{u} + f\Delta t,
\]

(3.2)

For the second second step, the pressure correction field is obtained as the solution to the following Poisson equation

\[
\nabla^2 p' = -\frac{1}{\Delta t} \nabla \cdot \tilde{u}.
\]

(3.3)
Equation 3.3 is solved with fast Fourier transform (FFT) (Brigham & Brigham 1988). Finally, the corrected velocity field $u^{n+1}$ is obtained as

$$u^{n+1} = \tilde{u} - \Delta t \nabla p'.$$

(3.4)

Central difference scheme is used for spatial discretisation of convective and diffusive terms and Adams-Bashforth scheme is used for temporal integration of convective terms.

### 3.1.2. Temporal integration of diffusive terms

As viscosity contrast is allowed between the fluid inside and outside of the capsules, the classical Fast Fourier spectral method cannot be readily used to evaluate the diffusive term $D u = \nabla \cdot (\mu [\nabla u + \nabla u^T])$. Indeed, the viscosity field being a function of space, this operator cannot be reduced to a constant coefficient Laplace operator. However, (Dodd & Ferrante 2014) have recently introduced a splitting operator technique able to overcome this drawback. Though it has initially been derived for the pressure Poisson equation, this splitting approach can easily be extended to the Helmholtz equation resulting from an implicit (or semi-implicit) integration of the diffusive terms,

$$(I - \Delta t D)u^{n+1} = \text{RHS}^n$$

(3.5)

where $I$ is the identify matrix, and $\text{RHS}^n$ the discretized right-hand side including the non-linear advection terms. Given the viscosity field $\mu^*(x) = 1 + \mu'(x)$,

(3.6)

where 1 is the constant part and $\mu'(x)$ the space-varying component, the diffusive term $D u$ can be re-written as

$$D u = \frac{1}{Re} \nabla^2 u + \frac{1}{Re} \nabla \cdot (\mu'(x) [\nabla u + \nabla u^T]).$$

(3.7)

The constant coefficients operator $D_1$ can then be treated implicitly while the variable coefficients operator $D_2$ is treated explicitly. The resulting Helmholtz equation then reads

$$(I - \Delta t D_1)u^{n+1} = \text{RHS}^n + \Delta t D_2 u^n.$$

(3.8)

Since $D_1$ is now a constant coefficient Laplace operator, equation (3.8) can be solved using a classical Helmholtz solver based on Fast Fourier transforms. Note that a similar Fast Fourier-based solver is used to solve the Poisson equation (3.3) for the pressure. This method enables us to choose larger time steps at lower Reynolds numbers compared to other explicit methods such as Runge-Kutta method (Breugem 2012) and computationally more efficient compared to fully implicit methods.
3.2. Numerical solution of the membrane equations

The membrane shape has been modeled as linear piece-wise functions on triangular meshes by (Pozrikidis 1995), (Ramamujan and Pozrikidis 1998) and (Li & Sarkar 2008) among others. The finite element method has also been employed by (Walter et al. 2010) for its generality and versatility. Another highly accurate method is the global spectral method. Fourier spectral interpolation and spherical harmonics have been used for two-dimensional (Freund 2007) and three-dimensional simulations (Kessler et al. 2008; Zhao et al. 2010). Here, the approach of (Zhao et al. 2010) is followed, previously implemented in (Zhu & Brandt 2015; Zhu et al. 2014, 2015; Rorai et al. 2015). This is briefly outlined below.

The capsule surface is mapped onto the surface of the unit reference sphere $S^2$, using the angles in spherical coordinates $(\theta, \phi)$ for the parametrization. The parameter space $\{(\theta, \phi) \mid 0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi\}$ is discretized by a quadrilateral grid using Gauss-Legendre (GL) quadrature intervals in $\theta$ and uniform spacing in the $\phi$ direction. All other surface quantities are stored on the same mesh, i.e. the grid is co-located. The surface coordinates $x(\theta, \phi)$ are expressed by a truncated series of spherical harmonic functions,

$$x(\theta, \phi) = \sum_{n=0}^{N_{SH}-1} \sum_{m=0}^{n} P_n^m(\cos \theta)(a_{nm} \cos m\phi + b_{nm} \sin m\phi),$$

yielding $N_{SH}^2$ spherical harmonic modes. The corresponding normalized Legendre polynomials are given by

$$P_n^m(x) = \frac{1}{2^n n!} \sqrt{\frac{(2n+1)(n-m)!}{2(n+m)!}} (1-x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2 - 1)^n.$$  

The SPHEREPACK library (Adams & Swarztrauber 1999; Swarztrauber & Spotz 2000) is employed for the forward and backward transformations. To deal with aliasing errors arising due to the nonlinearities in the membrane equations (products, roots and inverse operations needed to calculate the geometric quantities), an approximate de-aliasing is performed by performing the nonlinear operations on $M_{SH} > N_{SH}$ points and filtering the result back to $N_{SH}$ points. A detailed discussion on this issue is provided in (Freund & Zhao 2010).

Considering different viscosity inside and outside the cell, a space and time dependent viscosity field is defined by an indicator function $I(x, t)$ related to the membrane location,

$$\mu^*(x) = (1 - I(x)) + I(x) \lambda,$$

where $\lambda$ is the viscosity ratio. Here the definition of (Unverdi & Tryggvason 1992) for the indicator function is followed as the solution to the following Poisson equation

$$\nabla^2 I = \nabla \cdot G,$$
where the Green’s function $G = \int \delta(X - x)n \, ds$, and $n$ is the unit normal vector to the cell surface. Using the smooth Dirac delta function introduced below in the computation of $G$ makes the indicator function smoother near the boundary (Kim et al. 2015). Such indicator function is similar to the regularised Heaviside function used in the levelset framework.

3.3. Numerical solution of the filament equations

3.3.1. Two step approach for the Euler-Bernoulli equations

As mentioned in the previous chapter, the Euler-Bernoulli equations should be solved together with the tension equation to get position of the filaments. The tension equation is coupled with the Euler-Bernoulli equations and solving them at the same time requires solving non-linear sets of equations leading to high computational time. (Huang et al. 2007) proposed an efficient two-step method to avoid those complications. In this method all equations are discretised with finite difference method on a staggered grid then a predicted value for $X$ is computed based on the previous time steps

$$X^* = 2X^n - X^{n-1}, \quad (3.13)$$

where $X^n$ and $X^{n-1}$ are the positions in current and previous time steps respectively. The value of $X^*$ is then used to solve equation 2.31 for tension. The constraint of inextensibility should be imposed in the tension equation. One way is to set the first term in (RHS) of equation 2.31 to zero but by dropping that term the numerical errors introduced in the solution will not be corrected (Huang et al. 2007). The proper way is to impose the inextensibility condition in the discretised form of the mentioned term. By assuming $A = \frac{\partial X}{\partial s} \cdot \frac{\partial X}{\partial s}$, its second derivative in discretised form reads as

$$\frac{\partial^2 A}{\partial t^2} = \frac{A^{n-1} - 2A^n + A^{n+1}}{\Delta t^2}. \quad (3.14)$$

Now $A^{n+1}$ can be set to 1 as inextensibility condition

$$\frac{\partial^2 A}{\partial t^2} = \frac{A^{n-1} - 2A^n + 1}{\Delta t^2}. \quad (3.15)$$

By doing this, the numerical errors introduced in the previous time steps will be penalised (Huang et al. 2007). Finally a set of algebraic equations should be solved for the tension

$$a_{wi}T_{i-1} + a_{pi}T_i + a_{ei}T_{i+1} = S_{Ti} \quad (3.16)$$

where $S_{Ti}$ denotes the discretised form of the source terms. The set of equations form a tridiagonal matrix of coefficients which can be solved by Thomas algorithm. By having the tension in can be substituted in the discretised form of the Euler-Bernoulli equations and solve them for $X^{n+1}$. 


3.3.2. Inertial filaments

For inertial filaments equation 2.25 is discretised as

\[ \frac{X_{i}^{n+1} - 2X_{i}^{n} + X_{i}^{n-1}}{\Delta t^2} = RHS_{i}^{n+1} - F_{i}^{n}. \] (3.17)

Since the tension and bending terms are treated implicitly, there will be a set of equations in the form

\[ b_{wwi}X_{i-2}^{n+1} + b_{wi}X_{i-1}^{n+1} + b_{pi}X_{i}^{n+1} + b_{ti}X_{i+1}^{n+1} + b_{eii}X_{i+2}^{n+1} = S_{i}^{n}. \] (3.18)

forming a pentadiagonal matrix of coefficients which can be solved with Gaussian elimination method.

3.3.3. Neutrally buoyant filaments

When the filaments are neutrally buoyant, i.e. there is no density difference between the filaments and their surrounding fluid, the coefficient \( b_{pi} \) in equation 3.18 goes to zero and causes numerical issues for solving the equations. In order to avoid this problem, the Euler-Bernoulli equation explained in equation 2.27 is used and the fluid particle acceleration is treated as source term at step \( n \) (Pinelli et al. 2016)

\[ \frac{X_{i}^{n+1} - 2X_{i}^{n} + X_{i}^{n-1}}{\Delta t^2} = \frac{X_{i}^{n} - 2X_{i}^{n-1} + X_{i}^{n-2}}{\Delta t^2} + RHS_{i}^{n+1} - F_{i}^{n}. \] (3.19)

This kind of discretisation makes non-zero coefficients and Gaussian elimination is applicable to solve for \( X_{i}^{n+1} \).

3.4. Immersed boundary method

To couple the fluid and the solid motion, the immersed boundary method (IBM) is used which was first proposed by (Peskin 1972) to study blood flow inside heart. The main feature of the IBM is that the numerical grid does not need to conform to the geometry of the object, which is instead represented by a volume force distribution \( f \) that mimics the effect of the object on the fluid, typically no-slip and no-penetration at a solid surface. In this approach, two sets of grid points are needed: a fixed Eulerian grid for the fluid flow and a moving Lagrangian grid for the flowing deformable structures (see Fig.3.1). The volume force arising from the interaction of the deformable structure and flow is obtained by the convolution onto the Eulerian mesh of the singular forces estimated on the Lagrangian nodes; these are computed using the fluid velocity interpolated at the location of the Lagrangian points. This interpolation/spreading is usually performed by means of regularized delta functions, in our case the one proposed by Roma et al. (1999).

\[ \delta(X - X_{0}) = \delta(x - x_{0})\delta(y - y_{0})\delta(z - z_{0}), \] (3.20)
3. Numerical methods

Figure 3.1: Schematic of the Eulerian and Lagrangian grids

where

\[ \delta(x - x_0) = \frac{1}{h} \phi(x - x_0) \frac{h}{h}, \]  

(3.21)

where \( h \) is grid spacing and the function \( \phi \) is defined as

\[
\phi(r) = \begin{cases} 
\frac{1}{3}(5 - 3|r| - \sqrt{-3(1 - |r|)^2 + 1}), & 0.5 \leq |r| \leq 1.5. \\
\frac{1}{3}(1 + \sqrt{-3r^2 + 1}), & |r| \leq 0.5. \\
0, & \text{otherwise}, 
\end{cases}
\]  

(3.22)

where \( r \) is any component of \( \frac{X - X_0}{h} \).

3.4.1. Immersed boundary method for capsules

In general the immersed boundary method for capsules can be summarised as follows: At each time step, the fluid velocity defined on the Eulerian mesh is first interpolated onto the Lagrangian mesh,

\[ U_{ib}(X, t) = \int_{\Omega} u(x, t) \delta(X - x) d\Omega, \]  

(3.23)

where \( x \) and \( X \) are the Eulerian and Lagrangian coordinates and \( \delta \) is the smooth Dirac delta function (Roma et al. 1999). The elastic force per area \( q \) and surface normal vectors \( n \) are then computed from the membrane equations described above. As next step, the normal vectors are used to compute the indicator function \( I(x, t) \) on the Eulerian mesh. The force is then spread to Eulerian mesh and added to the momentum equations as
\[ f(x, t) = \int -q(X, t) \delta(x-X) ds. \]  

(3.24)

Thereafter, the positions of the Lagrangian points are updated according to

\[ X^{n+1} = X^n + \int_0^t U_{ib} dt. \]  

(3.25)

Note that equation (3.25) assumes an over-damped regime, i.e. the Lagrangian points go to their equilibrium position immediately after the elastic force is applied. Finally, the fluid flow is solved in the Eulerian framework as explained in section 3.1. A flowchart for computational procedure at each iteration is depicted in figure 3.2(a).

The method described above is not particularly efficient when the Reynolds number increases since it requires small time steps, which increases the computational time. At moderate and high Reynolds numbers for single capsules, a modification of the method by (Kim et al. 2015), is employed to be consistent with the assumption of inertialess membrane. In this approach, in addition to the Lagrangian coordinates \( X \), the additional immersed boundary points \( X_{ib} \) are introduced whose motion is governed by equation (3.25). Since the total force exerted on each element on the membrane surface is equal to the difference between its acceleration and the acceleration of fluid element at the same location, the motion of the real Lagrangian points is governed by

\[
\rho_{os} \frac{\partial^2 X}{\partial t^2} = \rho_{os} \frac{\partial^2 X_{ib}}{\partial t^2} + F_e - F_{FSI} + F_A,
\]  

(3.26)

where \( \rho_{os} \) is the surface density of the base fluid. The two sets of Lagrangian points, \( X \) and \( X_{ib} \), are connected to each other by a spring and damper, i.e. a fluid-solid interaction force \( F_{FSI} \) computed using the following feedback law

\[
F_{FSI} = -\kappa \left[(X_{ib} - X) + \Delta t (U_{ib} - U)\right].
\]  

(3.27)

The procedure for this modified method is as follows. At each time step, first \( U_{ib} \) and the fluid-solid interaction force \( F_{FSI} \) are computed from equation (3.27). The indicator function \( I(x, t) \) is then computed to identify the interior of the cell and impose viscosity contrasts, and the momentum equation solved to obtain the flow velocity \( u \). Finally, the positions of the Lagrangian points \( X \) are updated using equation (3.26). The non-dimensional form of equation (3.26) can be written as,

\[
d^* \frac{\partial^2 X}{\partial t^2} = d^* \frac{\partial^2 X_{ib}}{\partial t^2} + F_e - F_{FSI} + F_A,
\]  

(3.28)

where \( d^* = d/R \) is ratio between the membrane thickness and initial radius of the cell, assumed in the present study to be \( d^* = 0.01 \). In the above, \( F_A \) is the penalty force used to enforce volume conservation which will be discussed later.
3. Numerical methods

Initialise flow field and capsule positions
Interpolate velocity onto Lagrangian points
Compute elastic force and spread it onto Eulerian grid
 Solve Navier-Stokes equations for the fluid phase
Compute indicator function
Update position of Lagrangian points
Compute collision forces

(a)

Initialise flow field and filament positions
Interpolate velocity onto Lagrangian points
Compute Lagrangian force
Solve Navier-stokes equations for the fluid phase
Compute lubrication and collision forces
Update position of Lagrangian points
Spread Lagrangian force onto Eulerian grid

(b)

Figure 3.2: A flowchart of the computational procedure used for suspended (a) capsules and (b) filaments

This method is not efficient for multiple capsules where there are capsule-capsule interactions.

3.4.1.1. volume correction

However adding the elastic force to the flow, reduces flow motion across the membrane but flow penetration is not eliminated completely at the level of discretisation and volume of fluid that is enclosed by capsule membrane changes Pranay et al. (2010). There are different ways to enforce the volume conservation.
3.4. Immersed boundary method

One is adding a force to the capsule equation (if equation 3.28 is used) or to the elastic force $q$ (if the original immersed boundary method by Peskin 1972 is used). This force can be defined as (Kim et al. 2015)

$$
F_A = \Delta p \cdot \eta(\theta, \phi) \cdot e_n,
$$

$$
\Delta p = \frac{1}{\beta} \left( 1 - \frac{V}{V_0} \right) + \frac{1}{\beta} \int_0^t \left( 1 - \frac{V}{V_0} \right) dt'.
$$

(3.29)

Here $\Delta p$ represents the pressure generated by the volume change, $\eta(\theta, \phi)$ is the surface area of each element and $e_n$ the local unit normal vector and $\beta$ a constant value. In some cases, this method can cause large oscillations in the capsule volume and numerical instabilities.

Another more efficient method is proposed by (Pranay et al. 2010) suggesting to add a displacement correction to the Lagrangian points which can be done every time step or every $n > 1$ time steps. The displacement correction is defined as

$$
z = -3(V - V_0) A n,
$$

(3.30)

where $V$ and $V_0$ are instantaneous and initial volumes respectively, $A$ capsule surface area and $n$ is a unit normal to capsule surface area.

3.4.2. Immersed boundary method for filaments

The solution procedure for the filaments suspended in fluid flow can be summarised as follows for every time step. First the predicted fluid velocity is interpolated on the Lagrangian points

$$
U_{ib} = \int_V \hat{u} \delta (X - x) dV,
$$

(3.31)

Then the fluid-solid interaction force is computed based on the velocity difference between the fluid and solid at every Lagrangian point

$$
F = \frac{U - U_{ib}}{\Delta t},
$$

(3.32)

where $U_{ib}$ is the interpolated velocity on the Lagrangian points defining the filaments, $U$ the velocity of the Lagrangian points, and $\Delta t$ the time step. Note that in the case of inertial filaments, using the factor $\frac{1}{\Delta t}$ in equation 3.32 may cause numerical instabilities since $U - U_{ib}$ is larger compared to the neutrally buoyant filaments therefore it can be replaced with $\beta < \frac{1}{\Delta t}$ to ensure a stable solution. The force is then spread to the Eulerian grid as

$$
f = \hat{\rho} \int_{L_f} F \delta (X - x) ds,
$$

(3.33)

for inertial filaments and
\[ f = \frac{\pi}{4} r_P^2 \int_{L_f} F \delta (X - x) \, ds, \quad (3.34) \]

for neutrally buoyant filaments. In the equations above \( \tilde{\rho} = \frac{\rho}{\hat{\rho} r_P^2} \) and \( r_P = d/L \) is the filament aspect ratio defined as the ratio between filament diameter to the filament length. The factors in front of the integrals arise from choosing different scales for Eulerian and Lagrangian forces. In the next step the filament equations are solved to obtain new position of the filaments. Finally the Navier-Stokes equations are solved to update the flow field. A flowchart of the computational procedure is sketched in figure 3.2(b).

3.4.2.1. Consideration of shear moments

To correctly obtain the filament rotation due to shear moments within our one-dimensional model, four ghost points are considered at a small radial distance (\( \approx \Delta r = \frac{d}{4} \)) around each of the Lagrangian points used to compute the hydrodynamic forces which is described in details in the next section. These 4 points are then used to evaluate the moment exerted by the fluid on the filament

\[ M = r \times F, \quad (3.35) \]

where \( r \) is the position vector connecting the main points on the filaments to the ghost points. Note that, the moment at the two ends of the filaments should be set to \( M = -r \times F \) in order to satisfy the zero moment condition. The effect of the shear moment is then introduced in the Euler-Bernoulli equation (2.25 or 2.27) to provide the correct rotation

\[ \frac{\partial^2 X}{\partial t^2} = \frac{\partial^2 X_l}{\partial t^2} + \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right) - \gamma \frac{\partial^4 X}{\partial s^4} - \frac{\partial}{\partial s} D (M) - F + F^c, \quad (3.36) \]

where \( D \) is defined as

\[ D (M_i) = \sum_{i \neq j} M_j. \quad (3.37) \]

This extra force can be added to the hydrodynamic forces \( F \) by applying the same numerical scheme.

3.4.3. Immersed boundary method for rigid nucleus

In the case of nucleated capsules, the nucleus may be considered as rigid particles. For rigid particles the immersed boundary implementation by Breugem (Breugem 2012) is followed, which has been widely used in the framework of rigid particles, see e.g. (Lashgari et al. 2014). In this method, a moving Lagrangian mesh is adopted to impose no-slip and no-penetration on the surface of a rigid object. The numerical procedure is as follows: first, the prediction velocity \( \hat{u} \) is computed from equation 3.1 neglecting the fluid-solid interaction forces. This fluid velocity is then interpolated onto the Lagrangian mesh \( U_{ib} \) and the
3.5. Short range interactions between deformable objects

Fluid-solid interaction force computed, based on the difference between the fluid and the solid body velocity at each Lagrangian point,

\[ F_{FSI} = \frac{U_P - U_{ib}}{\Delta t}. \] (3.38)

This force is spread to the Eulerian grid and the second prediction velocity \( \tilde{u} \) obtained by solving the Navier-Stokes equations with the fluid-solid interaction force. The divergence-free constraint is then imposed on the velocity field by solving the pressure Poisson equation and correcting the velocity field appropriately. Finally, the total force and torque on each particle is computed, and the translational and rotational velocities of the particle obtained by integrating the Newton-Euler equations. Readers are also referred to (Uhlmann 2005) for further details.

3.5. Short range interactions between deformable objects

In a suspension, there might be interactions between the suspended bodies. The long range interactions are usually well resolved with the immersed boundary method while the capturing short range interactions needs fine enough Eulerian mesh which increases computational cost. One can use the models proposed for short range interactions to save in the computational time. In this section the models for capsules and filaments will be explained.

3.5.1. The approach for the interaction of deformable objects

To be able to compute the interaction forces, the nearby Lagrangian points should be distinguished whose distance is shorter than a cutoff length. For this aim, one can check every Lagrangian point against other Lagrangian points in the suspension which is computationally expensive. (Berg 2018) has used another method by generating a grid which is typically larger than the Eulerian grid. The grid size should be larger than the cutoff distance which is the distance above that the short range interactions are negligible. Thereafter the Lagrangian points are spread among the cells and the points in a cell is only checked against the points in its neighbour cells. By doing this, the computational time spent for the interaction of the bodies is reduce substantially.

3.5.2. Interaction between capsules

In the capsule suspensions, it is important to avoid overlapping. In order to avoid capsule-capule, capsule-particle, and capsule-wall overlapping specially at higher Reynolds numbers, a repulsive force in the form of Morse potential (Liu et al. 2004) is used if distance between two surfaces becomes less than length of two grid points. The general form of the potential is as follows

\[ \phi = D_e \left[ e^{-2a(r_L - r_c)} - 2e^{-a(r_L - r_c)} \right], \] (3.39)

where \( D_e \) is the interaction strength, \( a \) a geometrical scaling factor, \( r_L \) the distance between two surfaces and \( r_c \) the zero cut-off force distance which is
two grid cells here. The repulsive force is derivative of the potential \( F = -\frac{\partial \phi}{\partial r} d \),
where \( d \) is a unit vector joining two surfaces. The contact force at each
Lagrangian point should be spread to flow as equation 3.24.

3.5.3. Interaction between filaments

In order to capture short range interactions between filaments whose distance is
of the order of the numerical mesh size, the lubrication correction proposed by
Lindström & Uesaka (2008) is used. The model is based on the force between
two infinite cylinders as obtained in two cases: when the two cylinders are
parallel and when they are not. For the non-parallel case, Yamane et al. (1994)
derived a first order approximation of the lubrication force,

\[
F_l^1 = \frac{-12}{R \sin \alpha} \dot{h},
\]

where \( h \) denotes the shortest distance between the cylinders and \( \alpha \) the contact
angle. To use this in the Euler-Bernoulli equations governing the filament
dynamics, the force is converted to a force per unit length, i.e., it is divided by
\( \Delta s \) the Lagrangian grid spacing. Equation (3.40) cannot be used for lubrication
between parallel cylinders since \( F_l^1 \to \infty \) as \( \alpha \to 0 \); in this case, a first order
approximation of the force per unit length was derived by Kromkamp et al.
(2005):

\[
F_l^2 = \frac{-4}{\pi R \sin \alpha} \left( A_0 + A_1 \frac{h}{r} \right) \left( \frac{h}{r} \right)^{-3/2} \dot{h},
\]

\( A_0 = 3\pi \sqrt{2}/8, ~ A_1 = 207\pi \sqrt{2}/160, \)

where \( r \) is the radius of the cylinders \( r = d/2 \). Based on equations (3.40)
and (3.41), the following approximation of the lubrication force for two finite
cylinders can be derived (Lindström & Uesaka 2008):

\[
F_l^i = \min(F_l^1/s, F_l^2).
\]

Finally, the lubrication force between walls and filaments is found by considering
the walls as cylinders of infinite radius and assuming the contact area to be
that between two cylinders with equivalent radius, i.e., \( r_{eq} = r/2 \) (Lindström
& Uesaka 2008). In our simulations, when the shortest distance between two
Lagrangian point becomes lower than \( d/4 \), the lubrication correction \( F_l^{ic} = F_l^i - F_l^0 \)
is imposed, where \( F_l^0 \) is the lubrication force at a distance of \( d/4 \). Finally, the total lubrication force acting on the \( i \)-th element is obtained as:

\[
F_l^{ic} = \sum_{j \neq i}^{n_l} F_l^{ic}_{ij},
\]

where \( n_l \) is the number of Lagrangian points closer than the activation distance
\( d/4 \) to the \( i \)-th point.
3.6 Notes on the implementation, parallelisation and computational requirements

To avoid contacts and overlap between filaments and with the walls, a repulsive force is also implemented. This has the form of a Morse potential (Liu et al. 2004) which is explained in details in section 3.5.2. The total interaction force between the filaments are summation of the lubrication and the collision forces which is added to the Euler-Bernoulli equations as a linear force shown by $F^c$ in equation 2.23.

3.6 Notes on the implementation, parallelisation and computational requirements

The Eulerian mesh is decomposed using a 2D-pencil domain decomposition in the streamwise and spanwise direction. For that purpose, the library 2DECOMP & FFT Li & Laizet (2010) is used. The same library handles all of the transpose operations required for the Helmholtz and Poisson solvers based on the fast Fourier transforms. Regarding the parallelisation of each capsule/filament, each processor can either be master or slave. A processor is labelled master if it contains most of the Lagrangian points describing the given particle, while those containing only some of these points are labelled as slaves. The rest of the processors do not have any rule for the considered particle. Only the master processor has the information of the particle (e.g. Lagrangian points and their velocities) in its memory, though the slaves can access it for interpolation and spreading operations, which might require information from the neighbours. For the particle equations, the master is responsible for all the numerical procedures, e.g. transformation using spherical harmonics. Such parallelisation saves memory usage but requires communication between cores at each time step. A simple illustration of the particle parallelisation is illustrated in figure 3.3.

In order to obtain accurate results, the density of Eulerian and Lagrangian grid points should be similar. In some cases for capsules, it is nonetheless necessary to have a very fine Eulerian mesh, thus requiring very fine Lagrangian mesh. However, since the spherical harmonic calculations are costly, the overall computational time increases significantly. To make the code more efficient, two different sets of Lagrangian points are therefore considered: forcing points that are used for interpolation-spreading and the spherical-harmonic points that are used to define the shape of the cell and the elastic stresses. While the density of the forcing points has to be similar to that of the Eulerian points, fewer points are required for the spherical harmonics representation of the cell, especially in the case of stiffer membranes deforming less. At each time step, before computing the elastic forces, the spherical-harmonic points are obtained using spectral interpolation. These points are then used to compute the elastic forces and surface normal vectors. Once computed, the elastic forces and surface normal vectors are interpolated onto the finer mesh so that the elastic forces are spread on the Eulerian mesh. All spectral interpolations are done with the SPHEREPACK library (Adams & Swarztrauber 1999; Swarztrauber & Spotz 2000).

We have checked independence of the results from the computational domain,
grid, and time step size for all projects by running the simulations with different parameters and chose the optimum parameters. For deformable objects, in order to have an accurate and stable solution, the typical time step should be much smaller compared to the same case but rigid objects (with using the immersed boundary method for rigid objects) therefore longer computational time is needed for suspended deformable objects than the rigid ones which may take up to months even with proper parallelisation in particular for the filaments suspended in channel or shear flow while for the settling problem and the capsules, a statistically steady state can be reached in a few weeks and for single filament in 3-periodic turbulent flow, the total computational time is less than a week. As a conclusion it can be mentioned that the computational time is highly correlated with the flow configuration, interaction between the objects and flow regime.

3.7. Derivation of bulk stress

For suspensions of the deformable objects, in order to define rheological properties, it is necessary to compute bulk stresses. In this section we will discuss derivation of bulk stress for different objects.

3.7.1. Capsules

Considering a volume \( V \) that contains a large amount of particles, each of volume \( V_0 \) and surface area \( A_0 \), such that the suspension can be assumed homogeneous and assuming statistically stationary state, (Batchelor 1969) derived an expression for the bulk stress in suspension,

\[
\Sigma_{ij} = \frac{1}{V} \int (\sigma_{ij} - \rho u'_i u'_j) \, dV. \tag{3.44}
\]
For a Newtonian fluid, equation (3.44) is rewritten in non-dimensional form as (Batchelor 1969)

\[
\frac{\Sigma_{ij}}{\mu \dot{\gamma}} = \frac{Re}{V} \int_{V - V_0} \left\{ -p \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right\} dV + \frac{Re}{V} \int_{V_0} \sigma_{ij} dV - \frac{1}{V} \int u_i' u_j' dV,
\]

where \( u_i' u_j' \) is the fluctuation stress of the fluid, vanishing when inertia is negligible. In our simulations, it is found that the stress arising from the velocity fluctuations is negligible also at the higher Reynolds number considered, \( O(10) \), thus the contribution of the particles to the total stress can be rewritten for our purposes as

\[
\frac{\Sigma^P_{ij}}{\mu \dot{\gamma}} = \frac{Re}{V} \sum_{S_M} F_M x_j dS + \frac{Re}{V} \sum_{V_R} F_R x_j dV,
\]

where \( F_M \) denotes the elastic forces from the membranes, \( F_R \) the fluid-solid interaction forces from the rigid nucleus. The relative shear viscosity \( \eta \) is defined as

\[
\eta = \frac{\mu_{eff}}{\mu} = 1 + \frac{\Sigma^P_{ij}}{\mu \dot{\gamma}}
\]

where \( \mu_{eff} \) is the effective viscosity of the suspension and \( \dot{\gamma} \) is the shear rate. The first normal stress difference is defined as the difference between the streamwise and wall-normal component of the normal stresses,

\[
N_1 = \frac{\Sigma^P_{11} - \Sigma^P_{22}}{\mu \dot{\gamma}},
\]

whereas the second normal stress difference, \( N_2 \), is the difference between the wall-normal and spanwise component of the normal stresses.

### 3.7.2. Filaments

The rheological behaviour of the suspensions is presented in terms of the relative viscosity

\[
\eta = \frac{\mu_{eff}}{\mu},
\]

where \( \mu \) is the viscosity of the carrier fluid and \( \mu_{eff} \) is the effective viscosity of the suspension. The relative viscosity can be rewritten in terms of the bulk shear stress

\[
\eta = 1 + \Sigma^f_{xy},
\]
where $\bar{\Sigma}_{xy}$ is the time and space average of the shear stress arising from the presence of the filaments, non-dimensionalised by the imposed shear rate $\dot{\gamma}_{xy}$ and the viscosity $\mu$. The normal stress differences are used to describe the Non-Newtonian behaviour of the suspension, and are defined as

$$N_1 = \bar{\Sigma}_{xx} - \bar{\Sigma}_{yy}, \quad N_2 = \bar{\Sigma}_{yy} - \bar{\Sigma}_{zz}. \quad (3.51)$$

To compute the total stress in the suspension and to compute all the different contributions, the derivation by Batchelor (1970) is followed first proposed for a suspension of rigid spherical particles and adapt it to the case of flexible filaments, see also Batchelor (1971); Wu & Aidun (2010a). The dimensionless total stress reads

$$\bar{\Sigma}_{ij} = \text{Re} \left[ \frac{1}{V} \int_{V - \Sigma V_0} \left( -P \delta_{ij} + \frac{2}{\text{Re}} \varepsilon_{ij} \right) dV + \frac{1}{V} \sum_{V_0} \sigma_{ij}, dV - \frac{1}{V} \int_{V} u_i' u_j' dV \right], \quad (3.52)$$

where $V$ is the total volume under investigation and $V_0$ the volume of each filament, $\varepsilon_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}$ represents the strain rate tensor and $u'$ the velocity fluctuations. The first term on the right hand side of equation (3.52) represents the fluid bulk viscous stress tensor, the second term the stress generated by the fluid-solid interaction forces and the last term the stress generated by the velocity fluctuations in the fluid (the Reynolds stress tensor). The total stress may be written as the summation of the fluid and filament stress tensors:

$$\bar{\Sigma}_{ij} = \Sigma_{ij}^0 + \Sigma_{ij}^f, \quad (3.53)$$

where

$$\Sigma_{ij}^0 = \frac{\text{Re}}{V} \int_{V - \Sigma V_0} \left( -P \delta_{ij} + \frac{2}{\text{Re}} \varepsilon_{ij} \right) dV,$$

$$\Sigma_{ij}^f = \frac{\text{Re}}{V} \sum_{V_0} \sigma_{ij}, dV - \frac{\text{Re}}{V} \int_{V} u_i' u_j' dV. \quad (3.54)$$

The fluid-solid interaction stress can be decomposed into two parts (Batchelor 1970):

$$\int_{V_0} \sigma_{ij} dV = \int_{A_0} \sigma_{ik} x_j n_k dA - \int_{V_0} \frac{\partial \sigma_{ik}}{\partial x_k} x_j dV, \quad (3.55)$$

where $A_0$ represents the surface area of each filament. The first term is called the stresslet and the second term indicates the acceleration stress (Guazzelli & Morris 2011). For neutrally buoyant filaments, where the relative acceleration of fluid and the filament is zero, the second term in (3.55) is identically zero. $\sigma_{ik} n_k$ is the force per unit area acting on the filaments (Batchelor 1971), that for slender bodies can be rewritten as

$$\int_{A_0} \sigma_{ik} x_j n_k dA = -r_p^2 \int_{L} F_i x_j ds, \quad (3.56)$$

where the term $r_p^2$ arises from choosing the linear density instead of the volume density as scale for the fluid-solid interaction force. Finally, the filament stress
3.7. Derivation of bulk stress

is

$$
\Sigma_{ij}^f = -\frac{R e r_p^2}{V} \sum \int_L F_i x_j ds - \frac{R e}{V} \int_V u'_i u'_j dV. \quad (3.57)
$$

From the results of the simulations, it is observe that the last term, related to the velocity fluctuations, is very small compared to the stresslet and can be thus neglected for the range of Reynolds numbers considered here which is consistent with the behaviour of rigid particles for the same Reynolds numbers $O(10)$, as shown in Alghalibi et al. (2018).
Nucleated capsules in shear flow

In this chapter we have discussed a summary of the results for dynamics and rheological properties of capsules with a nucleus in shear flow, having a great importance for transport of Malaria infected blood cells or cancer cells in blood flow (Gounley et al. 2017). First, dynamics of a single nucleated capsule is discussed followed by the results for dynamics and rheological properties of nucleated capsule suspensions.

4.1. Single nucleated capsule

In this section a summary of the results for a nucleated capsule in shear flow is presented. The nucleus is considered as a capsule with very stiff membrane which its deformation is negligible. Both the capsule and the nucleus are initially located at the center of the computational domain therefore there is no translational motion. Capillary number is defined as the ratio of the viscous forces to the elastic forces

$$Ca = \frac{\mu \dot{\gamma} R^2}{G_s} = \frac{We}{Re},$$

(4.1)

where $\dot{\gamma}$ is the shear rate, $R$ initial radius of the capsule, $We = \frac{\rho U L}{G_s}$ the Weber number and $Re = \frac{\rho \dot{\gamma} R^2}{\mu}$ the Reynolds number. The Reynolds number is fixed at $Re = 0.1$ to avoid inertial effects unless the effect of inertia is studied. The non-dimensional bending stiffness is defined as

$$B = \frac{E_B}{\rho R^3 \dot{\gamma}^2},$$

(4.2)

where $E_B$ is the bending modulus. In order to provide a quantitative measure of the capsule deformation, the Taylor parameter is used. To compute it, an ellipsoid shape is fitted to each capsule such that it has the same moment of inertia as that of the different deformed capsules (Ramanujan and Pozrikidis 1998). By denoting the major and minor axes of the ellipse with $a$ and $b$, the deformation parameter reads

$$D = \frac{a - b}{a + b},$$

(4.3)
The domain is a box with the size $10 \times 10 \times 10$ in units of capsule initial radius. The Eulerian grid is $128^3$ whereas for the Lagrangian mesh $24 \times 48$ points are chosen in the latitudinal and longitudinal directions respectively resulting in 576 spherical harmonics with 24 modes.

Figure 4.1 depicts the deformation parameter as a function of the capillary number for viscosity ratios $\lambda = 1$ and 5 in the absence of bending resistance, both for capsules with and without a stiff nucleus. Note that the deformation parameter is computed on the outer membrane, the inner one not being noticeably deformed. As shown in this figure, the presence of a nucleus reduces the deformation, and this reduction is larger the higher the capillary number. The stiff nucleus reduces the outer membrane deformation since the minimum radius cannot be smaller than the radius of the nucleus. At higher Capillary numbers, the membrane would tend to deform more thus making the effect of the nucleus becomes more evident. It can be inferred from figure 4.1 that the deformation is smaller for the cases with a more viscous fluid between the outer membrane and the nucleus, $\lambda = 5$. In this case, viscous forces appear to work together with elastic forces to reduce the cell deformation.

The transient evolution of the deformation parameter to reach the final state is demonstrated in figure 4.2 for three different capillary numbers. The figure shows that larger capillary numbers require longer time to reach the final steady state. As for the steady state, the deformation is larger for higher capillary numbers.

The first two rows of figure 4.3(a) depict the steady shape of the cell for three different capillary numbers of the outer membrane and zero bending stiffness. Note that, in the first row, the cell considered has no nucleus. In the absence of nucleus, the cell assumes an ellipsoidal shape, while it has a thicker middle part in the presence of the nucleus. Cells with nucleus thus have a lower flexibility and may encounter more difficulties to pass through narrow vessels.

The effect of bending stiffness on the deformation parameter is presented in figure 4.1(b). It can be observed that cells with bending stiffness deform less and the reduction measured by the deformation parameter increases with the Capillary number. This effect is documented by the shape of capsules with bending stiffness reported in the lowest panels of figure 4.3. Here, one can see that the deformation is reduced mainly on the edges of the capsule. Indeed, figure 4.3 shows that the cell shape is closer to an ellipsoid when adding bending rigidity. The difference between the different cases shown in the figures demonstrates that the effect of the bending rigidity is not negligible in such conditions and should be accounted for to obtain more accurate predictions.

For a number of microfluidic applications, it may be important to understand the effect of flow inertia on the deformation of the transported cells. It is therefore reported in figure 4.4 the effect of increasing the Reynolds number on the deformation parameter. To prevent buckling, a small bending stiffness is considered in the simulations. It can be observed that when increasing the
Figure 4.1: (a) Deformation parameter of initially spherical cells with and without a stiff nucleus in homogeneous shear versus the Capillary number for viscosity ratios $\lambda = 1$ and 5 and no bending stiffness. (b) Cell deformation parameter versus the Capillary number for capsules with and without bending stiffness at viscosity ratio $\lambda = 1$ and $Re = 0.1$.

Figure 4.2: Time evolution of deformation parameter for an initially spherical cell with nucleus for different capillary numbers. Reynolds number $Re = 0.1$, bending stiffness $B = 0$.

Reynolds number the steady state deformation parameter first decreases for $Re = 1$ and then increases ($Re = 5$). The initial deformation rate is faster when increasing inertia. Note also some oscillations in the deformation for $Re = 5$, as observed in previous studies. These can be attributed to the formation of a pair of vortices inside the cell, on the two sides of the nucleus, in the transient stage (See figure 4.4(b)). Such vortices disappear at steady state but their formation and breakup results in oscillations of the cell membrane.

4.2. Suspensions of nucleated capsules

In this section the results for suspensions of nucleated capsules in shear flow at different capillary number and flow inertia is presented. In order to have
4.2. Suspensions of nucleated capsules

Figure 4.3: Steady-state shape of an elastic capsule in shear flow at $Re = 0.1$. (i) cell without nucleus, (ii) with nucleus and bending stiffness $B = 0$, (iii) with nucleus and $B = 10$. The Capillary number is (a) $Ca = 0.15$, (b) $Ca = 0.30$ and (c) $Ca = 0.60$.

Figure 4.4: (a) Time evolution of deformation parameter for an initially spherical cell with nucleus for different Reynolds numbers, (b) streamlines in the mid $x_1$ plane for $Re=5$ at $t=2.5$, black lines indicate location of the inner and outer membranes, $Ca = 0.3$, $B = 0.1$
stable solutions, a small bending stiffness, \( B = \frac{0.05}{W} \) is considered. The division by Weber number to have equal effect of bending resistance for all cases. The typical volume fraction of the capsules is 31.42\% unless it is mentioned. The computational domain is a box with size of \( 16 \times 10 \times 16 \) in streamwise, wall normal and spanwise directions in the units of capsule initial radius with \( 256 \times 160 \times 256 \) grid points. The capsule surface is typically represented with \( 36 \times 72 \) points in the latitudinal and longitudinal directions, corresponding to \( 2592 \) Lagrangian points on each capsule surface and to \( 1296 \) spherical harmonics and \( 36 \) modes. For a few cases, those exhibiting small deformations, i.e. low capillary and Reynolds numbers, \( 24 \times 48 \) points are used as this is found to be sufficient to resolve the capsule surface.

4.2.1. Nucleated capsule suspensions in shear flow

In this section, the dynamics of suspensions of nucleated capsules are examined for different Reynolds numbers, capillary numbers, and volume fractions and show that the competition between average deformation and orientation defines the rheological properties of the system. Figure 4.5 shows 4 snapshots of the capsules flowing in suspensions in the statistically steady state for the most deformable case, \( Ca = 0.5 \), and for different Reynolds numbers. The figure suggests more deformation at higher Reynolds number; moreover, the nucleated capsules exhibit overall lower deformations, they are thicker in the regions close to their nucleus while their membrane deformation is larger in the regions far from the nucleus, which is consistent with the results of (Alizad Banaei et al. 2017) on the dynamics of single nucleated cells. It can be observed that at \( Re = 0.1 \), negligible inertia, most of capsules have their major axis in the shear plane whereas at \( Re = 5 \) there are number of capsules with their major axis oriented in the spanwise direction. To quantify these observation and their effect on the global suspension behaviour, five observables will be compared, namely the relative shear viscosity, first normal stress difference, the orientation angle, elastic energy and Taylor parameter. The orientation angle \( \theta \) is defined as the angle between diameter of the box surrounding the capsule with the flow direction.

Figure 4.6 depicts the effect of capillary number and Reynolds number on the relative viscosity of simple and nucleated capsule suspensions. It shows that the relative viscosity decreases with the capillary number for both types of the capsules; shear thinning with deformability is in agreement with previous results for capsule at negligible inertia and deformable hyper-elastic particles Matsunaga et al. (2016); Rosti et al. (2018b); Rosti & Brandt (2018). Before discussing the effect of inertia it is important to mention that both relative viscosity, and the first normal stress difference discussed below, increase for increasing mean capsule deformation and mean inclination angle, whereas the first normal stress difference, on the contrary, decreases with the mean inclination angle, see also (Matsunaga et al. 2016).

The data in figure 4.6 shows that the suspension relative viscosity can increase or
4.2. Suspensions of nucleated capsules

Figure 4.5: Visualization of capsules with $Ca = 0.5$ and volume fraction $\phi = 0.31$ in the flowing suspension at statistically steady state for the cases: (a) $Re = 0.1$ without nucleus, (b) $Re = 5$ without nucleus, (c) $Re = 0.1$ with nucleus and (d) $Re = 5$ with nucleus.

decrease with the Reynolds number for a fixed capillary number. In particular, for the capsules without nucleus, it first decreases, see data at $Re = 1$ and higher values of $Ca$ investigated, and then increase at higher inertia, whereas the nucleated-capsule suspensions always display an increase of the effective viscosity with $Re$. The increase of the relative viscosity can be explained by an increase of the capsule deformation with the Reynolds number, which is quantified in figure 4.7 by the Taylor parameter, and by an increase of the orientation angle with inertia, displayed on the right panel of the same figure 4.7. The decrease of the relative viscosity with the Reynolds number observed at moderate inertia can be explained by the competition between two contrasting effects: the increased elastic stress due to larger deformations and the reduction in the stresslet induced by the capsule alignment with the local shear. In other words, the deformation increases with the Reynolds number, which increases the membrane shear stress; on the other hand, the orientation angle $\theta$ decreases with inertial effects, which decreases the capsule induced stresses. Some alignment is observed already at weak inertia, $Re = 1$, for the most deformable capsules considered here, so that the induced reduction is initially stronger, resulting in a global reduction of the relative viscosity. This effect is more pronounced in the absence of a rigid nucleus inside the capsules.

When there is a nucleus inside capsule, a third effect comes into play, namely the stresses induced by the nucleus, which combines with the capsule
deformation and orientation. The rigid nucleus adds more force on the flow and increases the total shear stress while the deformation and orientation can act in opposite ways. It can be observed in figure 4.6 that for \( Ca = 0.1 \) and \( Ca = 0.5 \) and \( Re \leq 1 \) the presence of the nucleus induces larger viscosities in the case of nucleated capsules, despite a significant reduction of the capsule deformation, so lower elastic stresses. Indeed the data in figure 4.7 clearly show that the presence of a rigid nucleus decreases the overall membrane deformation for all cases considered in this study. For \( Ca = 0.5 \) and \( Ca = 0.3 \) and \( Re = 5 \), a small difference in the relative viscosity of the simple and nucleated capsules is reported; in this case, the increased stresses due to the presence of the nucleus and the lower elastic stresses due to the decreased deformation almost exactly compensate for each other. Finally, regarding the cases with \( Ca = 0.1 \), the most stiff capsules under consideration. In this case, the cell membranes weakly deform and the presence of the nucleus does not affect the average deformation and orientation, the former being only function of inertia whereas the latter is almost constant, see figure 4.7. The lower effective viscosity in the presence of a nucleus can be explained by the fact that capsule behave more like rigid objects and the presence of a rigid sphere inside slightly decreases the deformation when increasing inertia.

Effect of volume fraction on the rheological properties as well as the mean deformation and orientation angle is studied for a constant capillary number, \( Ca = 0.3 \), and two Reynolds numbers, \( Re = 1 \) and \( Re = 5 \). The relative viscosity is depicted in figure 4.8 whereas the mean orientation angle and mean Taylor parameter are displayed in figure 4.9.

As expected, the relative viscosity increases with the volume fraction, see figure 4.8. First, it is noted that at \( Re = 1 \) and \( 0.1 \leq \phi \leq 0.2 \), there is very small
4.2. Suspensions of nucleated capsules

Figure 4.7: Mean Taylor parameter and averaged capsule orientation as function of \( Re \) and \( Ca \) for volume fraction \( \phi = 0.31 \). Solid lines correspond to capsules without nucleus and dashed line indicate the results for capsules with nucleus. Black, red, and blue colors denote \( Ca = 0.1 \), \( Ca = 0.3 \), and \( Ca = 0.5 \), respectively.

difference between the relative viscosity of the simple and the nucleated capsule suspensions; this can be explained by the balance of the two counteracting effects mentioned above. On one hand, the presence of a nucleus increases the mean shear stresses, on the other hand, it reduces the membrane deformation and thus reduces the elastic contribution to the total stresses, see figure 4.9. The same is not true at \( Re = 5 \), in which case the cells without nucleus display larger viscosity, indicating that the elastic stresses arising from the membrane deformation are stronger than those due to the rigid nucleus inside. When further increasing the volume fraction to \( \phi = 0.31 \), the alignment becomes more evident; the larger relative viscosity for the nucleated capsule suspensions at \( Re = 1 \) can then be explained by the presence of the nucleus and by the reduced elastic stresses due to alignment. At higher inertia, the deformation is more pronounced so that the elastic stresses increase in the case of capsules without nucleus. As a result, the suspension shear viscosity, which was larger for capsules with nucleus at \( Re = 1 \), becomes of the same order for the two types of capsules considered.
Figure 4.8: Relative viscosity of nucleated and denucleated capsules versus the volume fraction $\phi$ for $Ca = 0.3$. Solid and dashed lines represent capsule with and without nucleus, whereas blue and red indicate flows with $Re = 1$ and $Re = 5$.

Figure 4.9: Averaged deformation, in terms of the Taylor parameter, and average orientation of capsules for $Ca = 0.3$. Solid and dashed lines represent capsule with and without nucleus, whereas blue and red indicate flows with $Re = 1$ and $Re = 5$. 
Flexible filaments in different flow configurations

In this chapter we have discussed a summary of the results for dynamics and rheological properties of filaments in different flow configurations. First, the results for rheology of filament suspensions are presented in shear flow at finite inertia. Then quiescent settling of filaments is discussed followed by the results of single filament in a homogeneous isotropic turbulent flow. Finally drag reduction in turbulent channel flow with filaments are discussed briefly.

5.1. Rheology of flexible filament suspensions at finite inertia

Rheological data of filament suspensions is of great importance in pulp and paper industry and material reinforcing (Lundell et al. 2011; Lindström & Uesaka 2008). In this section the rheological properties and deformation statistics of neutrally buoyant filaments with aspect ratio $r_p = 0.0625$ are presented in shear flow at finite flow inertia. The filament Reynolds number is varied between 0.1 and 10 and the bending stiffness is varied between $(0.005 \leq \gamma \leq 0.5)$. The domain size is $5 \times 8 \times 5$ in units of filament length in streamwise, wall normal and spanwise directions with $80 \times 128 \times 80$ grid points. There are 17 Lagrangian points on each filament. The solid volume fraction of the suspension is

$$\phi = \frac{n_f \pi r_p^2}{4V},$$

where $n_f$ is the number of filaments in the computational box and $V$ the volume of the computational domain.

5.1.1. Selected results

The suspension behaviour is analysed at a fixed volume fraction, $\phi = 0.053$, and vary the Reynolds number and filament flexibility. First, in figure 5.1 the dependence of the suspension relative shear viscosity on the bending rigidity (left panel) and the Reynolds number (right panel) is reported. Figure 5.1a shows that the viscosity increases with the bending rigidity, i.e., the viscosity decreases as the filaments are more flexible, indicating that the suspensions exhibit a shear-thinning behaviour with increasing flexibility. This result is in agreement with the simulations by (Switzer III & Klingenberg 2003; Sepehr et al.)
Flexible filaments in different flow configurations

Figure 5.1: Relative viscosity of filament suspensions versus (a) the filament bending rigidity and (b) the Reynolds number. The suspension volume fraction is fixed to $\phi = 0.053$ for all cases.

2004) for flexible fibres, and also to the results pertaining the case of deformable particles, capsules and droplets, see e.g. (Reasor et al. 2013; Matsunaga et al. 2016; Rosti & Brandt 2018; Rosti et al. 2019). These observations are in contrast with the results of (Wu & Aidun 2010b) where larger viscosities are obtained for more flexible cases. Suspensions of elastic elongated objects can therefore display different behaviour: viscosity decreasing with deformability (Switzer III & Klingenberg 2003; Sepehr et al. 2004) or increasing with it (Wu & Aidun 2010b; Joung et al. 2001). This difference can be explained by the different physical objects under consideration: (Wu & Aidun 2010b) and (Joung et al. 2001) considered chains of interconnected rigid particles which can twist and bend in their joints, while in present results, continuously flexible filaments have been considered that can only bend. Note also that, although (Switzer III & Klingenberg 2003) and (Sepehr et al. 2004) adopt a model similar to the one used by (Wu & Aidun 2010b), they observe shear-thinning which may be explained by the different aspect ratio considered: indeed, the former consider fibres whose aspect ratio is at least 5 times smaller than those considered by (Wu & Aidun 2010b).

Figure 5.1b displays the same data of 5.1a, now as a function of the Reynolds number, in order to highlight how inertia affects the suspension viscosity. It is observed that $\eta$ increases with the Reynolds number, especially for the most stiff cases; this indicates that inertial effects are more evident for rigid rods than for flexible filaments.

To examine the filament dynamics and their deformation, one can consider the average distance between the two ends of each filament averaged over time and the number of filaments. The data pertaining all the different cases under investigation are shown in figure 5.2. The figure indicates that the end-to-end distance increases as the bending stiffness is increased, i.e., the filaments deformation decreases for larger values of $\tilde{\gamma}$. Moreover, the average end-to-end
5.2. Settling of flexible filament suspensions under gravity

Settling of inertial filaments/fibres is found in many applications in particular in pulp and paper industry (Provatas et al. 1996). In this thesis, the quiescent settling problem is studied for fibre suspensions with the aspect ratio \( r_p = 0.05 \) and the density ratio \( r = \rho_f / \rho = 1.1 \). By choosing the velocity scale as \( U_s = \sqrt{(r - 1)gL} \), the Reynolds number in the Navier-Stokes equations will be replaced with the Galileo number

\[
Ga = \sqrt{rgL^3/\nu},
\]

with \( \nu \) being the kinematic viscosity of the fluid. The Galileo number is set to \( Ga = 160 \) for all cases. The computational domain is a triperiodic box with the size \( 2\pi \times 4\pi \times 2\pi \) in units of fibre length (\( 4\pi \) is the settling direction) with 128 \( \times \) 256 \( \times \) 128 grid points. In order to have zero mean fluid velocity, every time step, the mean velocity is deduced from the fluid velocity field.

Formation of streamers in settling of fibre suspensions is an interesting phenomenon. Streamers are regions of high concentration of fibres that are correlated to high local settling velocities (Metzger et al. 2005; Gustavsson & Tornberg 2009). The formation of streamers also creates regions of low concentrations of fibres outside the streamers where fibres can move upward in the opposite direction of gravity. Figure 5.3 shows the snapshots of the structure of the streamers for rigid and flexible fibres at different fibre concentrations.
Flexible filaments in different flow configurations

Figure 5.3: Snapshots of the streamers and backflow regions. In the top row the fibres are colored by their settling velocity and in the bottom row they are colored by their local fibre concentration, $C$. Only the fibres with $w > 0.3$ or $w < -0.15$ are shown.

In this figure the streamers are identified as the fibres with settling velocities $w > 0.3$ and the fibres in the backflow region are distinguished by $w < -0.15$. Similar to the numerical simulations of (Gustavsson & Tornberg 2009) the structures of the streamers are persistent in time until eroded and dispersed on the edges and the streamers did not break down to smaller scale streamers as observed in laboratory experiments (Metzger et al. 2005). The streamers in figure 5.3 appear as oblique columns of fibres with their vertical connectivity being lost in some locations. The lateral size of the streamers and their vertical connected lengths are larger for higher values of $nL^3$ and also for rigid as opposed to flexible fibres. The larger size of the streamers can be attributed to lower local packing of the fibres that occurs due to the reduced mobility at high $nL^3$ or higher particle rigidity. Flexible fibres exhibit narrower but more packed streamers. At lower $nL^3$, the size of the streamers is smaller but their structure is similar to their higher $nL^3$ counterparts, and their packing is higher.

The mean settling velocity for different number density and bending rigidities are presented in figure 5.4. For each bending rigidity $\gamma$, the mean settling velocity decreases with increasing the number density due to the hindering effect by the adjacent fibres. The mean settling velocity increases with increasing the fibre flexibility and this effect is more evident at higher number densities. One can explain this by less projected surface area of the fibres decreasing as the fibres become more flexible and therefore their mean settling velocity increases. The fibre deformation is almost independent of the number density at higher concentrations since the fibres become less mobile and the effect of fibre deformations is negligible at high $nL^3$. The formation of streamers for
5.3. Single filament in homogeneous isotropic turbulence

$nL^3 > 10$ plays a more important role in settling of denser suspensions of fibres since dense clumps of fibres that settle rapidly and counterbalance the effects of hindering. The streamers create higher packings in flexible fibres therefore, the difference between the mean settling velocity of flexible and rigid fibres is more pronounced at higher $nL^3$. For flexible fibres, as the mobility of fibres reduces at high $nL^3$, the streamers in the flexible fibres reach self-similar structures and the settling velocities reach a plateau at high number densities. For rigid fibres, the reduced fibre mobility leads to weakened streamers with significantly less compact structures and the settling velocity continues to drop at high $nL^3$ due to the hindering effects.

5.3. Single filament in homogeneous isotropic turbulence

Motion of a flexible filament in turbulent flow is present in biological applications (Fish & Lauder 2006; Bagheri et al. 2012; McKinney & DeLaurier 1981; Boragno et al. 2012) and energy harvesting (McKinney & DeLaurier 1981; Boragno et al. 2012; Li et al. 2016; Zhao & Yang 2017). In this section dynamics of an inertial flexible fibre in homogeneous isotropic turbulent flow is studied to present a theory for description of how elastic fibres respond to the fluctuations of the flow (see figure 5.5). The computational domain is a triperiodic box with the size $2\pi$ in units of the longest fibre length and 128 grid points per side. The Reynolds number based on the Taylor microscale $Re_\Lambda$ is equal to 92 and the non-dimensional turbulent dissipation rate $\overline{\varepsilon' u'_{\text{rms}}^3}$ equal to 2.54 where $H$ is the computational domain size.

Regarding the motion of the fibre, two distinct types of motion is expected: over-damped and under-damped regimes. In the over-damped regime, the elastic forces are dominant and the elasticity is expected to strongly affect the fibre dynamics. In this regime, due to large elastic forces, any imposed deformation
by the turbulence will be followed by high-frequency oscillations to return the fibre to its undeformed configuration. On the other hand for under-damped case, due to small elastic forces, the fibre does not resist deformation and is thus slaved to the turbulent fluctuations. It can be inferred from the two regimes that a critical value for the bending stiffness $\gamma_{\text{crit}}$ should exist separating the two regimes. $\gamma_{\text{crit}}$ can be found from a resonance condition between the fibre elastic time scale $\tau_\gamma = \alpha (\rho_1 c^4/\gamma)^{1/2}$ with $\alpha = \pi/22.3733$ and $c$ the fibre length and the eddy turnover time $\tau(\tau) = \tau^{2/3} \epsilon^{-1/3}$ evaluated at the fibre scale $c$, $\epsilon$ being the turbulence dissipation rate of kinetic energy. The condition $\tau(c) \sim \tau_\gamma$ results in:

$$\alpha \left( \frac{c^4 \rho_1}{\gamma} \right)^{1/2} \sim c^{2/3} \epsilon^{-1/3} \Rightarrow \gamma_{\text{crit}} \sim c^{8/3} \epsilon^{2/3} \rho_1 \alpha^2 \quad . \quad (5.3)$$

Equation 5.3 can be written in non-dimensional form

$$\gamma_{\text{crit}} \sim \epsilon^{2/3} \alpha^2 \quad . \quad (5.4)$$

where $\epsilon = \frac{c^4}{\nu_{\text{eff}} r c}$. The predicted $\gamma_{\text{crit}}$ is verified with the DNS simulations by studying long time-series (corresponding to $\sim 20$ large-eddy turnover times), of the motion of 30 different fibres, corresponding to different combinations of 3 different densities $\rho_1$, 3 lengths $c$ and 9 bending rigidities $\gamma$, all the cases
5.4. Drag reduction in turbulent channel flow using flexible filaments

Filaments/fibres can be used to reduce drag force in turbulent channel flows (Vaseleski & Metzner 1974; Metzner 1977; Lee et al. 1974; Kale & Metzner 1976; Gillissen et al. 2008; McComb & Chan 1981). In this thesis, suspensions of neutrally buoyant filaments with aspect ratio $r_p = 0.05$ is considered in a turbulent channel flow with constant mass flow rate and the Reynolds number $Re_H = 2800$ based on the channel half height. The domain size is $54 \times 18 \times 27$ in units of filament length in streamwise, wall normal and spanwise directions.

Figure 5.6: The fibre oscillation frequencies (normalized by the turbulence frequency at the fibre length scale) as a function of the fibre bending rigidity (normalized by the critical value given in (5.3)). Diamonds: $c/H = 0.20$ and $\rho_1/\rho_0 H^2 = 0.042$; bullets: $c/H = 0.12$ and $\rho_1/\rho_0 H^2 = 0.042$; triangles: $c/H = 0.16$ and $\rho_1/\rho_0 H^2 = 0.042$; stars: $c/H = 0.16$ and $\rho_1/\rho_0 H^2 = 0.125$; squares: $c/H = 0.16$ and $\rho_1/\rho_0 H^2 = 0.014$.

belonging to the under-damped regime. The leading oscillation frequency $f$, extracted from the Fourier transform of the time history of the end-to-end distance and divided by $f_{turb} = 1/\tau(c)$, is reported in Fig. 5.6 as a function of $\gamma/\gamma_{crit}$. The outcome confirms our expectations and the good data collapse brings to the conclusion There is a sharp transition at $\gamma_{crit}$ separating the two distinct regimes;

The fact that for $\gamma/\gamma_{crit} < 1$ the fibre is locked to the frequency of the turbulent eddies with the same size of the fibre suggests that the fibre is able to reveal the turbulence velocity fluctuations. In other words, the fibre can be considered as a physical proxy of the celebrated turbulent eddies. This being the case, a massive fibre, which can be easily tracked in a turbulent flow, can reveal the features of eddies of different scales.
5. Flexible filaments in different flow configurations

Figure 5.7: Time and space averaged streamwise velocity distribution in wall normal direction for different filament flexibilities.

respectively with $1080 \times 360 \times 540$ grid points. There are 20 Lagrangian points on each filament. The filament length is 20 in units of inner length scale $\frac{u_\tau}{\nu}$ where $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$ with $\tau_w$ the wall shear stress. Effect of the filaments flexibility and volume fraction on the drag reduction and turbulent statistics is studied however in this thesis only the results for 1.5% volume fraction is presented.

Figure 5.7 depicts distribution of mean streamwise velocity averaged in time and space in wall normal direction for $\gamma = 30$ and $\gamma = 0.1$. For $\gamma = 30$ the filaments stay straight while for $\gamma = 0.1$ they exhibit finite deformation in wall region and very small bending at the turbulent core. The mean velocity profile for each case is scaled with its own shear velocity $u_\tau$. The figure shows that there is very small difference between velocity profiles of the stiff and the flexible cases. This small difference between the velocity profiles can be attributed to small deformation of the filaments for $\gamma = 0.1$. The maximum deformation happens around $y^+ = 40$ corresponding to the minimum value of average end-to-end distance $D_e = 0.9$ which seems to have negligible effect on the bulk behaviour.

The Reynolds number based on the friction velocity $Re_\tau = u_\tau h/\nu$ is 178 for single phase flow while it is 150 for the suspensions. The total drag reduction based on the pressure gradient is 28.8% for both flexibilities.

Figure 5.8 shows streamwise and wall normal Reynolds stress distribution in wall normal direction indicating that the streamwise fluctuations increase by adding filaments while there is less wall normal fluctuations for suspensions than single phase flow being in agreement with results of (Shahmardi et al. 2019; Dubief et al. 2004) for drag reduction with polymers. The fluctuations can be related to orientation angle of the filaments with the flow direction. Since most of the filaments are aligned with the flow direction, the wall normal

\[ y^+ \]

\[ \frac{\overline{u}}{u_\tau} \]

\[ \gamma = 30 \]

\[ \gamma = 0.1 \]

\[ \text{Single phase} \]
fluctuations are damped by filament elasticity while streamwise fluctuations are intensified by the filaments motion. As mentioned before the maximum deformation happens around $y^+ = 40$ where the Reynolds stresses have their maximum value therefore the Reynolds stresses have significant contribution to the filaments deformation.
Chapter 6

Conclusions and outlook

6.1. Capsules and deformable cells

In this thesis, a new numerical tool for the simulation of capsules with the possibility of having a nucleus inside has been developed. The capsule membrane is considered as a thin hyperelastic membrane enclosing a droplet with same density as the outer fluid but with a viscosity contrast. The membrane elasticity equations are solved with a spectral method by modelling the capsule shape as a truncated series of spherical harmonics. The inner nucleus can be either considered as a rigid particle or as a second capsule, typically stiffer. The fluid equations are solved with a semi-implicit finite volume solver. For the coupling between the fluid flow and the solid motion, two different versions of the Immersed Boundary Method are used for capsules and rigid particles. When simulating capsule suspensions, in order to avoid membrane-membrane, membrane-wall, and membrane-rigid particle overlapping, a short range repulsive force based on Morse potential is implemented. The code has been validated both for single capsule and capsule suspensions against data in the existing literature.

All the simulations have been performed for initially spherical capsules with Neo-Hookean membranes in shear flow. The nucleus initial radius is always set to half of the capsule initial radius. For single capsules, the results indicate that the presence of a nucleus inside decreases the deformation significantly. The capsules shape depends on the capillary number, the viscosity ratio, and the bending stiffness. For nucleated capsules with negligible bending stiffness, the capsule cross section in the shear plane has a diamond-like shape while for the rest of the cases considered it is more similar to an ellipse.

As regards capsule suspensions, the results indicate that, at a constant Reynolds number, the relative viscosity of the suspensions decreases with the capillary number, so the suspension is shear thinning with respect to deformability, as observed in previous studies on suspensions of flexible and deformable objects. The effect of the Reynolds number and of the presence of the nucleus results from the competition between the increased shear stresses due to increased deformation and the reduction due to capsule alignment to the mean flow direction. The deformation increases with inertia and decreases for capsules with a rigid nucleus; the presence of the nucleus reduces the capsule mean
6.2. Filaments

Here, we have presented a numerical code able to simulate flexible slender bodies, namely filaments/fibres suspended in a fluid flow. The filaments are considered as one-dimensional continuously flexible objects obeying the Euler-Bernoulli beam equation. The immersed boundary method is used to couple fluid and solid motion as in the case of capsules. For the short range interaction between the filaments, both lubrication correction and collision forces are considered. The code has been validated against different numerical and experimental data in different configurations such as the motion of single flexible filament under gravity, the rotation of single stiff filament in shear flow, the motion of flexible filaments in an oscillatory flow, and the settling of stiff filaments under gravity.

As concerns the rheology of filament suspensions, the effect of flexibility and flow inertia is studied in this thesis. It is observed that at fixed volume fraction, the filament suspension has a shear-thinning behaviour with respect to flexibility, as observed in previous studies and for other flexible objects, e.g. capsules, red blood cells and deformable particles. The shear-thinning is increased at finite inertia yet in a laminar flow. The relative viscosity increases with the Reynolds number due to the larger contribution of the fluid-solid interaction stress to the total stress. The first normal stress is positive as in polymer and other shear-thinning fluids, and increases with the Reynolds number.

By increasing the filament volume fraction, the suspension viscosity increases, except for stiff filaments at negligible inertia where there is a clear saturation.
The shear-thinning behaviour mentioned above is more pronounced at high Reynolds numbers, when the filaments exhibit more deformation. On the other hand, the shear thinning is also stronger at lower volume fraction and decreases with the volume fraction. This is due to the formation of a more ordered structure in the flow, where the filaments tend to be more aligned and move as an aggregate, which results in less filament-filament interactions. Interestingly, the fluid velocity fluctuations first display a maximum at intermediate volume fractions and then decrease at the highest packing considered here, which can be explained as a combination of two effects. In the case of rigid filaments, this is due to the formation of a packed structure at high \( \phi \), whereas in the case of flexible filaments this is attributed to an increased deformation resulting in reduced effect on the fluid. A possible extension to this work is therefore the study of the rheology of filaments suspended in a non-Newtonian fluid, as well as the system response to an oscillating shear as mentioned above for capsule suspensions.

Settling of flexible filaments in a quiescent fluid is studied at fixed Galileo number and density ratio. The effect of the flexibility and the filament volume fraction is examined in detail. We report the formation of regions of high concentration of fibres, known as streamers, characterised by high settling velocities. The streamers are strengthened by increasing the fibre volume fraction. The mean settling velocity decreases with increasing the volume fraction due to the hindering effect by the adjacent fibres. The mean settling velocity increases with increasing the fibre flexibility which can be attributed to a lower projected surface area as well as to the formation of the streamers. At higher volume fractions, the fibres become less mobile, in particular for more flexible cases and the mean settling speed and the mean fibre deformation tend to approach a constant value. An interesting extension to this work is to consider contact friction between the fibres which is expected to intensify the streamers.

WE have also studies the dynamics of a filament in homogeneous isotropic turbulence. The results show that there are two different regimes for the filament motion: over-damped and under-damped regime with a sharp transition from one to another for a critical bending rigidity \( \gamma_{\text{crit}} \). In the over-damped regime, the bending forces are dominant and the filament oscillates with higher frequencies than the fluid ones; in the under-damped regime, conversely, due to the small bending forces, the filament is slaved to the turbulent fluctuations which can be used to reveal two-point turbulent statistics. An interesting extension to this work is to study filament suspensions in homogeneous isotropic turbulence to find the maximum number of the filaments that can be used to reveal the two-point statistics without altering the background flow. Above this threshold concentration, filaments can dampen the turbulence, which also deserves further consideration.

Regarding turbulent channel flow with filaments, the work is at a more preliminary stage. We report here a relatively large drag reduction, about 29% for 1.5% filament volume fraction for both stiff and more flexible filament suspensions. The velocity and Reynolds stress profiles for the two different bending rigidities
are very similar which can be attributed to small deformation of the filaments for the flexible case. The maximum deformation of the filaments occurs at $y^+ = 40$, near the walls, where the Reynolds stress is maximum. However, this work is still in progress, so future work in the area should first explore a wider parameter range in terms of filament flexibility and length.
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Part II

Papers
Summary of the papers

Paper 1

Numerical simulations of elastic capsules with nucleus in shear flow

The shear-induced deformation of a capsule with a stiff nucleus, a model of eukaryotic cells, is studied numerically. The membrane of the cell and of its nucleus are modelled as a thin and impermeable elastic material obeying a Neo-Hookean constitutive law. The membranes are discretised by a Lagrangian mesh and their governing equations are solved in spectral space using spherical harmonics, while the fluid equations are solved on a staggered grid using a second-order finite differences scheme. The fluid-structure coupling is obtained using an immersed boundary method. The numerical approach is presented and validated for the case of a single capsule in a shear flow. The variations induced by the presence of the nucleus on the cell deformation are investigated when varying the viscosity ratio between the inner and outer fluids, the membrane elasticity and its bending stiffness. The deformation of the eukaryotic cell is smaller than that of the prokaryotic one. The reduction in deformation increases for larger values of the capillary number. The eukaryotic cell remains thicker in its middle part compared to the prokaryotic one, thus making it less flexible to pass through narrow capillaries. For a viscosity ratio of 5, the deformation of the cell is smaller than in the case of uniform viscosity. In addition, for non-zero bending stiffness of the membrane, the deformation decreases and the shape is closer to an ellipsoid. Finally, we compare the results obtained modeling the nucleus as an inner stiffer membrane with those obtained using a rigid particle.

Paper 2

Nucleated capsules at finite inertia

We study the rheology of suspensions of capsules with a rigid nucleus at negligible and finite flow inertia by means of numerical simulations. The capsule membrane is modelled as a thin Neo-Hookean hyperelastic material and the nucleus as a rigid particle with radius equal to half the radius of the undeformed spherical capsules. The fluid and solid motion are coupled with an immersed boundary method, validated for both the deformable membrane and the rigid nucleus. We examine the effect of the Reynolds number, capillary number and volume
fraction on the macroscopic properties of the suspensions, comparing with the case of capsules without nuclei. In addition to classic global rheological measures, we report the mean deformation of the capsules, the mean elastic energy and mean orientation angle. The results indicate that the relative viscosity decreases with the capillary number, i.e. increasing deformability, whereas the presence of the nucleus and inertial effects can be associated with variations of the mean orientation angle and mean deformation of the capsules, which affect the relative suspension viscosity in an opposite way. The first normal stress difference increases with the capillary number and decreases for capsules with nucleus while the shear viscosity, normal stress difference and deformation all increases with the Reynolds. Finally, the relative viscosity and the first normal stress difference increase with the capsule volume fraction, more so for the first normal stress difference than for the relative viscosity.

**Paper 3**

*Numerical study of filament suspensions at finite inertia*

We present a numerical study on the rheology of semi-dilute and concentrated filament suspensions for different bending stiffness and Reynolds number, with the immersed boundary method used for the coupling between fluid and solid. The filaments are considered as one-dimensional inextensible slender bodies with fixed aspect ratio, obeying the Euler-Bernoulli beam equation. At fixed volume fraction, the suspensions are found to be shear-thinning where the relative viscosity decreases by decreasing the non-dimensional bending rigidity. The relative viscosity increases when increasing the Reynolds number due to the larger contribution of the fluid-solid interaction stress to the total stress; moreover the shear-thinning increases at finite inertia, yet in the laminar regime considered here. The first normal stress is positive as in polymeric and other shear-thinning fluids, and increases with the Reynolds number. However, it has a peak for a certain value of the filament bending stiffness, which varies with the Reynolds number, moving towards more rigid suspensions at larger inertia. When increasing the filament volume fraction, we observe that the viscosity increases. On the other, the shear-thinning behavior with respect with deformability is stronger at lower volume fraction and decreases with the number of filaments. This is due to the formation of a more ordered structure in the flow, where filaments tend to be more aligned and move as an aggregate, which reduces the filament-filament interactions.

**Paper 4**

*Numerical study of settling of flexible fiber suspensions*

We study the inertial settling of suspensions of flexible and rigid fibers using an immersed boundary method. The fibers considered are inextensible and slender, with an aspect ratio of 20. For a single Galileo number of $Ga = 160$, we examine a range of bending rigidities and fiber concentrations that span dilute to concentrated regimes. The results show the formation of streamers, regions of
highly packed fibers, in semi-dilute and concentrated regimes where \( nL^3 > 10 \).

The fibers in the streamers exhibit high settling velocities, while the fibers in the low concentration regions outside the streamers either go upwards or have low settling velocities. Flexible fibers exhibit higher local fiber concentrations inside the streamers and smaller length scales of the streamers compared to rigid fibers. The velocity increase due to the formation of the streamers counterbalances the hindering of the settling velocity and the settling velocity becomes independent of \( nL^3 \) for \( nL^3 > 10 \) for flexible fibers. However, at high fiber concentrations the maximum packing of the fibers inside the streamers is hampered by the limited mobility of the fibers. Due to this limited mobility, the deformation of the fibers, their settling orientation, and horizontal velocity become insensitive to \( nL^3 \) when \( nL^3 > 10 \).

**Paper 5**

*A flexible fiber reveals the two-point statistical properties of turbulence*

We study the dynamics of a flexible fiber freely moving in a three-dimensional fully-developed turbulent field and present a phenomenological theory to describe the interaction between the fiber elasticity and the turbulent flow. This theory leads to the identification of two distinct regimes of flapping, which we validate against Direct Numerical Simulations (DNS) fully resolving the fiber dynamics. The main result of our analysis is the identification of a flapping regime where the fiber, despite its elasticity, is slaved to the turbulent fluctuations. In this regime the fiber can be used to measure two-point statistical observables of turbulence, including scaling exponents of velocity structure functions, the sign of the energy cascade and the energy flux of turbulence, as well as the characteristic times of the eddies within the inertial range of scales. Our results are expected to have a deep impact on the experimental turbulence research as a new way, accurate and efficient, to measure two-point, and more generally multi-point, statistics of turbulence.

**Paper 6**

*Flowing fibers as a proxy of turbulence statistics*

The flapping states of a flexible fiber fully coupled to a three-dimensional turbulent flow are investigated via state-of-the-art numerical methods. Two distinct flapping regimes are predicted by the phenomenological theory recently proposed by Rosti et al. [Phys. Rev. Lett. 121, 044501, 2018]: the under-damped regime, where the elasticity strongly affects the fiber dynamics, and the over-damped regime, where the elastic effects are strongly inhibited. In both cases we can identify a critical value of the bending rigidity of the fiber by a resonance condition, which further provides a distinction between different flapping behaviors, especially in the under-damped case. We validate the theory by means of direct numerical simulations and find that, both for the over-damped regime and for the under-damped one, fibers are effectively slaved to the turbulent fluctuations and can therefore be used as a proxy to measure
various two-point statistics of turbulence. Finally, we show that this holds true also in the case of a passive fiber, without any feedback force on the fluid.