The influence of inertia on the rotational dynamics of spheroidal particles suspended in shear flow

by

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Abstract

Dispersed particle flows occur in many industrial, biological and geophysical applications. The knowledge of how these flow behave can for example lead to improved material processes, better predictions of vascular diseases or more accurate climate models. These particle flows have certain properties that depend on single particle motion in fluid flows and especially how they are distributed both in terms of spatial position and, if they are non-spherical, in terms of orientation. Much is already known about the motion of perfectly spherical particles. For non-spherical particles, apart from their translation, it is important to know the rotational motion due to local velocity gradients. Such studies have usually been restricted by the assumption that particles are extremely small compared to fluid length scales. In this limit, both inertia of the particle and inertia of the fluid can be neglected for the particle motion. This thesis gives a complete picture of how a spheroidal particle (a particle described by a rotation of an ellipse around one of its principal axes) behave in a linear shear flow when including both fluid and particle inertia, using numerical simulations. It is observed that this very simple problem possess very interesting dynamical behavior with different stable rotational states appearing as a competition between the two types of inertia. The effect of particle inertia leads to a rotation where the mass of the particle is concentrated as far away from the rotational axis as possible, i.e. a rotation around the minor axis. Typically, the effect of fluid inertia is instead that it tries to force the particle in a rotation where the streamlines of the flow remain as straight as possible. The first effect of fluid inertia is thus the opposite of particle inertia and instead leads to a particle rotation around the major axis. Depending on rotational state, the particles also affect the apparent viscosity of the particle dispersion. The different transitions and bifurcations between rotational states are characterized in terms of non-linear dynamics, which reveal that the particle motion probably can be described by some reduced model. The results in this theses provides fundamental knowledge and is necessary to understand flows containing non-spherical particles.

Descriptors: Fluid mechanics, dispersed particle flows, inertia, non-spherical particles, non-linear dynamics.
Sammanfattning


Descriptors: Strömningsmekanik, flöden med dispergerade partiklar, tröghet, icke-sfäriska partiklar, icke-linjär dynamik.
Preface

In this thesis, the rotational motion of both prolate and oblate spheroidal particles suspended in a linear shear flow is considered. The thesis is divided into two parts. The first part starts off with describing some of the prerequisite concepts within rigid body dynamics, fluid mechanics and describes some examples of simple dynamical systems. Later on, the particular flow problem is introduced and the numerical method is explained. Finally the important results and conclusions are presented and discussed.

The second part consists of three papers, which are provided for the reader that wants to know more about the methodology leading to the results;

**Paper 1** Tomas Rosén, Fredrik Lundell and Cyrus K. Aidun;  
*Effect of fluid inertia on the dynamics and scaling of neutrally buoyant particles in shear flow*

**Paper 2** Tomas Rosén, Fredrik Lundell, Minh Do-Quang and Cyrus K. Aidun;  
*The dynamical states of a prolate spheroidal particle suspended in shear flow as a consequence of particle and fluid inertia*

**Paper 3** Tomas Rosén, Fredrik Lundell, Minh Do-Quang and Cyrus K. Aidun;  
*Effect of fluid and particle inertia on the rotation of an oblate spheroidal particle suspended in linear shear flow*

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I am enough of an artist to draw freely upon my imagination. Imagination is more important than knowledge. Knowledge is limited. Imagination encircles the world.

– A. Einstein
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Part I

Overview & summary
In our everyday surroundings we encounter dispersed particle flows everywhere. Even though they usually go unnoticed, the microscopic motion of individual dispersed particles in a fluid can have significant effect on macroscopic properties, which are of interest in many fields of science and engineering. For some applications, the individual particle distribution and interaction is of interest. In other cases, the effect of the particle on the suspending fluid is sought. For example, the presence of solid particles in the fluid is particularly influencing the effective viscosity of the solid-fluid dispersion.

Every time you take a breath, millions of particles are accompanying the inhaled air. This type of dispersion, where solid particles are suspended within air or another gas, is called an aerosol. Aerosols have been observed to cause severe health problems in urban areas, where elevated concentrations due to motor vehicle emissions and industrial emissions are associated with e.g. decreased lung function, asthma and cardiovascular diseases (Morawska et al. 1998; Morawska & Zhang 2002). The harmful particles can be e.g. asbestos particles used as isolation material in buildings. These can directly be linked to lung cancer (Miserocchi et al. 2008), and knowledge about the transport and deposition of such particles in the airways are important for improving health protection (Gradoň et al. 1991; Gavze & Shapiro 1998; Balkovsky et al. 2001). The same mechanism can be used also for usage of pharmaceutical aerosols in order to target drug delivery in the lungs (Martin & Finlay 2008). All aerosols are thus not harmful for the environment, and the spreading of some particles might actually rather be linked to creating life, such as the spreading of seeds and pollen (Okubo & Levin 1989; Kuparinen et al. 2009).

Higher up in the atmosphere, aerosols can have large effects on the global climate since they directly scatter light and comes in as an important parameter in the global radiation budget (Holländer 1993). The atmospheric aerosol particles also act as condensation nuclei for cloud droplet formation, and their behavior in turbulent flows are essential for explaining how rain is initiated (Balkovsky et al. 2001; Falkovich et al. 2002). The motion and collisions of particles in the clouds also determine the growth of ice crystals (Gavze et al. 2012) for example in the upper part of Cumulonimbus clouds leading to heavy rainfall and thunderstorms. Within the category of atmospheric aerosols, also
understanding the emission of ash from large volcanic eruptions is crucial for correct risk assessment within the aviation industry and can result in severe social and economical disruption (Stohl et al. 2011).

Volcanic eruptions also cause other geophysical flows, for example lava flows, where the motion of suspended crystal particles not only affect the effective viscosity of the flow (Mueller et al. 2011), but also determine the geological texture of the solidified flow, i.e. the formation of rock (Ventura et al. 1996).

Another example are rapid pyroclastic flows of hot ash particles along the sides of the volcano, destroying everything in its way. These flows are very hard to study, but the distribution of the sedimanted particles can give valuable insights to the flow situation prior to sedimentation (Sarocchi et al. 2008). Other geophysical gravity driven flows can also be better understood by the dispersed particle behavior, for example avalanches (Hutter 1996). Not only does the snow crystal distribution cause weak layers within the snow, crucial for avalanche initiation, the dynamics of the avalanche itself is dependent on dynamics of snow particles.

Continuing exploring dispersed particle flows within nature, we encounter several examples of solid particles that are suspended in a liquid instead of a gas. Below the surface of the ocean, plankton are more or less moving passively with the fluid flow. Due to turbulent environments, plankton can be clustered in certain regions, influencing the feeding, mating and capture rates of these small organisms (Guasto et al. 2012; Pécely et al. 2012). The motion of elongated plankton has an effect on the light scattered in the upper layers of the ocean, which affects the maximum depth where photosynthesis is possible. This in turn has a significant effect on how much carbon in the water that can be turned into organic compounds (Marcos et al. 2011; Guasto et al. 2012). The light scattering also has an effect on the reflectivity of the oceans, which influences global climate. Furthermore, velocity gradients in the flow can cause bacteria to have apreferential swimming direction, and thus be unevenly distributed within the ocean layers (Marcos et al. 2012; Stocker 2012).

Other examples of solid-liquid dispersions are found within the human body. At every instant, the flow of blood is crucial for our survival, carrying nutritions to the cells and carrying oxygen to all bodily tissues. The blood is a dispersion of blood plasma containing red blood cells (which carry oxygen from the lungs to the cells), white blood cells (which are important for the immune defense) and platelets (which are important for coagulation of blood). The blood effective viscosity is dependent on the particle motion just as in any dispersion and can thus be different for different flow situations. At the same time, clustering of particles can cause lethal diseases such as atherosclerosis. Understanding such formations, requires knowledge about particle behavior in flows and has attracted a lot of attention in the past years (Pozkiridis 2006; Laadhari et al. 2012; Reasor et al. 2013).
Predicting the behavior of dispersed particle flows is not only valuable in these naturally occurring examples. We can also use this knowledge in many industrial applications. In papermaking for example, the behavior of the paper fibers in a pulp flow determine the tensile properties of the final product (Lundell 2011a). The same is true for carbon fibers in composite moulding used for example to produce strong lightweight panels in cars (Le et al. 2008). Controlling the orientation of carbon nanotubes in polymer composites, can allow us create new materials with high electrical conductivity with small carbon content (Lanticse et al. 2006). Many materials are coated with a substrate for protection (e.g. lacquer), or in order to have e.g. certain optical (e.g. paint) or electrical properties. The substrate often consists of particles dispersed in some liquid and is sprayed onto the surface. Understanding the substrate properties can give us valuable information on how to optimize the design of spray nozzles in order to control both bonding properties and substrate distribution on the surface (Jen et al. 2005; Li et al. 2005). Transport and usage of coal-water mixtures for fuel requires knowledge of effective viscosity and settling rates of coal particles (Turian et al. 1992). Within food industry, where many products are dispersed particle flows, the effective viscosity of the product can be directly linked to mouthfeel, which is one of the main features that a consumer uses to choose between products (Finney Jr. 1973). Perhaps the most famous example within food industry is the so-called ketchup effect, where the dispersion seems to have lower viscosity when applying more stress to it, for example when shaking the ketchup bottle (a property called shear-thinning). This is also a property that can be understood through the interaction of particles dispersed in fluid (Bayod & Willers 2002).

All these examples indicate a tremendous potential benefit of understanding dispersed particle flows. Much research has already been done, but a large part of it is restricted by assuming perfectly spherical particles and/or assuming that particles are so small that all inertial effects are neglected leading to an ideal behavior where particles follow the streamlines of the flow.

The aim of the research presented in this paper is to provide fundamental knowledge of the behavior of non-spherical particles in fluid flows and in particular when inertia is taken into account. This can be a valuable input in order to answer important questions within science and engineering: How do aerosols spread? How do clouds form? How does blood flow? How can we improve drug delivery? How can we invent new materials and improve present material processes? What is the response of the global biosphere to a changing climate?
1. INTRODUCTION
CHAPTER 2

Prerequisite concepts

Before describing in detail how particles behave in flows, a short introduction will be given to the field of mechanics. Mechanics is used for predicting motion of an object when it is subject to a force. If we have an object located in space at \( \mathbf{x} = \mathbf{x}_0 \) moving with constant velocity \( \dot{\mathbf{x}} = \frac{d\mathbf{x}}{dt} = \mathbf{v}_0 \) at time \( t = 0 \), we know that the object will be located at \( \mathbf{x}(t) = \mathbf{v}_0 t + \mathbf{x}_0 \) at time \( t \). If the object has a constant acceleration, i.e. \( \ddot{\mathbf{x}} = \mathbf{a}_0 \), the position of the object is known at any time \( t \) through the relation \( \mathbf{x}(t) = \frac{1}{2} \mathbf{a}_0 t^2 + \mathbf{v}_0 t + \mathbf{x}_0 \). Since the acceleration of an object is related to the forces acted upon them, knowing the forces leads to full understanding of the motion of an object.

2.1. Rigid body dynamics

The field of mechanics was pioneered by Isaac Newton in 1687, when a few simple laws were presented, which related motion of objects to forces acted upon them. These can be summarized as follows:

1. In a non-accelerating reference system, an object will be at rest or move with constant velocity \( \mathbf{v} \) if not subject to an external force.
2. An object will be accelerated in proportion to the magnitude of an external net force \( \mathbf{F} \) and in the same direction. The magnitude of acceleration \( \mathbf{a} \) is inversely proportional to the mass \( m \). Mathematically this is written
   \[
   \mathbf{F} = m\mathbf{a}. \tag{2.1}
   \]

3. For every force from an object A on an object B, there will be a reaction force of the same magnitude and in opposite direction from B on A.

The equation 2.1 can be expressed as a conservation law of the quantity \( \mathbf{\phi} = m\mathbf{v} \), called momentum, by writing
   \[
   \mathbf{F} = \frac{d\mathbf{\phi}}{dt} = \dot{\mathbf{\phi}}. \tag{2.2}
   \]

The conservation of momentum thus implies that the time derivative of an
object’s momentum must equal the net force acted upon it. Consider two colliding particles with momentum \( \varphi_1 \) and \( \varphi_2 \) prior to the collision without any external forces (see figure 2.1). During the collision, particle 1 is affected by a force \( F_{12} \) from particle 2 during a short collision time \( \Delta t \), which changes its momentum to \( \varphi'_1 \). Equation 2.2 gives thus \( F_{12} \Delta t = \varphi'_1 - \varphi_1 \). Similarly, particle 2 will change its momentum according to \( F_{21} \Delta t = \varphi'_2 - \varphi_2 \). Then from Newton’s third law we know that the force from particle 2 on particle 1 is \( F_{21} = F_{12} \). The relations can be combined into

\[
\varphi'_1 + \varphi'_2 = \varphi_1 + \varphi_2,
\]

i.e. the total momentum of the two particle system is constant during the collision, and is said to be conserved. Even though this relation is not sufficient to determine the individual momentum of each particle after collision, we can state two things about a closed colliding particle system in the absence of external forces:

1. The total mass of the particles will be conserved.
2. The total momentum of the particles will be conserved.

A conservation law for a particle’s rotation can similarly be derived from equation 2.2 if the particle is rigid (i.e. all points within the particle have the same relative distance between one another at any time), where the time derivative of the angular momentum around point \( O \), \( \dot{L}_O \) equals the net torque \( M_O \) acting on the object, i.e.

\[
M_O = \dot{L}_O = I \ddot{\omega} + \omega \times (I \cdot \omega),
\]

where \( I \) is called the inertial tensor of the particle and \( \omega \) is the angular velocity of the particle. Analogue to the conservation for momentum in terms of particle translation, angular momentum is also a conserved quantity for particle rotation. This means that a particle can’t gain angular momentum without being subject to an external torque.
2.1. RIGID BODY DYNAMICS

2.1.1. Understanding inertia

This thesis will mainly talk about the effect of inertia, and therefore it is important to understand what these effects come from.

Suppose you are sitting in a car moving with constant velocity (see figure 2.2). This system can be referred to as a *inertial frame of reference*, since all objects with mass $m$ within the car will get the acceleration $a = F/m$ relative to the car if it is subject to a force $F$. If the car is now braking with a constant acceleration $a_0$, you feel some force that is pushing you forward against the seatbelt. What did this force come from? This force can be referred to as an *inertial force* and appears during the deceleration of the car. The car becomes a non-inertial frame of reference since it is accelerated relative to the earth (which can be thought of as an inertial frame of reference). The inertial force that you are feeling is exactly equal to $F_{\text{inertia}} = ma_0$. During the deceleration, an object with mass $m$ will namely get the acceleration $a = \frac{F + \text{max}}{m}$ relative to the car if it is subject to a force $F$.

Another example is if you are sitting in a carousel spinning with angular velocity $\omega_0$. In order to maintain your rotational motion, you are always affected by an acceleration towards the center of the carousel. This means that
a reference frame traveling with you is not an inertial frame of reference and
you thus feel a force pushing you away from the center. This inertial force is
called a centrifugal force. Again we can treat dynamics in this rotating frame
of reference as an inertial frame of reference by introducing fictitious inertial
forces. Another important consequence of the centrifugal forces acting on an
object with mass rotating around an axis, is that it will always tend to rotate
in such a way that mass of the particle is concentrated as far away as possible
from the rotational axis.

2.2. Fluid dynamics and the Navier-Stokes equations

Within a gas and a liquid molecules move around more or less freely accord-
ing to the laws presented in the previous section, i.e. conserving mass and
momentum as long as no external forces act on the system. However the ex-
change of momentum between molecules is much more complicated than just
through direct collisions. The rate at which momentum is transported through
the medium can be found at a macroscopic scale as a type of friction, or a
resistance to deformation of the medium. This friction is referred to as the
dynamic viscosity $\mu$ of the gas or liquid and has the units $\text{Pa} \cdot \text{s}$. In a gas,
molecules are not so close together, giving them lower probability to interact
and the momentum transport is low. Therefore the dynamic viscosity is low.
In a liquid, molecules are more closely packed allowing them to interact more
and therefore have a higher dynamic viscosity. Even though the microscopic in-
teractions are very different between liquids and gases, in terms of macroscopic
motion, a liquid and a gas have exactly the same behavior, but of course still
with differences in density and dynamic viscosity. Therefore gases and liquids
will further on be referred to as fluids. In terms of motion of the fluid, it is
usually more convenient to use the kinematic viscosity $\nu = \mu/\rho_f$, where $\rho_f$ is
the fluid density. A fluid with constant viscosity is called a Newtonian fluid,
but it should be noted that this is a theoretical assumption and is not always
valid for all real fluids.

Even though the motion and interactions between molecules within the
fluid are well known and could be described with the principles provided in the
previous section, the individual motion of more than $10^{23}$ molecules, usually
encountered in fluid flows, is a lot harder to predict. Instead, in fluid dynamics,
the fluid is usually treated as a continuum, i.e. fluid occupies every single ponit
in space. At each point, the motion of the fluid is described by its velocity
$\mathbf{u}$, pressure $p$ and density $\rho_f$ at every time instant $t$. When the flow is slow
relative to the sound speed through the medium, the fluid can be assumed
incompressible. This means that there can be no variations of density within
the medium, i.e. $\rho_f$ is a constant. Still, when treating the fluid as a continuum,
it must still obey the laws of mass and momentum conservation. Applying
Newton’s laws to a small control volume in the fluid, we can write the mass
conservation criteria as
2.3. DIMENSIONAL ANALYSIS

\[ \nabla \cdot \mathbf{u} = 0, \quad (2.5) \]

and the momentum conservation (without any external forces acting on the fluid) as

\[ \rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \rho_f \nu \nabla^2 \mathbf{u}, \quad (2.6) \]

where the left hand side denotes the rate of change of momentum in the control volume and the right hand side denotes the stresses on the control volume due to pressure forces and viscous diffusion of momentum from/to the surrounding fluid. These two equations, called the isothermal incompressible Navier-Stokes equations, combined with desired boundary conditions are sufficient for describing the full fluid motion. However, due to the non-linear \((\mathbf{u} \cdot \nabla) \mathbf{u}\) term on the left hand side, a solution can usually not be found analytically. Nevertheless, through the help of computers nowadays, solutions can be obtained by numerical integration.

If a viscous fluid is flowing over a solid wall, transfer of momentum will also take place between the wall and the fluid closest to the wall. The consequence is that molecules close to the wall, on average will assume the same velocity as the wall. This is called a no slip condition, and is true as long as the fluid can be described as a continuum. The momentum transfer leads to a force per unit area in the flow direction, i.e. a shear stress \(\tau_w\), on the solid wall. If we define the flow in \(x\)-direction, and \(y\) as the wall normal direction (see figure 2.3), the wall shear stress can be expressed as

\[ \tau_w = \rho_f \nu G_w \mathbf{e}_x, \quad (2.7) \]

where \(G_w = \partial u_x / \partial y\) is the gradient of the velocity, or the shear rate at the wall. This type of force is the typical force that will be affecting the particle in the flow in this thesis.

2.3. Dimensional analysis

In the previous section the Navier-Stokes equations were presented (eqs. 2.5 and 2.6), which determine the fluid motion. In order to analyze the properties of such equations, it is very useful to write them down in non-dimensional form. Suppose we have a flow over a spherical particle. We can already assume that the flow will look different if we change the viscosity \(\mu\), fluid density \(\rho_f\), size of particle \(L\) and/or incoming velocity \(U\), i.e. 4 free parameters. Analyzing the dependence on all these independent physical parameters might be tedious work. This can be significantly simplified through a scaling of the equations. This is explained by Buckingham’s II theorem (Buckingham 1914),
which states that any physically meaningful equation with \( n \) physical variables and \( k \) fundamental dimensions, can be rescaled in a way that the equation only depends on \( n - k \) non-dimensional variables. In mechanics, the fundamental dimensions are usually just mass, length and time, i.e. \( k = 3 \). This means that the Navier-Stokes equations can be rescaled in a way that it only depends on one dimensionless parameter. We can do this by doing the following scalings (non-dimensional quantities/operators, denoted with primes): 

\[
\begin{align*}
\mathbf{u} &= U' \mathbf{u}', x = Lx', y = Ly', z = Lz', t = (L/U)t', \nabla = (1/L)\nabla'.
\end{align*}
\]

The scaling of the pressure is not obvious, and we can choose to scale it either scales with the dynamic forces, i.e. \( p = \rho f U'^2 p' \) (typical for high speed flows) or viscous forces, i.e. \( p = (\rho f U \nu / L)p' \) (typical for low speed flows). Introducing this in eqs. 2.5 and 2.6, we arrive at the non-dimensional form of the mass conservation equation

\[
\nabla' \cdot \mathbf{u}' = 0, \tag{2.8}
\]

and the momentum conservation, either using \( p = \rho f U'^2 p' \)

\[
\frac{\partial \mathbf{u}'}{\partial t'} + (\mathbf{u}' \cdot \nabla') \mathbf{u}' = -\nabla' p' + \frac{\nu}{UL} \nabla'^2 \mathbf{u}', \tag{2.9}
\]

or using \( p = (\rho f U \nu / L)p' \)

\[
\frac{UL}{\nu} \left( \frac{\partial \mathbf{u}'}{\partial t'} + (\mathbf{u}' \cdot \nabla') \mathbf{u}' \right) = -\nabla' p' + \nabla'^2 \mathbf{u}'. \tag{2.10}
\]

The equations thus only depend on one single non-dimensional parameter,
2.3. DIMENSIONAL ANALYSIS

called a Reynolds number, \( Re = UL/\nu \) and can be seen as a measure of inertia in the flow, i.e. how much the flow at current time is depending on the the flow at previous time. For high speed flows, when \( Re \rightarrow \infty \), the viscous term in eq. 2.9 become vanishingly small compared to the inertial terms on the left hand side. Small eddies and swirls can’t be damped out, and the flow becomes turbulent. For low speed flows, when \( Re \rightarrow 0 \), the left hand side in eq. 2.10 vanishes, which means that there is no inertia in the flow and the momentum conservation equation simplifies to

\[
\nabla' \rho' = \nabla'^2 \mathbf{u}'.
\]  

(2.11)

The flow is in this case not dependent on time, and will instantly assume the flow field that balances pressure forces with viscous diffusion of momentum. This type of flow is called Stokes flow.

The same type of dimensional analysis can be done for the particle equations of motion in eqs. 2.2 and 2.4. In the flow situation that will be considered in this thesis, the flow can be assumed to be low speed (compared to the time scale of the particle), and the pressure forces will rather scale with viscous forces (the type of forces we considered in eq. 2.7). This means that pressure in the flow scales with \( p = (\rho_f U \nu/L) \rho_p \) and the characteristic force and torque on the particle thus becomes \( \mathbf{F} = L^3 \cdot (\rho_f U \nu/L) \rho_p \mathbf{F}' \) and \( \mathbf{M_O} = L^3 \cdot (\rho_f U \nu/L) \mathbf{M_O}' \), respectively. Time is scaled as before, \( t = (L/U) t' \) and other scalings that will be used are: \( \mathbf{\varphi} = \rho_p L^3 \mathbf{\varphi}' \), \( \mathbf{I} = \rho_p L^5 \mathbf{I}' \), \( \omega = (U/L) \omega' \). The non-dimensional form of the particle equations of motion becomes

\[
\mathbf{F}' = \frac{\rho_p}{\rho_f} \frac{U L d \mathbf{\varphi}'}{\nu dt'}
\]  

(2.12)

\[
\mathbf{M_O}' = \frac{\rho_p}{\rho_f} \frac{U L}{\nu} (I' \dot{\omega'} + \omega' \times (I' \cdot \omega')).
\]  

(2.13)

The non-dimensional group seen at the right hand side of both equations is called a Stokes number, \( St = (\rho_p/\rho_f) \cdot (UL/\nu) = (\rho_p/\rho_f) Re \). This number is a measure of the influence of inertia of the particle. As we see however, it is dependent on the inertia of the fluid through a linear dependence of the Reynolds number, \( Re \). If particles are extremely light or extremely small, such that \( St \rightarrow 0 \), the right hand side of both equation 2.12 and 2.13 will equal zero, and the particles will act as passive tracers that are following the streamlines of the flow. To summarize, if we want to analyze the effect of both fluid and particle inertia on the dynamics of particles in flows, the following set of equation must be solved:

\[
\nabla' \cdot \mathbf{u}' = 0
\]  

(2.14)
2. PREREQUISITE CONCEPTS

\[ Re \left( \frac{\partial u'}{\partial t'} + (u' \cdot \nabla') u' \right) = -\nabla' p' + \nabla'^2 u', \quad (2.15) \]

for the fluid motion, with no slip condition on the particle surface (plus other suitable boundary conditions depending on flow problem) and

\[ F' = St \cdot \frac{d\phi'}{dt'} \quad (2.16) \]

\[ M'O' = St \cdot (I' \dot{\omega}' + \omega' \times (I' \cdot \omega')). \quad (2.17) \]

for the particle motion, where force and torque on the particle are obtained through the shear stress and pressure on the particle surface. The motion of the particle can thus be determined by varying two parameters \( Re \) and \( St \).

The specific flow problem that will be covered in this thesis will be described in detail in the next chapter.

2.4. Non-linear dynamics and bifurcations

In order to understand the behavior of non-linear dynamical systems, one must know what type of motions we can expect in different types of systems and which transitions that are typically encountered. In this section, some fundamental behavior will be described through a set of examples. The importance of these examples in order to understand the particle behavior in flows will be seen later in this thesis. The concepts presented in this section can also be found in other literature (Holmes & Rand 1980; Hale & Koçak 1991; Strogatz 1994; Schenk-Hoppé 1996).

2.4.1. The pendulum

This section will describe the motion of a pendulum with a mass \( m \) attached to a massless rod of length \( l \), with the other end attached in space. The motion is constrained to a one-dimensional rotation around the attached end of the rod, with an angle \( \phi \in [-\pi, \pi] \) between the rod and the vertical direction along which there is a gravitational acceleration \( g \) (see figure 2.4).

The general motion of a pendulum is described with the following equation:

\[ ml^2 \ddot{\phi} = M_{grav.} + M_{diss.} + M_{ext.}, \quad (2.18) \]

where \( M_{grav.} = -mgl \sin \phi \) is the torque from the gravity force, \( M_{diss.} \) is the torque from friction forces and \( M_{ext.} \) is some other external torque.
2.4. NON-LINEAR DYNAMICS AND BIFURCATIONS

2.4.1a. No energy dissipation. In the case of no friction and no external torque, the equation simplifies to

\[ \ddot{\phi} = -\frac{g}{l} \sin \phi. \]  

(2.19)

Since no energy is dissipated, the system is conservative and the oscillations of the pendulum will be determined by the initial angle \( \phi \) and angular velocity \( \dot{\phi} \). If the pendulum is released at \( \phi = \dot{\phi} = 0 \), the pendulum will be at equilibrium and not oscillate and stay there since \( \ddot{\phi} = 0 \). Small deviations from this initial orientation will lead to small oscillations according to \( \ddot{\phi} = -\frac{g}{l} \phi \) (for small angles, \( \sin \phi \approx \phi \)). This special case at \( \phi = \dot{\phi} = 0 \) is called a center. When the pendulum is released from \( \phi = \pm \pi \) and \( \dot{\phi} = 0 \), this will also be at an equilibrium since \( \phi = \dot{\phi} = 0 \), but small deviations will grow exponentially, and this unstable location is called a saddle. A hypothetical orbit where the pendulum starts from the saddle, rotates and reaches the same saddle again is said to be a homoclinic orbit. Apart from these special cases, there are an infinite amount of closed orbits depending on the initial angle and angular velocity that can be illustrated with a phase diagram in figure 2.5a.

2.4.1b. The damped pendulum. Adding damping to the pendulum, means that there will be some friction that is trying to resist the motion. This can be realized for example by putting the pendulum in a very viscous fluid, and the momentum of the pendulum will be transferred to momentum in the fluid. The damping term will in this case be linear according to \( M_{\text{diss.}} = -C \dot{\phi} \), where \( C \) is a positive constant.

\[ \ddot{\phi} = -\frac{g}{l} \sin \phi - \frac{C}{ml^2} \dot{\phi}. \]  

(2.20)
The system will in this case always (unless exactly released at the saddle at $\phi = \pm \pi$ and $\dot{\phi} = 0$) lose energy until reaching the point of minimum potential energy at $\phi = \dot{\phi} = 0$. What previously was a center at this location is transformed into a stable fixed point in the damped case. In order to characterize the behavior close to this point, it is useful to linearize the system around $\phi = \dot{\phi} = 0$ (where $\sin \phi \approx \phi$) according to:

$$
\begin{pmatrix}
\dot{\phi} \\
\ddot{\phi}
\end{pmatrix} =
\begin{pmatrix}
0 & 1 \\
-g/l & -C/ml^2
\end{pmatrix}
\begin{pmatrix}
\phi \\
\dot{\phi}
\end{pmatrix}.
$$

(2.21)

The eigenvalues of the matrix $A$ are given by

$$
\lambda_{1,2} = \frac{Tr(A)}{2} \pm \sqrt{\frac{Tr(A)^2}{4} - Det(A)}.
$$

(2.22)

As long as the trace of $A$ is negative, the fixed point will be stable, i.e. if $Tr(A) = -C/(ml^2) < 0$ all nearby trajectories will approach the fixed point. If $Tr(A)^2 < 4 \cdot Det(A)$, i.e. if $C^2/(m^2 l^4) < 4g/l$, the eigenvalues will be imaginary and the trajectories will spiral towards the fixed point. The system is weakly damped and the pendulum will make small oscillations around the equilibrium position until they eventually die out. On the other hand if $C^2/(m^2 l^4) > 4g/l$, the system is strongly damped and the eigenvalues will be real and negative. The pendulum will then tend to approach the fixed point along the eigendirection of the lowest (and also slowest) eigenvalue. The phase diagram of the damped pendulum is shown in figure 2.5b.
2.4. NON-LINEAR DYNAMICS AND BIFURCATIONS

2.4.1c. *The driven and strongly damped pendulum.* Assume now that we apply a constant external torque to the pendulum, i.e. $M_{\text{ext}} = M$. The governing equation then becomes

$$\ddot{\phi} = -\frac{g}{l} \sin \phi - \frac{C}{ml^2} \dot{\phi} + \frac{M}{ml^2}.$$  \hspace{1cm} (2.23)

If the system is strongly damped $m^2 gl^3/C^2 \rightarrow 0$ (found through dimensional analysis), the inertia of the system can be neglected, i.e. $\ddot{\phi} = 0$ always, and the angular velocity $\dot{\phi}$ is just a function of the orientation.

$$\dot{\phi} = \frac{M}{C} - \frac{mgl}{C} \sin \phi.$$ \hspace{1cm} (2.24)

If $M > mgl$, the motion will be a periodic rotation and the angular velocity of the pendulum will have a minimum at $\phi_0 = \pi/2$, where the gravitational torque is largest and counteracting the external torque (see figure 2.6a). When $M < mgl$, two fixed points are created where $\sin \phi = M/mgl$, one stable and one unstable (see figure 2.6c). The long term behavior of the pendulum will in this case be restricted to a motionless state at the stable orientation where the external torque is balanced by the gravitational torque. The transition from a periodic rotation to a steady state is through an infinite-period saddle-node bifurcation. Close to the transition at $M \lesssim mgl$, the period of the rotation is determined by how long time it spends in a region $\phi_1 \lesssim \phi_0 \lesssim \phi_2$. In this region, the angular velocity can be expanded using $\sin \phi = \cos (\phi - \phi_0) \approx 1 - (\phi - \phi_0)^2$

$$\dot{\phi} = \epsilon + A(\phi - \phi_0)^2,$$ \hspace{1cm} (2.25)

where $\epsilon = (M - mgl)/C$ and $A = mgl/C$. The period of the rotation can thus be found to be

$$T = \int_{-\pi}^{\pi} \frac{d\phi}{\epsilon + A(\phi - \phi_0)^2} \approx \int_{0}^{2\pi} \frac{d\phi}{\epsilon + A(\phi - \phi_0)^2} \approx \int_{0}^{2\pi} \frac{d\phi}{\epsilon + A(\phi - \phi_0)^2} \approx \int_{-\infty}^{\infty} \frac{dx}{x^2} = \frac{\pi}{\sqrt{\epsilon}}.$$ \hspace{1cm} (2.26)

The divergence of the period according to $T \propto \epsilon^{-1/2}$ is typical for an infinite-period saddle-node bifurcation in any dynamical system and the transition parameter $\epsilon$ can be any parameter that leads to the bifurcation at $\epsilon = 0$.

2.4.1d. *The driven and weakly damped pendulum.* If the damping is low, the motion is governed by the full equation 2.23. For this case, fixed points are also created in a saddle-node bifurcation at $M = mgl$, but the period does not diverge at this point, and a periodic rotation can be found even for $M < mgl$. The reason is that the damping close to the fixed points is not enough to make
Figure 2.6. Schematic phase diagram of a damped pendulum with an external torque $M_{\text{ext}} = M$: (a) $M > mgl$ (strong damping); (b) $M > mgl$ (weak damping), inertia will cause $\dot{\phi}$ to be almost constant during the period; (c) $M < mgl$ (strong damping); (d) $M < mgl$ (weak damping and $M \lesssim M_c$); (e) $M = M_c < mgl$; (f) $M_c < M < mgl$; the blue area in figure show the conditions enclosed by the stable manifold of the saddle (SM) that lead to the steady state; one unstable manifold of the saddle (UM) leads to steady state and one leads to the periodic orbit.
the pendulum stop and the inertia of the pendulum is causing it to maintain its rotation. The fixed points still exist, and the pendulum will stay in a motionless state if it is released at rest close to the stable fixed point. The system thus is *bistable* and both a periodic and a steady state are co-existing and depending on initial angle and angular velocity. If in the periodic rotation, eventually at some critical driving torque, $M = M_c < mgl$, the period will diverge and the steady state will be the only long term solution of the system. The bifurcation occurring at $M = M_c$ is called a *homoclinic bifurcation* and is best illustrated in a phase diagram in figure 2.6d-f.

At $M = mgl$, one stable fixed point $\phi_c$ and one unstable saddle $\phi_{us}$ are created and as long as $M < M_c$, both unstable manifolds of the saddle are leading to the stable fixed point, i.e. the steady state (see figure 2.6d). At $M = M_c$, the stable and unstable manifolds are merged, creating a *homoclinic orbit*, where the saddle is connected to itself (see figure 2.6e). At $M_c < M < mgl$, the steady state is co-existing with the periodic orbit as a long term solution of the motion (see figure 2.6f). One of the unstable manifolds of the saddle is leading to the periodic orbit and one to the stable fixed point. The stable manifold of the saddle acts as a delimiter between trajectories leading to the periodic orbit and trajectories leading to the stable fixed point. Close to the bifurcation at $M = M_c$, the periodic orbit $\phi(\dot{\phi})$ has a non-differentiable appearance and the square-root scaling that was seen in the strongly damped case does not apply. Instead it can be shown that the period diverges according to $T \propto \ln |M - M_c|$ for the homoclinic bifurcation.

When the mass of the pendulum $m$ is very large, inertia will cause the pendulum not to be accelerated so rapidly by gravity at $\phi = -\pi/2$, but also not being easily decelerated when reaching $\phi = \pi/2$. The result is that the angular velocity of the pendulum becomes almost constant, seen in figure 2.6b.

The dynamics of the driven damped pendulum can be summarized in a state diagram in figure 2.7, illustrating the possible long term solutions for the system depending on the magnitude of the damping and the driving torque.

### 2.4.2. The bead on a rod

Now we are going to turn to another dynamical system, which is a bead on a rod which can slide along a rod in the $x$-direction, illustrated in figure 2.8. The bead with mass $m$ is attached at $x = 0$ with a restoring force, for example a spring, proportional to the distance to the center and friction between bead and rod causes a damping force proportional to the velocity $\dot{x}$. The motion is thus governed by the following equation of motion

$$\ddot{x} = \alpha x + \beta \dot{x}. \quad (2.27)$$
2. PREREQUISITE CONCEPTS

![Diagram](image)

**Figure 2.7.** Schematic state diagram showing the different long term dynamical solutions of the pendulum with damping \( C \) and external torque \( M \): three types of bifurcations can occur: an infinite-period saddle-node bifurcation (IP-SN), a saddle-node bifurcation (SN) or a homoclinic bifurcation (HC).

![Diagram](image)

**Figure 2.8.** Illustration of the dynamical problem of a bead that can slide in the \( x \)-direction along a rod; the bead is experiencing restoring forces illustrated with a spring and damping forces that typically can arise from friction between bead and rod.

As long as \( \alpha \) and \( \beta \) are even functions of \( x \), the system will have odd symmetry, i.e. \( -\ddot{x}(x, \dot{x}) = \ddot{x}(-x, -\dot{x}) \).

**2.4.2a. Linear spring and linear damping.** The simplest case, is when \( \alpha = \mu_1 \) and \( \beta = \mu_2 \) are constants.

\[
\ddot{x} = \mu_1 x + \mu_2 \dot{x}.
\] (2.28)

The eigenvalues of this linear system can be found as in section 2.4.1b as:
2.4. NON-LINEAR DYNAMICS AND BIFURCATIONS

\[ \mu_1 \phi + \mu_2 \dot{\phi} = \phi \dot{\phi} \]

Figure 2.9. Typical phase diagrams for the bead on a rod with linear spring and linear damping depending on parameters \( \mu_1 \) and \( \mu_2 \).

\[ \lambda_{1,2} = \frac{\mu_2}{2} \pm \sqrt{\frac{\mu_2^2}{4} + \mu_1}. \quad (2.29) \]

If \( \mu_1 < 0 \) and \( \mu_2 = 0 \), equation 2.28 is describing a harmonic oscillator, where the position at \( x = \dot{x} = 0 \) is a center and an infinite amount of periodic oscillations are allowed depending on initial position. If \( \mu_1 < 0 \) and \( \mu_2 < 0 \), which is the usual case for a real spring and physical damping, the eigenvalues will always have a negative real part, and all trajectories will lead to \( x = \dot{x} = 0 \). This point is then a stable fixed point. Depending on the choice of \( \mu_1 \) and \( \mu_2 \) we will get different phase diagrams (see figure 2.9).

2.4.2b. Non-linear spring and linear damping (Duffing oscillator). If we now assume that the restoring force has a non-linear appearance with \( \alpha = \mu_1 - x^2 \) and \( \beta = \mu_2 \), we arrive at the Duffing oscillator

\[ \ddot{x} = \mu_1 x + \mu_2 \dot{x} - x^3. \quad (2.30) \]

We start by observing the case where \( \mu_2 < 0 \), i.e. damping is always resisting the motion. On long distances from the center, the restoring force will always be towards the center. However, if \( \mu_1 > 0 \), the center will be unstable and the motion will be away from the center. There will thus be two symmetrical stable fixed points at \( \pm \sqrt{\mu_1} \). The bifurcation occurring at \( \mu_1 = 0, \mu_2 < 0 \) is
called a *supercritical pitchfork bifurcation*. The phase diagrams of this system depending on parameters $\mu_1$ and $\mu_2$ is seen in figure 2.10.

2.4.2c. Linear spring and non-linear damping (Van der Pol oscillator). If we keep the restoring force linear, but instead make the damping non-linear with $\alpha = \mu_1$ and $\beta = \mu_2 + x^2$, we arrive at the Van der Pol oscillator

$$\ddot{x} = \mu_1 x + \mu_2 \dot{x} + x^2 \dot{x}. \quad (2.31)$$

We start by considering $\mu_1 < 0$, i.e. the restoring force is always to the center. The non-linear term is amplifying large disturbances. If $\mu_2 < 0$, small disturbances are damped and $x = \dot{x} = 0$ is a stable fixed point. For some oscillations, the amplification and damping cancel out, and there is an unstable limit cycle, outside which trajectories will go to infinity while trajectories inside go to $x = \dot{x} = 0$. Increasing $\mu_2$, the limit cycle will shrink and at $\mu_2 > 0$, it has vanished and all disturbances are amplified. The bifurcation that has occurred at $\mu_2 = 0, \mu_1 < 0$ is called a *subcritical Hopf bifurcation*. The figure 2.11 show the different phase diagrams for the Van der Pol oscillator.

2.4.2d. Non-linear spring and non-linear damping (Duffing-Van der Pol oscillator). Now we combine the two systems, such that we have both non-linear restoring force and non-linear damping with $\alpha = \mu_1 - x^2$ and $\beta = \mu_2 + x^2$. The result is the Duffing-Van der Pol oscillator

---

**Figure 2.10.** Typical phase diagrams for the bead on a rod with non-linear spring and linear damping (Duffing oscillator) depending on parameters $\mu_1$ and $\mu_2$. 
2.4. NON-LINEAR DYNAMICS AND BIFURCATIONS

\[ \ddot{x} = \mu_1 x + \mu_2 \dot{x} - x^3 + x^2 \dot{x}. \]  

(2.32)

This system is a bit more complicated but has both the characteristics of the Duffing oscillator and the Van der Pol oscillator as seen from the phase diagrams in figure 2.12. There still is a subcritical Hopf bifurcation at \( \mu_1 < 0, \mu_2 = 0 \) and still a supercritical pitchfork bifurcation at \( \mu_2 < 0, \mu_1 = 0 \). Additionally one can observe a \textit{supercritical Hopf bifurcation} at line I, a \textit{breaking of the saddle connection} at line II and a \textit{saddle-node bifurcation of limit cycles} at line III.

We will see later on in this thesis, that this special system is very relevant when it comes to describing the motion of prolate spheroidal particles in shear flows.
Figure 2.12. Typical phase diagrams for the bead on a rod with non-linear spring and non-linear damping (Duffing-Van der Pol oscillator) depending on parameters $\mu_1$ and $\mu_2$. 
Flow problem and historical perspective

The long term goal of this field of work is to understand and predict dispersed particle flows encountered both in nature and in industry. The flow situations can be very complex, but on smaller scales, i.e. on the length scales of the particles, the flow fields are usually a lot simpler. On these scales, the flow velocity can be linearized around the location of the particle \( x_0 \) according to

\[
U(x, t) = U(x_0, t) + \nabla U(x_0, t) \cdot (x - x_0).
\]  

(3.33)

The first term denotes a flow with constant velocity, and a particle released in such a flow will experience a force leading to a translation according to equation 2.16 and will thus not affect particle orientation. The second term denotes a linear gradient of the velocity, and a particle in this type of flow will experience a torque leading to a rotation according to equation 2.17 if the gradient is perpendicular to the flow direction. Assuming that the particle is not accelerated too much, one can consider a translating inertial frame of reference with the particle at the center and the particle is only experiencing a linear shear flow and a rotational motion (see figure 3.1). However, the rotational motion of non-spherical particles in a linear shear flow is not fully understood. The first order approximation of a non-spherical particle is a spheroid, and this type of particle considered here.

The main goal of this thesis is to describe the rotational behavior of spheroidal particles in a simple shear flow and to analyze the consequences this has for a suspension of such particles.

3.1. The simple shear flow

The simple shear flow can be described by the equation

\[
\begin{pmatrix}
u_x \\
u_y \\
u_z
\end{pmatrix} = \begin{pmatrix}
0 & G & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} \begin{pmatrix}x \\y \\z
\end{pmatrix},
\]  

(3.34)
3. FLOW PROBLEM AND HISTORICAL PERSPECTIVE

![Image of flow problem and historical perspective](image)

**Figure 3.1.** Illustration of the principle of linearizing the flow around a suspended particle.

**Figure 3.2.** Linear decomposition of the simple shear flow into strain and vorticity flow.

with $G$ as the shear rate of the flow. The matrix can be decomposed into a symmetric and an anti-symmetric part

$$
\begin{pmatrix}
0 & G & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
= 
\begin{pmatrix}
0 & G/2 & 0 \\
G/2 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
+ 
\begin{pmatrix}
0 & G/2 & 0 \\
-G/2 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix},
$$

(3.35)

where the symmetric part is denoting a strain flow ($\mathbf{u} = \mathbf{D}\mathbf{x}$) and the anti-symmetric part is denoting a rotating flow ($\mathbf{u} = \mathbf{V}\mathbf{x}$). The simple shear flow is thus just a linear combination of these two flows (illustrated in figure 3.2).

The easiest way of creating a linear shear flow is to have fluid contained between two parallel walls moving in $x$-direction with velocity $U_w$ and $-U_w$, respectively, and separated with distance $N$. This creates a shear flow with
3.2. The Spheroid

In this thesis, all particles are treated as rigid bodies. The particles will thus not deform and their motion is solely determined by its translation (determined by equation 2.16) and rotation (determined by equation 2.17). In the case of a single particle in a flow, the net force and torque will be given by the surrounding fluid acting on the particle surface.

This work is intending to describe the motion of non-spherical particles, and one of the most general form of a non-spherical particle is a spheroid. A spheroidal particle can be seen as a spherical particle that either is "pulled out" or "squished together". In mathematical terms, the particle surface is described by:

\[
\frac{x'^2}{a^2} + \frac{y'^2}{b^2} + \frac{z'^2}{b^2} = 1,
\]

where \((x', y', z')\) denotes a body-fixed coordinate system, \(a\) is an axis of rotational symmetry and \(b\) is the equatorial radius. If \(a = b\), we recover the equation for a sphere with radius \(b\). If \(a > b\), the particle has the shape similar to that of a grain of rice and is called a *prolate* spheroid (figure 3.3a). If \(a < b\),

---

**Figure 3.3.** Illustration of a spheroid; (a) a prolate spheroid; (b) an oblate spheroid; the red arrow indicates the axis of rotational symmetry.

constant shear rate \(G = 2U_w / N\). However, introducing walls has an influence on the particle rotation, which is minimized by keeping the confinement \(\kappa = l / N\) low (\(l\) is the length of the particle major axis). The space-fixed Cartesian coordinate system will be oriented, such that \(x\) is aligned with the flow direction, \(y\) is aligned in the velocity gradient direction and \(z\) is aligned with the vorticity direction.
the particle has the shape of a disc and is called an *oblate* spheroid (figure 3.3b). In this thesis, the aspect ratio of the particle $r_p$ will always be a quantity larger than unity and is thus defined as $r_p = a/b$ for a prolate spheroid and $r_p = b/a$ for an oblate spheroid. The inertial tensor $I$ in dimensional form for the spheroidal particle is

$$I = \frac{\rho_p V_p}{5} \begin{pmatrix} 2b^2 & 0 & 0 \\ 0 & a^2 + b^2 & 0 \\ 0 & 0 & a^2 + b^2 \end{pmatrix},$$ (3.37)

where $\rho_p$ is the density and $V_p = 4\pi ab^2/3$ is the volume of the particle. The orientation of the particles will be described by the Euler angles $(\phi, \theta, \psi)$, where $\phi$ is the angle between the $x$-axis and the projection of the particle symmetry axis on the $xy$-plane, $\theta$ is the angle between the $z$-axis and the particle symmetry axis and $\psi$ is the angle around the symmetry axis (this angle is of less
interest, due to the rotational symmetry of the particle). The flow problem is illustrated in figure 3.4.

3.3. Governing equations

In the previous chapter, the non-dimensional form of the incompressible Navier-Stokes equations and the particle equations of motion were introduced. They showed a dependence on two dimensionless numbers, the Reynolds number $Re = UL/ν$ and the Stokes number $St = (ρ_p/ρ_f)·Re$. To define these numbers, a suitable velocity scale $U$ and length scale $L$ must be chosen for the problem. The natural choice for a length scale is the length of the particle major axis, i.e. $L = l = 2a$ for a prolate spheroid and $L = l = 2b$ for an oblate spheroid. The velocity scale chosen for the problem is the maximum fluid velocity difference along the particle, i.e. $U = G·l$. Furthermore, the translation of the particle is not of interest here, since there is no net force acting on the particle due to the symmetrical flow problem. The governing equations are thus (primes for showing non-dimensional quantities are dropped):

\[ \nabla \cdot \mathbf{u} = 0 \quad (3.38) \]

\[ Re_p \cdot \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla^2 \mathbf{u}, \quad (3.39) \]

for the fluid motion, with $\mathbf{u} = \mathbf{ω} \times \mathbf{r}$ on the particle surface to ensure the no slip condition (plus other suitable boundary conditions further away from the particle) and

\[ M_O = St \cdot (I\dot{\mathbf{ω}} + \mathbf{ω} \times (I \cdot \mathbf{ω})). \quad (3.40) \]

for the particle rotation. The dimensionless numbers $Re_p$ and $St$ are defined as:

\[ Re_p = \frac{Gl^2}{ν} \quad (3.41) \]

\[ St = ω \cdot Re_p, \quad (3.42) \]

with solid-to-fluid density ratio $ω = ρ_p/ρ_f$. If the particle has the same density as the fluid, i.e. $ω = 1$, the particle is said to be *neutrally buoyant*. 
### 3. FLOW PROBLEM AND HISTORICAL PERSPECTIVE

<table>
<thead>
<tr>
<th>Name</th>
<th>Abbr.</th>
<th>Description of motion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tumbling</td>
<td>T</td>
<td>Particle rotates with the axis of symmetry in the flow-gradient plane. The angular velocity is dependent on the orientation.</td>
</tr>
<tr>
<td>Rotating</td>
<td>R</td>
<td>Particle rotates with the axis of symmetry in the flow-gradient plane. The angular velocity is almost constant.</td>
</tr>
<tr>
<td>Log-rolling</td>
<td>LR</td>
<td>Particle rotates around its axis of symmetry, which is aligned in the vorticity direction. The angular velocity is constant.</td>
</tr>
<tr>
<td>Kayaking</td>
<td>K</td>
<td>Particle performs a precession and nutation around the vorticity direction. The angular velocity is dependent on the orientation.</td>
</tr>
<tr>
<td>Inclined rolling</td>
<td>IR</td>
<td>Particle rotates around its axis of symmetry, which is not aligned in the vorticity direction. The angular velocity is constant.</td>
</tr>
<tr>
<td>Inclined kayaking</td>
<td>IK</td>
<td>Particle performs a precession and nutation around an inclined axis. The angular velocity is dependent on the orientation.</td>
</tr>
<tr>
<td>Steady state</td>
<td>S</td>
<td>Particle is motionless with the axis of symmetry in the flow-gradient plane and with a constant angle $\phi_c$. The angular velocity is zero.</td>
</tr>
</tbody>
</table>

**Table 1.** Description of rotational states as found by Jeffery (1922); Ding & Aidun (2000); Qi & Luo (2003); Yu et al. (2007); Lundell & Carlsson (2010); Huang et al. (2012a) and others.

#### 3.4. Description of rotational states

The choice of $Re_p$ and $St$ has previously been seen to cause several stable rotational states of the particle, which will be reviewed in the next sections. No new rotational states are found in this thesis, and the states are defined in table 1 and illustrated in figure 3.5 and 3.6.

#### 3.5. Jeffery’s equations

In the case of $Re_p = 0$, the equations 3.38 and 3.39 can be solved analytically since the non-linear terms of the velocity vanish. Suitable boundary conditions for this problem, apart from no-slip on the particle surface, is that the velocity field assumes a linear shear flow far away from the particle, i.e. $u \rightarrow Gy_0 e_x$ as $|r| \rightarrow \infty$ ($r$ is the orientation vector relative to the particle). The hydrodynamic torque $M_D(\omega)$ acting on a particle rotating with angular velocity $\omega$ can then
3.5. JEFFERY’S EQUATIONS

be found analytically through solving the velocity field and integrating the fluid stresses over the spheroidal particle surface. With $St = 0$, equation 3.40 can be easily rearranged in order to obtain an analytical solution of $\omega(\phi, \theta)$. This was exactly what was done in the pioneering work by Jeffery (1922). The resulting rotational motion of the spheroidal particle is determined by:

$$\dot{\phi} = -\frac{G}{a^2 + b^2} \left( a^2 \sin^2 \phi + b^2 \cos^2 \phi \right)$$  \hspace{1cm} (3.43)

$$\dot{\theta} = \frac{a^2 - b^2 G}{a^2 + b^2} \frac{1}{4} \sin 2\phi \sin 2\theta.$$  \hspace{1cm} (3.44)

Analyzing the integrated motion in time, one finds that the particle performs periodic orbits with a conserved quantity $C$, called the orbit constant, depending on initial conditions, defined as

$$C = \frac{a}{b^2} \tan \theta \sqrt{a^2 \sin^2 \phi + b^2 \cos^2 \phi}.$$  \hspace{1cm} (3.45)

For all orbits, the rotation period is the same and equals to
3. FLOW PROBLEM AND HISTORICAL PERSPECTIVE

Figure 3.6. Rotational states for an oblate spheroidal particle in a linear shear flow; (a) Tumbling; (b) Log-rolling; (c) Kayaking; (d) Inclined rolling; (e) Steady state

\[
T_J = \frac{2\pi}{G} \left( r_p + \frac{1}{r_p} \right). \tag{3.46}
\]

Since there are an infinite number of initial orientations, there are an infinite amount of periodic orbits with a certain value of \(C\). One limiting orbits is \(C = 0\), which corresponds to Log-rolling. The other limiting orbit, as \(C = \infty\) \((\theta = \pi/2)\), is a Tumbling motion. The state for the intermediate orbits \(0 < C < \infty\) are called Kayaking, since the motion for a prolate spheroid resembles that of a kayak paddle.

The equations of motion for the spheroidal particles according to Jeffery (1922) have been widely used, especially in simulations of dispersions of many particles, and seen to give good prediction of particle behavior for small light particles where the assumption of \(Re_p \approx 0\) and \(St \approx 0\) are valid. It was later found by Bretherton (1962) that Jeffery’s equations are valid for any axi-symmetric particle given the correct scaling.

3.6. Apparent viscosity and Jeffery’s hypothesis

In order to shear a volume of fluid, some external work must be done, which is proportional to the fluid viscosity. Putting a particle in this volume, more
work must be done since the particle does not deform in the same way as the surrounding fluid. The additional work that has to be performed can be interpreted as the dispersion having a higher viscosity than the suspending liquid itself. This is called apparent viscosity. For a low volume fraction of particles in the fluid, i.e. a dilute dispersion, the apparent viscosity \( \nu_{\text{disp}} \) can be described by:

\[ \nu_{\text{disp}} = \nu (1 + \eta \Phi) \]  

where \( \Phi \) is the volume fraction and \( \eta \) is the intrinsic viscosity. For spherical particles and neglecting inertia, Einstein (1906, 1911) found that the intrinsic viscosity was \( \eta = 2.5 \). For spheroids, the instant contribution to the intrinsic viscosity depending on orientation is found by Jeffery (1922) and later analyzed by Mueller et al. (2009). For each orbit \( C \), the value of the instant intrinsic viscosity can be integrated over a period to yield a single value of \( \eta(C) \).

The energy injected into the system through the external work gets dissipated, as the fluid is forced to go around the particle and the streamlines get distorted. The higher value of \( \eta(C) \) also means higher energy dissipation in the dispersion of particles. In his paper, Jeffery hypothesized also what the influence of fluid inertia would be and stated that the particles will tend to adopt that motion which, of all the motions possible under the approximated equations, corresponds to the least dissipation of energy. In principle this means that Jeffery believed that the influence from fluid inertia would be that a prolate spheroid would go to a Log-rolling motion and an oblate particle would go to a Tumbling motion. This hypothesis has been debated over the last century and will be discussed in this work as well.

3.7. Previous work

The orientation of spheroidal particles in shear flows have been studied by several people during the last century. Taylor (1923) made experiments with spheroids of moderate aspect ratio \( r_p \approx 2 \) and observed that the particles assumed the orbits according to Jeffery’s hypothesis. Binder (1939) found in experiments with cylindrical rods, that particles with low aspect ratio were Log-rolling while high aspect ratio particles were Tumbling. In experiments of high aspect ratio fibers by Trevelyan & Mason (1951) and Mason & Manley (1956) no such preferential orbit could be found. Saffman (1956) derived that the effect of fluid inertia should indeed lead to a preferential orbit according to Jeffery’s hypothesis but that the effect should be much smaller than previously observed in experiments. However this analysis was only valid for low aspect ratio particles. In experiments by Karnis et al. (1963) with rods and discs in a flow through a straight pipe, preferential orbits could be found. With low \( Re_p \), these orbits followed the minimum dissipation hypothesis of Jeffery, but with
higher $Re_p$, they instead assumed orbits of maximum dissipation. Several other works have been presented on this topic (e.g. Harper & I-Dee Chang 1968; Leal 1980) but a clear consensus of what the effect of inertia really is on spheroidal particles in shear flows is still lacking.

During the last decades, computational methods have made it possible to explore the full solution of the Navier-Stokes equation beyond what is possible analytically. Ding & Aidun (2000) simulated the behavior of a Tumbling spheroid, and found that the Tumbling period was increasing with $Re_p$ and diverged past a critical Reynolds number $Re_p = Re_c$. At $Re_p > Re_c$, the spheroid would thus be in a motionless Steady state with a constant orientation $(\theta, \phi) = (\pi/2, \phi_c)$. This was seen to be true also in the two-dimensional problem of an elliptical cylinder in a linear shear flow, and was verified in experiments by Zettner & Yoda (2001).

The extreme cases of a nearly spherical particle ($r_p \approx 1$) and an infinitely slender fiber ($r_p \to \infty$) in a shear flow were investigated theoretically by Subramanian & Koch (2005) and Subramanian & Koch (2006). Their analysis, which was restricted to low but finite $Re_p$, showed that a neutrally buoyant ($\alpha = 1$) slender fiber drifted towards Tumbling and also found, just like Ding & Aidun (2000), that there is a critical Reynolds number $Re_p = Re_c$, past which the particle remains in a Steady state. Subramanian & Koch (2006) explored the influence of particle inertia on the rotational state and found that a nearly spherical particle behaved very differently if $St \gg Re_p$ or if $St = Re_p$. In the case of $St \gg Re_p$, particle inertia is dominating and the spheroid rotates in orbits corresponding to maximum dissipation (prolate spheroid is Tumbling and oblate spheroid is Log-rolling). In the neutrally buoyant case, the spheroids instead assume the rotations corresponding to minimum dissipation (prolate spheroid is Log-rolling and oblate spheroid is Tumbling).

By coupling the torque on the particle in a creeping shear flow with the full equation of motion of the particle in equation 3.40, it is possible to analyze the rotational behavior of a particle with finite $St$, although the torques in principle are valid just for $Re_p = 0$. This was done by Lundell & Carlsson (2010). The motivation is that the solution of the Stokes equation can be approximately valid even for small $Re_p > 0$. Not only did this analysis show that the spheroidal particles drifted towards orbits of maximum dissipation. It was also found that there is a transition from Tumbling, with $\dot{\phi}$ according to eq. 3.43 as $St = 0$, to a Rotation (with constant angular velocity) with $\dot{\phi} = -G/2$ as $St \to \infty$. This period thus also changes from $T = T_J$ (eq. 3.46) as $St = 0$ to $T = T_H = 4\pi$ as $St \to \infty$. The transition was characterized by a critical Stokes number $St_{0.5}$, which is the Stokes number where the particle is Tumbling with a period $T = (T_J + T_H)/2$.

The influence of fluid inertia on the three-dimensional rotation of a neutrally buoyant spheroidal particle in a linear shear flow was studied numerically
3.8. Aim of the Thesis

The present work is aiming towards full understanding of the behavior of a single spheroidal particle in a linear shear flow independently of confinement, i.e. the distance between the walls should be large enough not to influence the particle rotation. Furthermore, any influence of Brownian motion on the particle rotation is neglected. The previous work and dimensional analysis of the problem suggests that the final rotational state of the spheroidal particle is determined through a competition of fluid and particle inertial effects. Therefore, the problem should solely depend on $Re_p$, $St$, $r_p$ and initial conditions. The dependence on these parameters will be studied in detail to give a good physical explanation of the dynamical system with the help of some model examples and knowledge about non-linear dynamics and bifurcations. What the consequence will be for suspension rheology due to the rotational behavior of

by Qi & Luo (2003). They found that the prolate spheroid was Tumbling at low $Re_p$, but Log-rolling at high $Re_p$. An oblate spheroid was Log-rolling at low $Re_p$, but at higher it demonstrated Inclined rolling.

The same case was analyzed by Yu et al. (2007), who additionally found that with increasing $Re_p$, the prolate spheroid went from Tumbling to Log-rolling to Inclined rolling. The oblate spheroid was seen to go from Log-rolling to Inclined rolling to Steady state. They also found that the final state could be dependent on the initial orientation and that some rotational states co-exist at the same $Re_p$.

Huang et al. (2012a) also studied this problem numerically, increasing the simulation time and using many initial orientations. In their study they found additionally stable rotational states of Inclined kayaking and Kayaking. They found that a prolate spheroid had the following transitions with increasing $Re_p$: Tumbling to Tumbling/Log-rolling (with both states stable and depending on initial orientation) to Tumbling/Inclined rolling to Tumbling/Inclined kayaking to Tumbling/Kayaking to Tumbling/Inclined kayaking to Tumbling/Inclined kayaking to Steady state. The oblate spheroid was seen to undergo the same transitions as found by Yu et al. (2007), but without states co-existing at a fixed $Re_p$. Huang et al. (2012a) combined with later work (Huang et al. 2012b) also investigated the influence that the rotational states have on the intrinsic viscosity of a particle suspension.

The results from some of the mentioned studies of a single spheroid in a linear shear flow are summarized in table 2. Even though many question marks were cleared out through the recent numerical work, the studies were either limited by high confinement ($\kappa \geq 0.4$), neutrally buoyant particles ($\alpha = 1$), short simulation times ($Gt < 200$), constant aspect ratio (usually only $r_p = 2$ is considered) and/or few initial conditions (some times only one or two). The main problem is that a clear description of the physics is lacking from these numerical studies, and therefore it is difficult to generalize the behavior when varying for example $\alpha$, $r_p$ and $\kappa$.

3.8. Aim of the thesis

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spheroids in shear will also be covered. The present investigation will be done numerically with the help of the lattice Boltzmann method described in the next chapter.
### Table 2. Summary of previous work of the rotation of a single spheroidal particle in a linear shear flow; T=Tumbling, R=Rotating, LR=Log-rolling, IR=Inclined rolling, IK=Inclined kayaking, K=Kayaking, S=Steady state.

<table>
<thead>
<tr>
<th>Ref.</th>
<th>Method</th>
<th>$\kappa$</th>
<th>$\alpha$</th>
<th>$Re_p$</th>
<th>$St$</th>
<th>Rot. states (prolate)</th>
<th>Rot. states (oblate)</th>
<th>Other limitations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jeffery (1922)</td>
<td>Theoretical</td>
<td>$\infty$</td>
<td>Any</td>
<td>0</td>
<td>0</td>
<td>$T/K/LR$ (no drift) LR</td>
<td>$T/K/LR$ (no drift) $T$</td>
<td></td>
</tr>
<tr>
<td>Ding &amp; Aidun (2000)</td>
<td>Numerical</td>
<td>$&lt; 0.2$</td>
<td>2</td>
<td>$5 - 90$</td>
<td>$5 - 90$ ($\alpha = 1$)</td>
<td>-</td>
<td>Incr. $Re_p$: $T \to S$</td>
<td>Limited to rotation with $\theta = \pi/2$</td>
</tr>
<tr>
<td>Subramanian &amp; Koch (2005)</td>
<td>Theoretical</td>
<td>$\infty$</td>
<td>$&lt; 1$</td>
<td>$&lt; 1$ ($\alpha = 1$)</td>
<td>Incr. $Re_p$: $T \to S$</td>
<td>-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Subramanian &amp; Koch (2006)</td>
<td>Theoretical</td>
<td>$\approx 1$</td>
<td>$&lt; 1$ ($\alpha = 1$)</td>
<td>$LR$</td>
<td>$T$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Subramanian &amp; Koch (2006)</td>
<td>Theoretical</td>
<td>$\approx 1$</td>
<td>$&lt; 1$ ($\alpha = 1$)</td>
<td>$LR$</td>
<td>$T$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lundell &amp; Carlson (2010)</td>
<td>Analytical/Numerical</td>
<td>$\infty$</td>
<td>Any</td>
<td>0</td>
<td>$0 - 10^5$</td>
<td>Incr. $St$: $T \to R$</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Qi &amp; Luo (2003)</td>
<td>Numerical</td>
<td>0.5</td>
<td>2</td>
<td>$0.1 - 467$ ($\alpha = 1$)</td>
<td>Incr. $Re_p$: $T \to LR$</td>
<td>Incr. $Re_p$: $LR \to IR$</td>
<td>Only investigated two initial orientations.</td>
<td></td>
</tr>
<tr>
<td>Yu et al. (2007)</td>
<td>Numerical</td>
<td>0.4</td>
<td>2</td>
<td>$0.5 - 256$ ($\alpha = 1.001$)</td>
<td>Incr. $Re_p$: $T \to LR \to T/IR$</td>
<td>Incr. $Re_p$: $LR \to LR/IR \to S$</td>
<td>Only investigated two initial orientations. Short simulation time.</td>
<td></td>
</tr>
<tr>
<td>Huang et al. (2012a)</td>
<td>Numerical</td>
<td>0.5</td>
<td>2</td>
<td>$0.5 - 700$ ($\alpha = 1$)</td>
<td>Incr. $Re_p$: $T \to T/LR \to T/IR \to T/IK \to T/K \to T \to T/S$</td>
<td>Incr. $Re_p$: $LR \to IR \to S$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 4

Numerical method

4.1. Numerical setup

The flow problem described in the previous chapter is simulated by placing a spheroidal particle in a cubical domain with sides \( N \) as illustrated in figure 3.4. The flow is bounded in the \( y \)-direction by walls moving in the \( x \)-direction with velocity \( U_w \) and \(-U_w\) respectively creating a linear shear with constant shear rate \( G = 2U_w/N \). The boundaries in the \( x \)- and \( z \)-directions are treated with periodic boundary conditions meaning that fluid that exits the domain on one side will re-enter on the other side of the domain. The fluid and particle motion are simultaneously simulated using the lattice Boltzmann method with external boundary forcing (LB-EBF).

4.2. Description of the LB-EBF method

This section will describe the simulation steps performed in the lattice Boltzmann method with external boundary forcing (LB-EBF), which was described in detail by Wu & Aidun (2010) and also presented in Paper 2.

4.2.1. Fluid grid

The fluid is defined on a cubic Eulerian grid denoted as:

\[
x^e \in \Pi_f
\]  

(4.48)

The nodes are separated with the distance \( \Delta x \) in each direction. The domain is bounded by walls at \( y = 0 \) and \( y = N \) with velocity \( U_w \) and \(-U_w\) in \( x \) direction, which are treated with non-slip condition and periodic boundary conditions are applied at \( x = 0, x = N, z = 0, z = N \).

4.2.2. Particle grid

The spheroidal particle is defined with a Lagrangian grid consisting of boundary nodes, denoted as (for the \( j \)-th node):

\[
x^p_j \in \Gamma_s.
\]  

(4.49)
Each boundary node along the surface of the spheroid is representing an area element of size $\Delta A_j$, and gets a characteristic volume $\Delta v_j = \Delta A_j^{3/2}$. The best results are obtained by keeping $\Delta A_j \approx (\Delta x)^2$.

### 4.2.3. The discrete Dirac function

Since the fluid and particle nodes are not at the same position, the mapping of forces and velocities between fluid and particle grids is done through a discrete Dirac function defined by Peskin (2002) as:

$$ D(x) = \begin{cases} \frac{1}{64\Delta x^3} \left( 1 + \cos \left( \frac{\pi x}{2\Delta x} \right) \right) \left( 1 + \cos \left( \frac{\pi y}{2\Delta x} \right) \right) \left( 1 + \cos \left( \frac{\pi z}{2\Delta x} \right) \right), & |x| \leq 2\Delta x \\ 0, & |x| > 2\Delta x. \end{cases} $$

(4.50)

### 4.2.4. Principle of the lattice Boltzmann method (LBM)

The lattice Boltzmann (LB) method is based on the streaming and colliding of particle distribution functions $f_i(x^e, t)$, which has 19 components ($i = 0...18$ for a D3Q19 lattice) and is defined in each fluid grid node $x^e$. Each component can be seen as a probability for a fluid particle to have an associated velocity $c_i = (c_{i,x}, c_{i,y}, c_{i,z})$, where $x + c_i \in \Pi_f$. In the streaming step each distribution $f_i(x^e, t)$ is translated to $f_i(x^e + c_i, t + 1)$. Macroscopic quantities can be obtained in each fluid node through:

$$ \rho_f(x, t) = \sum_{i=0}^{18} f_i(x^e, t) $$

(4.51)

$$ \rho_f u_f(x, t) = \sum_{i=0}^{18} c_i f_i(x^e, t) $$

(4.52)

In the collision step, the particle distributions $f_i(x^e, t)$ are locally redistributed towards a local equilibrium distribution $f_i^{eq}(x^e, t)$, still preserving local density and momentum. The equilibrium distribution is defined as:

$$ f_i^{eq}(x^e, t) = w_i \rho_f \left( 1 + 3c_i \cdot u_f + \frac{9}{2} (c_i \cdot u_f)^2 - \frac{3}{2} u_f^2 \right). $$

(4.53)

where $w_0 = 1/3$, $w_{1-6} = 1/18$ and $w_{7-18} = 1/36$. 
4.2. DESCRIPTION OF THE LB-EBF METHOD

4.2.5. Simulation steps

4.2.5a. Initialization.
1. The initial particle node position $x_l^j$ and velocity $U_p(x_l^j, t_0)$ are calculated by using information about particle initial position, orientation, velocity and angular velocity.
2. The initial fluid velocity at $x_e$ is set to the linear velocity profile defined by wall velocity $U$.
3. The density is set to $\rho_f(x_e, t_0) = \rho_0$.
4. The populations are set to equilibrium $f_a(x_e, t_0) = f_{eq}^a(x_e, t_0)$.

4.2.5b. Iterative steps.
1. Streaming. New pre-collisional populations $f_{i}^{pre}(x_e, t)$ are obtained through
   \[ f_{i}^{pre}(x_e, t) = f_i(x_e - c_i, t - 1). \] \hspace{1cm} (4.54)
   Velocity $u(x_e, t)$ and density $\rho(x_e, t)$ are calculated through equations 4.51 and 4.52.
2. The fluid velocity on the particle boundary is calculated through
   \[ u(x_l^j, t) = \sum_{x_e \in \Pi_j} u(x_e, t) D(x_e - x_l^j)(\Delta x)^3. \] \hspace{1cm} (4.55)
3. The force acting on the particle nodes is calculated through
   \[ F_{fsi}(x_l^j, t) = f_{fsi}(x_l^j, t) \cdot \Delta v_j = \rho_0(u(x_l^j, t) - U_p(x_l^j, t - 1)) \cdot \Delta v_j \] \hspace{1cm} (4.56)
   with $f_{fsi}(x_l^j, t)$ defined as a force density.
4. The particle force $F$ and torque $T$ is determined by summation of the contributions from the nodes:
   \[ F(t) = \sum_{x_l^j \in \Gamma_s} F_{fsi}(x_l^j, t) \] \hspace{1cm} (4.57)
   \[ T(t) = \sum_{x_l^j \in \Gamma_s} (x_l^j - x^{lc}) \times F_{fsi}(x_l^j, t) \] \hspace{1cm} (4.58)
   where $x^{lc}$ is the center of gravity of the particle.
5. The velocity and angular velocity of the particle at \( t \) is determined by integration of

\[
\frac{dU}{dt} = \frac{F}{M} \tag{4.59}
\]

\[
I \frac{d\omega}{dt} + \omega \times (I \cdot \omega) = T \tag{4.60}
\]

where \( M \) and \( I \) is the particle mass and inertia tensor respectively and \( \omega \) denotes the particle angular velocity. From this the new position \( x_{p}^{i}(t) \) and velocity \( U_{p}(x_{p}^{i}, t) \) of the particle nodes is obtained through a fourth order accurate Runge-Kutta integration procedure.

6. The force acting on the fluid is determined by

\[
g(x^{e}, t) = - \sum_{x_{p}^{i} \in \Gamma_{s}} f^{sis}(x_{p}^{i}, t) D(x^{e} - x_{p}^{i}) \Delta v_{j}. \tag{4.61}
\]

7. Collision step. The post-collision distribution \( f_{i} \) is obtained by colliding the pre-collision distribution \( f_{i}^{pre} \) towards the local equilibrium distribution \( f_{i}^{eq} \), accounting for the external boundary force \( g \):

\[
f_{i}(x^{e}, t) = f_{i}^{pre}(x^{e}, t) + \frac{1}{\tau} [f_{i}^{eq}(x^{e}, t) - f_{i}^{pre}(x^{e}, t)] + 3w_{i}g(x^{e}, t) \cdot c_{i}. \tag{4.62}
\]

8. Repeat from step 1 for \( t = t + 1 \).

The sound speed in this model is a constant and equal to \( c_{s} = \sqrt{1/3} \) and the kinematic viscosity \( \nu \) is related to the relaxation time \( \tau \) in the last equation through \( \nu = c_{s}^{2} (\tau - 0.5) \). The current formulation of the method is only valid as long as the particle is not adapting too quickly to the surrounding fluid. Therefore it has been seen that the simulation fails as we make the density of the particle lighter than \( \rho_{p} = 0.8 \cdot \rho_{f} \). Throughout this study, we thus set a lower limit on the particle density to be equal to the density of the fluid, i.e. \( \alpha = \rho_{p} / \rho_{f} \geq 1 \). Light particles can be studied using another condition at the boundary and might be a topic for future work.

### 4.3. Obtaining intrinsic viscosity \( \eta \)

The procedure of obtaining the intrinsic viscosity of the one-particle suspension is identical to the one used by Huang et al. (2012b,a). In the lattice Boltzmann
scheme employed in this study, the local shear stress can be evaluated in each fluid node according to

$$\sigma(x^e,t) = -\left(1 - \frac{1}{2\tau}\right) \sum_{i=0}^{18} (f_i(x^e,t) - f_i^{eq}(x^e,t))c_{ix_i}c_{iy_i}. \quad (4.63)$$

The total shear stress on the moving walls $\sigma_w(t)$ is evaluated by taking the mean value of all nodes closest to the walls (i.e. at $y = 1$ and $y = N - 1$). The time dependent intrinsic viscosity $\eta^*(t)$ is calculated through:

$$\eta^*(t) = \frac{1}{\Phi} \left(\frac{\sigma_w(t)}{\rho_0\nu G} - 1\right), \quad (4.64)$$

where $\Phi$ is the volume fraction calculated through:

$$\Phi = \left(\frac{V_p}{N^3}\right), \quad (4.65)$$

where $V_p$ is the volume of a spheroid and $N^3$ is the volume of the simulation domain. In order to evaluate the intrinsic viscosity for a certain rotational state at a certain $Re_p$, the simulation is initialized at rest in an orientation where the particle assumes the stable rotational state quickly. The simulation is running to $G \cdot t = 1000$, which was seen to be enough for the value of $\eta^*(t)$ to converge at the walls for $0 < Re_p < 200$. The final (time-independent) value of $\eta$ was evaluated through a time-average of $\eta^*(t)$ from $G \cdot t = 667$ to $G \cdot t = 1000$.

### 4.4. Dependence on Knudsen and Mach numbers

Presently, there are many numerical methods to simulate fluid dynamics and the complete Navier-Stokes equations, for example finite-volume methods, finite element methods and distributed Lagrangian multiplier based fictitious domain methods. Lattice-Boltzmann methods have been attracting more and more interest during the last decade, especially due to straightforward parallelization and grid handling together with flexibility for introducing new physics. However, the simplicity of the presented model comes also with some drawbacks that one should be aware of.

The simulation method is based on the motion and collisions of gas molecules and no continuum assumption is made, which is needed for the fluid to be described by the Navier-Stokes equations. Due to this also, the code is never simulating a strictly incompressible fluid since compressibility is required for how information travels in the simulated fluid. The effects of compressibility is governed by the Mach number $Ma = U/c_s$, with $U$ as the characteristic velocity in the flow. The present model is making an assumption that $Ma \ll 1$ in order to allow the expansion of the equilibrium distributions in equation...
4.53. The non-continuum description of the fluid also means that there is a definable characteristic length that molecules travel between collisions \( l_f \). This is related to the dissipation of momentum within the fluid and thus also the viscosity. When the characteristic length in the flow \( L \) becomes of the same order of magnitude as \( l_f \), the continuum assumption of the fluid fails and we start seeing that consequently also the no slip condition fails and thus also the momentum transfer to the particle. These effects are characterized by the Knudsen number \( Kn = l_f/L = \nu/(cs\cdot L) \). However, it can be showed, that as long as \( Kn \ll 1 \), the lattice-Boltzmann fluid solver is equivalent to solving the incompressible Navier-Stokes equations.

The condition to keep \( Ma \) and \( Kn \) low, is not as easily realizable as it sounds. The problem is that the characteristic velocity \( U \) is also determining the time resolution of the flow, given by \( G^{-1} \), i.e. low \( Ma \) number also means high time resolution. This in turn means that simulation times might be unacceptably long and no long term motion can be determined. The biggest problem arrives when simulating low \( Re_p = Ma/Kn \), since \( Kn \) has an upper limit to assure the continuum description. Throughout this study, the time resolution will be constant (\( G = 1/600 \) if not stated otherwise) and thus the Mach number is also constant. The \( Re_p \) will be varied by changing the viscosity and thus also \( Kn \). But to assure that \( Kn < 10^{-2} \), the minimum Reynolds number studied is \( Re_p = 10 \).

4.5. Dependence on confinement \( \kappa \)

The aim of this work is to have results of the spheroidal particle rotational motion in a general linear shear flow. It is therefore desired to remove any effects that might come from the fact that the simulations are done in a confined domain, and the results should be domain size independent. There might be several issues related to the domain size of the problem.

First, a too short distance between the walls influences the particle since streamlines close to the wall are forced in the flow direction, and might thus also affect the shape of the streamlines around the particle.

Second, the particle motion induces a motion in the fluid. If the domain is too small in \( x \)- and \( z \)- directions, this induced flow might translate through the periodic boundaries and thus affect the particle itself.

Third, having a too large domain might also cause problems due to the flow becoming unstable. The stability of the flow is characterized by the channel Reynolds number \( Re_H = GN^2/\nu = \kappa^{-2} \cdot Re_p \).

In paper 1 it was found that the confinement needed to be at most \( \kappa = 0.2 \) for domain size independent results for the prolate spheroid and this is therefore chosen as the confinement in all the cases in the thesis. However, by setting a condition that the flow must remain stable for at least \( G \cdot t = 1000 \), the maximum Reynolds number that could be considered without the flow
becoming turbulent was around $Re_p = 300$. It is important to note that Qi & Luo (2003), and Huang et al. (2012a) could reach higher $Re_p$ since they have much higher confinement, $\kappa = 0.5$.

4.6. Dependence on resolution

In all computational fluid dynamics, changing the temporal and spatial resolution might influence the results, and by refining the resolution, the accuracy increases. At some point the results converge and become independent on the resolution and the resolution is chosen based on the desired accuracy. In the non-inertial case at $Re_p = 0.5$, excellent agreement was found compared with the theoretical orbits by Jeffery (1922) (see paper 1), and could be found regardless of resolution (as long as $Kn, Ma \ll 1$). The resolution dependence is investigated by simulating a prolate spheroid of $r_p = 4$.

The dependence on spatial resolution was investigated by keeping temporal resolution constant, i.e. the shear rate $G$ is constant and changing the size of the domain and particle while still keeping $\kappa = 0.2$. If spatial resolution is too low, the fluid will not be well resolved around the particle and the interpolation of forces on the particle surface might be incorrect. This will be especially problematic in the Log-rolling motion of a prolate spheroid, since the motion is mainly dependent on the resolution around the minor axis. It is seen that an error starts to occur when the minor semi-axis is $b < 3$ (see figure 4.1). Therefore, throughout this study, the minor semi-axis of the spheroid is always limited to be $\geq 3$. It should also be mentioned that the flow around the Log-rolling prolate spheroid is much less complex since the relevant particle Reynolds number rather should be based on $b$, i.e. $Re_{p,LR} = Re_p/r_p^2$.

In this study, we are interested in transitions between rotational states at a certain critical $Re_p$, and therefore we must know how the resolution influences the value of these numbers. It is seen that a Steady state arises with sufficiently high fluid inertia at $Re_p = Re_c$, and since the particle is motionless, particle inertia can’t influence this transition (this will be discussed more in next chapter). Therefore, the influence of spatial and temporal resolution on this number is investigated.

With $G = 1/2400$, the value of $Re_c$ is increasing with spatial resolution and seemingly converging (see figure 4.2). At the same time, if we keep spatial resolution constant at $N = 120$, we observe that $Re_c$ is decreasing when increasing time resolution (i.e. decreasing $G$) and seemingly converging. However, given the slow convergence rate it is not possible to state anything about what value is reached with very high resolution in time and space.

In order to determine $Re_c$, a moving grid is not actually needed, since it is defined as the minimum $Re_p$ for which there exist an orientation $\phi (\theta = \pi/2)$ where there is zero torque on the particle. This definition allows us to determine $Re_c$ using a Navier-Stokes based solver with a fixed grid for the particle and
Figure 4.1. Evolution of the $\theta$–angle as a prolate spheroid is simulated in the Log-rolling motion at different $Re_p$ and changing spatial resolution from (a) to (d); particle has $r_p = a/b = 4$ and is placed in a domain with confinement $\kappa = 0.2$; (a) $a = 8$, $b = 2$, $N = 80$; (b) $a = 10$, $b = 2.5$, $N = 100$; (c) $a = 12$, $b = 3$, $N = 120$; (d) $a = 24$, $b = 6$, $N = 240$

fluid with high grid refinement close to the particle. This type of model is set up in Comsol Multiphysics and resulted in a seemingly converged value of $Re_c = 131 \pm 5$ for a prolate spheroid of $r_p = 4$. Comparing this value with the ones obtained from the LB-EBF code in figure 4.2, it seems probable that this is the value that we would get given extremely high resolution in time and space (the value using $G = 1/2400$ seems to be well above $Re_c = 131$, but the value will be decreased with higher time resolution).

It is obvious, that it is extremely computationally expensive to get the exact converged number of $Re_c$ using LB-EBF (a rough estimate to get $Re_c$ with an accuracy of $\pm 1$ will be several years running on 12 CPUs). It might not even be possible to reach the converged value, since the low LB relaxation time $\tau$ needed for such a simulation might also affect the solution.

The critical Reynolds number $Re_c$ arises from a sensitive balance between negative torque $T^-$ from the primary flow and positive torque $T^+$ from the secondary flow as described by Ding & Aidun (2000). Using the previously
4.6. DEPENDENCE ON RESOLUTION

Figure 4.2. Critical Reynolds number $Re_c$ for a prolate spheroid of $r_p = 4$ depending on spatial resolution $N$ (left) and temporal resolution $G^{-1}$ (right); the dependence on the temporal resolution is also denoted with blue crosses in the left figure; the value of $Re_c \approx 131$ is obtained with Comsol.

mentioned Comsol model, it is found that a small error of $\pm 1\%$ in determining $T^+$ or $T^-$, will lead to an error of $\pm 7$ of the value of $Re_c$. The value of $Re_c$ is thus very sensitive to any small changes to the fluid field that can arise from changes in resolution, and it seems highly likely that no numerical method can obtain an accurate value without very high local grid refinement around the particle. The exact nature of this resolution dependence in LB-EBF is still not fully understood but is believed to arise in the computation of the forces on the particle. It is likely that the effective viscosity close to the particle depends on both spatial and temporal resolution and might be different from the one that is set. If so, this in turn also means that the effective Reynolds number of the flow around the particle would depend on the resolution.

For the present work it is more interesting to know the qualitative rotational behavior of the particles when increasing or decreasing $Re_p$, and the exact physical numbers is of less interest. Using different values of temporal and spatial resolutions did not change any qualitative behavior when changing $Re_p$, and the same sequence of transitions could be found independently of resolution. There are also indications that if we keep temporal and spatial resolution constant, the relation between $Re_{p,\text{true}}$ and $Re_{p,\text{set}}$ is linear, thus meaning that if a critical value of $Re_p = Re_1$ is found through simulations to be twice as large as another critical $Re_p = Re_2 \approx Re_1/2$, then the same is true also for the physical transitions.

The goal with the thesis is to find the long term behavior of the particle rotation and therefore the time resolution is set to be fairly low at $G = 1/600$
to be able to simulate up to $G \cdot t = 1000$ within an acceptable time. The spatial resolution is set by restricting the particle to either having the major axis limited to $l \geq 24$ or the minor axis limited to $w \geq 6$, and always keeping confinement $\kappa = l/N = 0.2$.

4.7. Interpretation and usage of the results in this thesis

The issues discussed in the previous section means that the results in this work must be interpreted correctly. The transitions between rotational states will most probably occur at different $Re_p$ in an experiment than the numbers presented here. However, since spatial and temporal resolution is kept constant, all the numbers can be relatively compared. This work is meant to give insight into the physical processes involved in this flow problem, and by knowing this, we can correctly predict what will happen when increasing and decreasing $Re_p$, $St$ and $r_p$, since the qualitative behavior is resolution independent. But in order to pinpoint the physical values of critical Reynolds numbers and intrinsic viscosities, other methods should be employed.

As a remark it should be mentioned that all these issues are believed to have been issues also for other previous numerical works, for example in the ones by Qi & Luo (2003), Yu et al. (2007) and Huang et al. (2012a), since the flow problem is not believed to have been sufficiently resolved. This is strengthened by the fact that the critical Reynolds numbers match almost perfectly with Huang et al. (2012a) when using the same parameters (seen in paper 1).
CHAPTER 5

Summary of results

5.1. Rotational states

The rotational states presented in chapter 3 are describing both a dynamical state for the fluid and for the particle and arise from a competition of fluid and particle inertia. Since we know the preferred states with dominating particle inertia (Lundell & Carlsson 2010), each state can be described by the dominating inertial effect. For the prolate case, generally fluid inertia is dominating when the particle orientation is constant (fluid is in a steady state) and particle inertia is dominating when particle is rotating around its minor axis (fluid is in a time-periodic state). For the oblate case, generally particle inertia is dominating when the symmetry axis is close to the vorticity direction and fluid inertia is dominating when the symmetry axis is close to the flow-gradient plane. It is also convenient for the discussion of the prolate particle, to separate between planar and non-planar rotational states. For planar states, the symmetry axis is always in the flow-gradient plane ($\theta = \pi/2$) and the dynamics can be described with the angle $\phi$. This includes Tumbling, Rotating and Steady state. For non-planar states, the symmetry axis is not in the flow-gradient plane ($0 < \theta < \pi/2$) and the rotation of all three rotational angles ($\phi, \theta, \psi$) might be needed to describe the motion. This includes Log-rolling, Inclined rolling, Kayaking and Inclined kayaking. The description of the rotational states for both prolate and oblate spheroids is summarized in table 1 and table 2.

5.1.1. Prolate spheroid of $r_p = 4$

Figure 5.1 shows which rotational states are stable depending on the choice of $Re_p$ and $St$ for a prolate spheroid of $r_p = 4$. How the different transitional lines are found is described in paper 2. In this diagram it is seen that a planar rotational state exists everywhere. Below a certain $Re_p < Re_c$, this planar rotation corresponds to the Tumbling or Rotating states. Due to fluid inertia, this planar state co-exists with a non-planar state at $Re_{LR} < Re_p < Re_T$, where the particle symmetry axis is close to perpendicular to the gradient direction. The particle thus does not gain so much angular momentum for particle inertia effects to be important. For a particle in a non-planar rotation, both increasing $Re_p$ above $Re_T$ or decreasing $Re_p$ below $Re_{LR}$, will eventually lead to a planar Tumbling motion. The particle will not return again to the
5. SUMMARY OF RESULTS

<table>
<thead>
<tr>
<th>Rot. state (abbr.)</th>
<th>Dynamical state (fluid)</th>
<th>Dynamical state (particle)</th>
<th>Planar/non-planar</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Time-periodic</td>
<td>Time-periodic</td>
<td>Planar</td>
<td>P</td>
</tr>
<tr>
<td>R</td>
<td>Time-periodic</td>
<td>Time-periodic</td>
<td>Planar</td>
<td>P</td>
</tr>
<tr>
<td>LR</td>
<td>Steady state</td>
<td>Time-periodic</td>
<td>Non-planar</td>
<td>F</td>
</tr>
<tr>
<td>K</td>
<td>Time-periodic</td>
<td>Quasi-periodic</td>
<td>Non-planar</td>
<td>P &amp; F</td>
</tr>
<tr>
<td>IK</td>
<td>Time-periodic</td>
<td>Quasi-periodic</td>
<td>Non-planar</td>
<td>P &amp; F</td>
</tr>
<tr>
<td>S</td>
<td>Steady state</td>
<td>Steady state</td>
<td>Planar</td>
<td>F</td>
</tr>
</tbody>
</table>

Table 1. Description of the rotational states of the prolate particle and the corresponding states in terms of fluid and particle dynamics; T=Tumbling, R=Rotating, LR=Log-rolling, IR=Inclined rolling, IK=Inclined kayaking, K=Kayaking, S=Steady state.

<table>
<thead>
<tr>
<th>Rot. state (abbr.)</th>
<th>Dynamical state (fluid)</th>
<th>Dynamical state (particle)</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Time-periodic</td>
<td>Time-periodic</td>
<td>F</td>
</tr>
<tr>
<td>LR</td>
<td>Steady state</td>
<td>Time-periodic</td>
<td>P</td>
</tr>
<tr>
<td>IR</td>
<td>Steady state</td>
<td>Time-periodic</td>
<td>P &amp; F</td>
</tr>
<tr>
<td>S</td>
<td>Steady state</td>
<td>Steady state</td>
<td>F</td>
</tr>
</tbody>
</table>

Table 2. Description of the rotational states of the oblate particle and the corresponding states in terms of fluid and particle dynamics; T=Tumbling, LR=Log-rolling, IR=Inclined rolling, S=Steady state.

non-planar rotation when changing back $Re_p$ since the particle is "stuck" in the Tumbling state.

At $Re_p > Re_c$, only planar rotation is possible and can be either Steady state or a rotation around the minor axis (Tumbling or Rotating). If the particle is heavy enough, i.e. $St > St_c$, both these states can co-exist.

5.1.2. Aspect ratio dependence

Making the particle more slender (i.e. increasing $r_p$) leads to the following consequences (detailed description in paper 2):

1. Transitions due to fluid inertia, for example $Re_c$ and $Re_{PF}$, will decrease.
2. Transitions due to particle inertia, for example $St_c$, will increase.
3. The probability to end up in a non-planar rotational state decreases, i.e. the more slender the particle, the likelier it is for the particle to be in a planar rotation.

5.1.3. Oblate spheroid of $r_p = 4$

The $Re_p/St$-diagram for an oblate spheroid of $r_p = 4$ is shown in figure 5.2 and described in detail in paper 3. At low $Re_p$, the particle is Log-rolling and at high $Re_p$, the particle is in a Steady state. In an intermediate region $Re_c < Re_p < Re_PF$, both states co-exist. For light particles, there is a possibility of a slow Tumbling motion to be stable at $Re_p \lesssim Re_c$.

5.1.4. Aspect ratio dependence

Making the oblate spheroid flatter (i.e. increasing $r_p$) will lead to the following (detailed description in paper 3):

1. Transitions due to fluid inertia, for example $Re_c$ and $Re_PF$, will decrease.
2. Transitions due to particle inertia, for example $St_T$, will increase. This also means that there is a higher probability for a light flat particle at $Re_p < Re_c$ to be in a Tumbling motion.
5.2. Comments on confinement dependence

In section 4.5, it was discussed how confinement could influence the simulated results. For the prolate case it was found that, as long as the particle wasn’t extremely confined ($\kappa \geq 0.5$), then the transitional Reynolds numbers due to fluid inertia $Re_c$ and $Re_{PF}$ were steadily decreasing with decreased $\kappa$ (see figure 5.3a). It was particularly observed that when $\kappa \leq 0.2$, $Re_c$ and $Re_{PF}$ were converging to one single value and the results can be seen as domain size independent. However, even the confined particle at $0.2 < \kappa < 0.5$ still undergoes the same sequence of transitions with increasing $Re_p$ and there are no qualitative changes to the $Re_p/St$ diagram shown in figure 5.1.

For the oblate case, it is a bit different. Looking at the two numbers $Re_c$ and $Re_{PF}$, which are concluded to be transitions due to fluid inertia, they do not have the same behavior when changing confinement $\kappa$ (see figure 5.3b). Just as the prolate case, $Re_c$ is decreasing when making the domain bigger, but $Re_{PF}$ is increasing. The consequence is that there is a critical confinement around $\kappa_c \approx 0.24$ where $Re_c = Re_{PF}$. When the particle is confined at $\kappa > \kappa_c$ and $Re_{PF} < Re_c$, the $Re_p/St$ diagram looks different as seen in figure 5.4.

The particle is still Log-rolling at low $Re_p$ and in a Steady state at high $Re_c$. In an intermediate region, at $Re_{PF} < Re_p < Re_c$, there are no co-existing states and instead the particle will be in a stable Inclined rolling state. Since it seems that $Re_{PF} \to \infty$ as $\kappa \to 0$, it seems that the transition at this critical Reynolds number is actually caused by having a confined domain and is likely not to occur for an unconfined particle.
5.2. COMMENTS ON CONFINEMENT DEPENDENCE

Figure 5.3. The critical Reynolds numbers $Re_c$ and $Re_{PF}$ as function of confinement $\kappa$; (a) prolate spheroid of $r_p = 4$; (b) oblate spheroid of $r_p = 2$; black lines indicating approximate trends.

Figure 5.4. Rotational states of an oblate spheroid with $r_p = 2$ depending on $Re_p$ and $St$: (a) $\kappa = 0.2$; (b) $\kappa = 0.5$. 
5.3. Bifurcations and dynamical transitions

In order to gain some physical intuition about what is happening in the dynamical system, it is desired to characterize the transitions leading to the different rotational states. An easy way of illustrating the dynamical behavior is by looking at the trajectory of the symmetry axis projected on the flow-gradient plane through \((s_x, s_y) = (\sin \theta \cos \phi, \sin \theta \sin \phi)\).

5.3.1. Prolate case

The projected trajectories for a neutrally buoyant particle of \(r_p = 4\) at different \(Re_p\) are schematically drawn in figure 5.5. To describe the transitions and bifurcations, it is convenient to treat the non-planar and planar rotation separately.

The bifurcations occurring in the non-planar rotation are summarized and characterized in table 3. A stable non-planar rotation is stabilized at a subcritical Hopf bifurcation at \(Re_p = Re_{LR}\) along with a creation of an unstable limit cycle that determines if an initial orientation will go to the non-planar state or diverge towards a distant attractor, which in this case is a planar rotation. At \(Re_p = Re_T\), the unstable limit cycle is annihilated and all initial orientations will go towards the distant attractor. Recalling the dynamical systems in chapter 2, it is seen that this behavior is exactly the type of behavior that we can see for a Duffing-Van der Pol oscillator, changing the linear parts of the non-linear damping and non-linear restoring forces. With this analogue, it seems that it is fluid inertia that causes the damping of small oscillations and particle inertia that amplifies large oscillations. The existence of the non-linear restoring forces is not fully understood. However, the Duffing-Van der Pol oscillator can also be seen as the general behavior of a non-linear dynamical system with odd symmetry around the origin, with a double-zero eigenvalue. It is therefore believed that, with a certain choice of parameters \(Re_p\) and \(St\), we should be able to find a case where the Log-rolling solution has a double-zero eigenvalue. Consequently, since the system per definition is non-linear and has odd symmetry around the origin, i.e. the projected trajectories of \((s_x, s_y)\) are equivalent to \((-s_x, -s_y)\), all the bifurcations/transitions presented in table 3 will exist if there is such a case.

The bifurcations occurring in the planar rotation are summarized in table 4. At \(Re_p = Re_c\), a Steady state is created in a saddle-node bifurcation, which can be an infinite-period saddle-node bifurcation if \(St < St_{cd}\). In this case the Tumbling period will diverge according to \(T \propto (Re_c - Re_p)^{-1/2}\). At \(Re_p > Re_c\), a Tumbling solution can co-exist with the Steady state if the particle is heavy enough, i.e. \(St > St_c\). Decreasing \(St\), a transition from Tumbling to Steady state can also occur at \(St = St_c\) in a homoclinic bifurcation. In this case the Tumbling period will diverge according to \(T \propto \ln(St - St_c)\). This behavior, along with the viscous damping elimination for very heavy particles,
5.3. BIFURCATIONS AND DYNAMICAL TRANSITIONS

<table>
<thead>
<tr>
<th>Figure (fig. 5.5)</th>
<th>Crit. Reynolds number</th>
<th>Dynamical transition/bifurcation</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>(b)→ (c)</td>
<td>$Re_{LR}$</td>
<td>Subcritical Hopf bifurcation</td>
<td>$F$ &amp; $P$</td>
</tr>
<tr>
<td>(c)→ (d)</td>
<td>$Re_{PF}$</td>
<td>Supercritical Pitchfork bifurcation</td>
<td>$F$</td>
</tr>
<tr>
<td>(d)→ (e)</td>
<td>$Re_{HOPF}$</td>
<td>Supercritical Hopf bifurcation</td>
<td>$F$ &amp; $P$</td>
</tr>
<tr>
<td>(e)→ (f)</td>
<td>-</td>
<td>Breaking of homoclinic connection</td>
<td>$F$ &amp; $P$</td>
</tr>
<tr>
<td>(f)→ (g)</td>
<td>$Re_{T}$</td>
<td>Saddle-node bifurcation of limit cycles</td>
<td>$F$ &amp; $P$</td>
</tr>
</tbody>
</table>

Table 3. Summary of all non-planar dynamical transitions of a prolate spheroidal particle in a linear shear flow; the transitions are illustrated in figure 5.5.

is exactly the same behavior that was described for the damped driven pendulum in chapter 2. As was described in chapter 3, the linear shear flow can be seen as a decomposition of a combination of vorticity and strain. The vorticity part will give a constant torque regardless of orientation, while the strain part will try to align the particle along the strain direction (at $\phi = \pi/4$). This is the reason behind the intermittent Tumbling motion. In the pendulum example it was gravity that acted in a certain direction and the constant torque was added from an external source. Due to the balance between external torque and the torque from the gravitational alignment, a steady state could be found. Using this analogue, it seems that fluid inertia in some way cause the strain part of the flow to be stronger than the vorticity part locally around the particle and this is the reason behind the saddle-node bifurcation for the prolate spheroid.
## 5. SUMMARY OF RESULTS

<table>
<thead>
<tr>
<th>Stokes number</th>
<th>Reynolds number</th>
<th>Dynamical transition/bifurcation</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>$St &lt; St_{cd2}$</td>
<td>$Re_p = Re_c$</td>
<td>Infinite-period saddle-node bifurcation</td>
<td>$F$</td>
</tr>
<tr>
<td>$St &gt; St_{cd2}$</td>
<td>$Re_p = Re_c$</td>
<td>Saddle-node bifurcation</td>
<td>$F$</td>
</tr>
<tr>
<td>$St = St_c$</td>
<td>$Re_p &gt; Re_c$</td>
<td>Homoclinic bifurcation</td>
<td>$P$</td>
</tr>
<tr>
<td>$St_{0.5}$</td>
<td>-</td>
<td>Elimination of viscous damping effects</td>
<td>$P$</td>
</tr>
</tbody>
</table>

*Table 4. Summary of all planar dynamical transitions of a prolate spheroidal particle in a linear shear flow*
5.3. BIFURCATIONS AND DYNAMICAL TRANSITIONS

Figure 5.5. Schematic illustration of the projected trajectories \((s_x, s_y) = (\sin \theta \cos \phi, \sin \theta \sin \phi)\) for a neutrally buoyant prolate spheroid of \(r_p = 4\): (a) \(Re_p = 0\) (Jeffery orbits); (b) \(Re_p \approx 10\); (c) \(Re_p \approx 30\); (d) \(Re_p \approx 60\); (e) \(Re_p \approx 65\); (f) \(Re_p \approx 70\); (g) \(Re_p \approx 73\); (h) \(Re_p \approx 75\); (i) \(Re_p \approx 80\); (j) \(Re_p \approx 85\); (k) \(Re_p = Re_c \approx 89\); (l) \(Re_p \approx 100\); filled and open circles indicate stable and unstable fixed points, respectively; thick solid and dashed lines indicate stable and unstable orbits, respectively.
5. SUMMARY OF RESULTS

5.3.2. Oblate case

In the previous section it was described how the dynamics of an oblate spheroidal particle was qualitatively different depending on confinement. The projected trajectories of a neutrally buoyant particle in low confinement ($\kappa \approx 0.2$) are schematically drawn in figure 5.6, while the trajectories for a highly confined particle ($\kappa \approx 0.5$) are drawn in figure 5.7. The transitions are characterized in tables 5 and 6.

Even though the dynamics of the oblate spheroidal particle is fully characterized, no analogue to a simple dynamical system has been found, as was done for the prolate case.

Figure 5.6. Schematic illustration of the projected trajectories $(s_x, s_y) = (\sin \theta \cos \phi, \sin \theta \sin \phi)$ for a neutrally buoyant oblate spheroid of $r_p = 4$ in a domain with $\kappa = 0.2$; (a) $Re_p = 10$; (b) $Re_p = 26$; (c) $Re_p = 31$; (d) $Re_p = 32$; (e) $Re_p = 36$; (f) $Re_p = 52$. 

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Even though the dynamics of the oblate spheroidal particle is fully characterized, no analogue to a simple dynamical system has been found, as was done for the prolate case.
5.3. BIFURCATIONS AND DYNAMICAL TRANSITIONS

Figure 5.7. Schematic illustration of the projected trajectories \((s_x, s_y) = (\sin \theta \cos \phi, \sin \theta \sin \phi)\) for a neutrally buoyant oblate spheroid of \(r_p = 2\) in a highly confined domain \(\kappa = 0.5\); (a) \(Re_p \approx 100\); (b) \(Re_p \approx 130\); (c) \(Re_p \approx 160\).

<table>
<thead>
<tr>
<th>Stokes number (St = St_T)</th>
<th>Reynolds number (Re_p = Re_c)</th>
<th>Dynamical transition/bifurcation</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>(St &lt; St_{cd2})</td>
<td>(Re_p = Re_c)</td>
<td>Infinite-period saddle-node bifurcation</td>
<td>(F)</td>
</tr>
<tr>
<td>(St &gt; St_{cd2})</td>
<td>(Re_p = Re_c)</td>
<td>Saddle-node bifurcation</td>
<td>(F)</td>
</tr>
<tr>
<td>-</td>
<td>(Re_p = Re_{PF})</td>
<td>Subcritical pitchfork bifurcation</td>
<td>(F)</td>
</tr>
</tbody>
</table>

Table 5. Summary of all dynamical transitions of an oblate spheroidal particle in a linear shear flow with low confinement.
## 5. SUMMARY OF RESULTS

<table>
<thead>
<tr>
<th>Stokes number</th>
<th>Reynolds number</th>
<th>Dynamical transition/bifurcation</th>
<th>Dominating inertial effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>-</td>
<td>$Re_p = Re_{PF}$</td>
<td>Supercritical pitchfork bifurcation</td>
<td>F</td>
</tr>
<tr>
<td>$St &gt; St_{cd2}$</td>
<td>$Re_p = Re_c$</td>
<td>Saddle-node bifurcation</td>
<td>F</td>
</tr>
</tbody>
</table>

Table 6. Summary of all dynamical transitions of an oblate spheroidal particle in a linear shear flow with high confinement.
5.4. Consequences for dispersion rheology

The influence that the rotational states have on the rheology of a dilute dispersed particle flow containing spheroidal particles can be found by evaluating the shear stress on the walls as described in section 4.3. What is interesting is the non-Newtonian behavior that such a dispersion can have due to inertial effects. A Newtonian fluid will always have the same viscosity $\nu$ regardless of the shear rate $G$. Typical non-Newtonian behavior is that $\nu$ is either an increasing function of $G$, called shear-thickening, or a decreasing function of $G$, called shear-thinning. Using the same dispersed particles and the same fluid in an experiment, $\text{Re}_p$ is only a function of $G$ and can thus be seen as a dimensionless shear rate. From section 3.6, we know that the apparent viscosity of the dispersion $\nu_{\text{disp}}$ can be expressed as

$$\nu_{\text{disp}} = \nu(1 + \eta \Phi), \quad (5.66)$$

where $\Phi$ is the volume fraction and $\eta$ is the intrinsic viscosity. It was also found by Jeffery (1922) that $\eta$ was a function of the rotational state of the particles. Since the particle rotational motion is dependent on the shear rate through $\text{Re}_p$, it is quite intuitive that we will encounter non-Newtonian behavior when including inertial effects.

5.4.1. Prolate case

The intrinsic viscosity $\eta$ as function of $\text{Re}_p$, solid-to-fluid density ratio $\alpha$ and rotational state is shown in figure 5.8 for a spheroidal particle of $r_p = 4$. Generally a shear-thickening behavior is seen for $\alpha = 1$ everywhere apart from a region on the Tumbling branch at $\text{Re}_p \lessapprox \text{Re}_c$. This can be accredited to the diverging period of the Tumbling motion. As the particle becomes heavier and heavier, the Tumbling branch becomes more shear-thickening as the diverging period disappears. Since the other rotational states are unaffected by $\alpha$, it is safe to assume that a dispersion of these particles will always become more shear-thickening when having heavier particles.

The effect of aspect ratio is studied for neutrally buoyant particles of $r_p = 4.5$ and 6 in figure 5.9. As the particle becomes more slender, it was already known from Jeffery (1922) that $\eta$ increases for the Tumbling motion at $\text{Re}_p = 0$. At the same time in these results it is seen that $\eta$ decreases close to $\text{Re}_p = \text{Re}_c$. The Tumbling branch will thus be more shear-thinning with more slender particles. It is also obvious that the slope of the Steady state branch changes and the dispersion becomes less shear-thickening with increasing $r_p$. It is however not believed that a dispersion of slender particles will ever be truly shear-thinning at $\text{Re}_p > \text{Re}_c$. The non-planar rotation branch is not affected significantly by the slenderness, which is also true for the non-inertial case at $\text{Re}_p = 0$. But it can safely be assumed that a dispersion of prolate particles...
will always become more shear-thinning when having particles of higher aspect ratio.

5.4.2. Oblate case

The intrinsic viscosity for a neutrally buoyant oblate particle of $r_p = 4$ is shown in figure 5.10 as a function of $Re_p$ and rotational state. Since the Log-rolling and Steady state for the particle corresponds to steady states for the fluid, the motion is not affected by the solid-to-fluid density ratio. However, as was seen in the previous section, the stable Tumbling motion vanishes with higher $\alpha$. Generally the dispersion of oblate spheroids is shear-thickening, but just as for the prolate particle, the dispersion can show a slight shear-thinning behavior in the Tumbling motion. Since the Tumbling motion is more probable for thinner
5.4. CONSEQUENCES FOR DISPERSION RHEOLOGY

Figure 5.9. Intrinsic viscosity $\eta$ as function of $Re_p$ and rotational state for a neutrally buoyant prolate spheroid of $r_p = 4$ (thick lines) compared with $r_p = 5$ and 6 (thin lines); the dashed lines is connecting the simulated data to the analytical value at $Re_p = 0$; black arrows indicate the trends as $r_p$ is increased.

particles, it is also possible that a dispersion of oblate spheroids with high $r_p$ can experience shear-thinning at $Re_p < Re_c$. 
Intrinsic viscosity $\eta$ as function of $Re_p$ and rotational state for an oblate spheroid of $r_p = 4$; the dashed line is connecting the simulated data to the analytical value at $Re_p = 0$. 

Figure 5.10.
6.1. Summary

This thesis has described the rotational motion of a single spheroidal particle in a simple shear flow and the influence of inertia, which depends on mainly three parameters: Reynolds number $Re_p$, Stokes number $St = \alpha \cdot Re_p$ ($\alpha$ is the solid-to-fluid density ratio) and aspect ratio $r_p$. Given a certain flow situation with typical local $Re_p$, it is possible to predict the rotational behavior of any spheroidal particle with certain $\alpha$ and $r_p$ using the results in the previous chapter. This is summarized in table 1 and 2 for prolate and oblate particles respectively. The tables also indicate what type of rheological behavior that can be expected for the dilute particle suspension.

6.2. Discussion

How can the results from this thesis be used practically?

Consider a steady laminar flow between two parallel walls driven by some external pressure gradient (illustrated in figure 6.1). The velocity gets a parabolic profile in wall normal direction and this type of flow is called a Poiseuille flow. In this flow, we add small spheroidal particles uniformly and we want to know how they orient and how the flow might change due to differences in apparent viscosity. This type of flow might be a good description for understanding some industrial or natural process described in the introduction.

The particles can be assumed to follow the straight streamlines and their translational motion is constant according to the distance from the wall. The particles are small, such that the surrounding flow can be assumed to be linear with a local shear rate according to the slope of the parabolic velocity profile. We thus get a local $Re_p$ depending on distance from the wall. In the middle of the channel, $Re_p$ is zero, but closer to the walls, $Re_p$ increases due to increasing shear. We divide the channel into three regions: (I) Middle region of the channel with low $Re_p$, (II) Intermediate region of the channel with moderate $Re_p$ and (III) Wall region of the channel with high $Re_p$.

As the base case we assume that we have neutrally buoyant spheroids of $r_p \approx 4$ and that $Re_p \approx 0 - 150$. First question we ask ourselves is whether
### 6. CONCLUSIONS

Typical rotational states of a prolate spheroidal particle in a shear flow depending on $Re_p$, $\alpha$ and $r_p$; superscript indicating if rotational state is leading to shear-thickening (+) or shear-thinning (−) of the dilute particle suspension; no superscript indicates that a dilute suspension behaves almost Newtonian; T=Tumbling, R=Rotating, LR=Log-rolling (or other non-planar states), S=Steady state

<table>
<thead>
<tr>
<th>$Re_p$</th>
<th>Light ($\alpha \leq 1$)</th>
<th>Neutrally buoyant ($\alpha \approx 1$)</th>
<th>Heavy ($\alpha \gg 1$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low $Re_p$ $Re_p \leq 30$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: LR$^+$ High $r_p$: LR$^+$</td>
<td>Low $r_p$: T$^+$ $r_p \approx 4$: T High $r_p$: T$^-$</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+$ High $r_p$: R$^+$</td>
</tr>
<tr>
<td>Middle $Re_p$ $Re_p \approx 30 - 70$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: LR$^+$ High $r_p$: S</td>
<td>Low $r_p$: T$^+/LR^+$ $r_p \approx 4$: T/LR$^+$ High $r_p$: S</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+$ High $r_p$: R$^+/S^+$</td>
</tr>
<tr>
<td>High $Re_p$ $Re_p \approx 70 - 150$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S</td>
<td>Low $r_p$: T$^-$/LR$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+/S^+$ High $r_p$: R$^+/S^+$</td>
</tr>
<tr>
<td>Very high $Re_p$ $Re_p \geq 150$</td>
<td>Low $r_p$: S$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+/S^+$ High $r_p$: S$^+$</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Typical rotational states of a prolate spheroidal particle in a shear flow depending on $Re_p$, $\alpha$ and $r_p$; superscript indicating if rotational state is leading to shear-thickening (+) or shear-thinning (−) of the dilute particle suspension; no superscript indicates that a dilute suspension behaves almost Newtonian; T=Tumbling, R=Rotating, LR=Log-rolling (or other non-planar states), S=Steady state

<table>
<thead>
<tr>
<th>$Re_p$</th>
<th>Light ($\alpha \leq 1$)</th>
<th>Neutrally buoyant ($\alpha \approx 1$)</th>
<th>Heavy ($\alpha \gg 1$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low $Re_p$ $Re_p \leq 30$</td>
<td>Low $r_p$: T $r_p \approx 4$: T$^-$ High $r_p$: T$^-$/S$^+$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: LR$^+$ High $r_p$: T$^-$/LR$^+$/$S^+$</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+$ High $r_p$: S$^+$</td>
</tr>
<tr>
<td>Middle $Re_p$ $Re_p \approx 30 - 70$</td>
<td>Low $r_p$: T$^-$ $r_p \approx 4$: T$^-$/S$^+$ High $r_p$: S$^+$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: LR$^+/S^+$ High $r_p$: S$^+$</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: R$^+/S^+$ High $r_p$: S$^+$</td>
</tr>
<tr>
<td>High $Re_p$ $Re_p \approx 70 - 150$</td>
<td>Low $r_p$: T $r_p \approx 4$: S$^+$ High $r_p$: S$^+$</td>
<td>Low $r_p$: LR$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S$^+$</td>
<td>Low $r_p$: R$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S$^+$</td>
</tr>
<tr>
<td>Very high $Re_p$ $Re_p \geq 150$</td>
<td>Low $r_p$: S$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S$^+$</td>
<td>Low $r_p$: S$^+$ $r_p \approx 4$: S$^+$ High $r_p$: S$^+$</td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Typical rotational states of an oblate spheroidal particle in a shear flow depending on $Re_p$, $\alpha$ and $r_p$; superscript indicating if rotational state is leading to shear-thickening (+) or shear-thinning (−) of the dilute particle suspension; no superscript indicates that a dilute suspension behaves almost Newtonian; T=Tumbling, LR=Log-rolling, S=Steady state
6.2. DISCUSSION

Figure 6.1. Illustration of a Poiseuille flow between two parallel plates with spheroidal particles; the particles are approximately translated with constant velocity and the flow in a moving inertial frame of reference around a particle can be approximated with a linear shear flow; the flow is divided into three regions: I = middle region, II = intermediate region, III = wall region.

<table>
<thead>
<tr>
<th>Region</th>
<th>Probable rot. states (Prolate)</th>
<th>Probable rot. states (Oblate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I)</td>
<td>T</td>
<td>LR</td>
</tr>
<tr>
<td>(II)</td>
<td>T/LR</td>
<td>LR/S</td>
</tr>
<tr>
<td>(III)</td>
<td>S</td>
<td>S</td>
</tr>
</tbody>
</table>

Table 3. Typical rotational states of neutrally buoyant spheroidal particles of $r_p = 4$ in a Poiseuille flow with $Re_p \approx 0-150$.

this range of $Re_p$ is physically relevant. Assume that the maximum velocity is given by $U_{\text{max}}$ and the size of the channel is $H$, then the maximum shear rate is given by $G = 4U_{\text{max}}/H \text{ s}^{-1}$. Say that we are considering $H = 10^{-2} \text{ m}$ with a particle length of $l = 10^{-3} \text{ m}$ in water with $\nu = 10^{-6} \text{ m}^2/\text{s}$. To reach $Re_p = 150$, we need a flow of $U_{\text{max}} = (Re_p \cdot \nu \cdot H)/4l^2 = 0.375 \text{ m/s}$, which does not seem unreasonably high.

A probable distribution of rotational states is described in table 3 and illustrated in figure 6.2, where also an approximate viscosity profile is drawn. The viscosity profile for the prolate particles will be fairly constant in region (I) and (II) and then increase closer too the wall when particles are assuming Steady state. For the oblate case there will be an initial increase in region (I), then a decrease in region (II) as more and more particles start to assume Steady state, and then an increase again in region (III) where all particles have assumed Steady state.
### Figure 6.2
An approximate distribution of rotational states in the plane Poiseuille flow with $Re_p \approx 0 - 150$ and a schematic profile of the apparent viscosity of the particle suspension consisting of neutrally buoyant prolate (left) and oblate (right) spheroids of $r_p = 4$.

### Figure 6.3
An approximate distribution of rotational states in the plane Poiseuille flow with $Re_p \approx 0 - 150$ and a schematic profile of the apparent viscosity of the particle suspension consisting of neutrally buoyant prolate (left) and oblate (right) spheroids with high aspect ratio, $r_p$.

**Increasing $r_p$**

Increasing $r_p$ will mainly influence the intermediate region (II) as seen in figure 6.3 and table 4. For the prolate particles, it will be less probable that particles assume Log-rolling and rather only be in a planar rotation. For the oblate particles, the Tumbling state might be more probable in region (II). The viscosity profiles are also changing as seen in figure 6.3. For the prolate case, the viscosity is initially decreasing towards the wall due to shear-thinning of the Tumbling spheroids. In region (III) there is a small increase again as the particles assume Steady state. For the oblate case, the viscosity stays rather constant in the middle region as a net result of shear-thinning Tumbling and shear-thickening Log-rolling.
### Table 4.

Typical rotational states of neutrally buoyant spheroidal particles of high $r_p$ in a Poiseuille flow with $Re_p \approx 0-150$.  

<table>
<thead>
<tr>
<th>Region</th>
<th>Probable rot. states (Prolate)</th>
<th>Probable rot. states (Oblate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I)</td>
<td>$T$</td>
<td>$T/LR/S$</td>
</tr>
<tr>
<td>(II)</td>
<td>$S$</td>
<td>$S$</td>
</tr>
<tr>
<td>(III)</td>
<td>$S$</td>
<td>$S$</td>
</tr>
</tbody>
</table>

#### Figure 6.4.

An approximate distribution of rotational states in the plane Poiseuille flow with $Re_p \approx 0-150$ and a schematic profile of the apparent viscosity of the particle suspension consisting of neutrally buoyant prolate (left) and oblate (right) spheroids with low aspect ratio, $r_p$.

**Decreasing $r_p$**

Keeping the same flow conditions, but decreasing the aspect ratio of the particles, means that we probably will not reach $Re_p = Re_c$ in the wall region (III). The consequence is that the prolate particles will probably either be Tumbling or Log-rolling while oblate particles are only Log-rolling (see figure 6.4 and table 5). The viscosity in both the prolate and oblate case will be a steadily increasing function towards the wall.

**Increasing $\alpha$**

Assuming there is no gravity causing sedimentation of the particles, an increase of the particle density does not have any big influence on oblate spheroids seen in figure 6.5 and table 6. For prolate spheroids, the increase in $\alpha$ will increase the probability for Tumbling particles. Also, since particle inertia effects are strong, there might be Tumbling particles in region (III). Since there is no diverging Tumbling period for the heavy prolate spheroids, the viscosity will be steadily increasing towards the wall.
6. CONCLUSIONS

<table>
<thead>
<tr>
<th>Region</th>
<th>Probable rot. states (Prolate)</th>
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<tbody>
<tr>
<td>(I)</td>
<td>T</td>
<td>LR</td>
</tr>
<tr>
<td>(II)</td>
<td>T/LR</td>
<td>LR</td>
</tr>
<tr>
<td>(III)</td>
<td>T/LR</td>
<td>LR</td>
</tr>
</tbody>
</table>

Table 5. Typical rotational states of neutrally buoyant spheroidal particles of low $r_p$ in a Poiseuille flow with $Re_p \approx 0 - 150$.

![Figure 6.5. An approximate distribution of rotational states in the plane Poiseuille flow with $Re_p \approx 0 - 150$ and a schematic profile of the apparent viscosity of the particle suspension consisting of heavy prolate (left) and oblate (right) spheroids with $r_p = 4$.](image)

<table>
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<th>Region</th>
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<th>Probable rot. states (Oblate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I)</td>
<td>T</td>
<td>LR</td>
</tr>
<tr>
<td>(II)</td>
<td>T</td>
<td>LR/S</td>
</tr>
<tr>
<td>(III)</td>
<td>T/S</td>
<td>S</td>
</tr>
</tbody>
</table>

Table 6. Typical rotational states of heavy spheroidal particles of $r_p = 4$ in a Poiseuille flow with $Re_p \approx 0 - 150$.

**Decreasing $\alpha$**

The thesis showed no results of what is happening at $\alpha < 1$, but using physical intuition we can still assume what will happen as particle inertia becomes less important. This is illustrated in figure 6.6 and described in table 7. For prolate spheroids, this means probably that there will be no drift to Tumbling and the typical states will be either Log-rolling or Steady state. This probably also
6.3. CONCLUDING REMARKS

Figure 6.6. An approximate distribution of rotational states in the plane Poiseuille flow with $Re_p \approx 0 - 150$ and a schematic profile of the apparent viscosity of the particle suspension consisting of light prolate (left) and oblate (right) spheroids with $r_p = 4$.

<table>
<thead>
<tr>
<th>Region</th>
<th>Probable rot. states (Prolate)</th>
<th>Probable rot. states (Oblate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I)</td>
<td>LR</td>
<td>T</td>
</tr>
<tr>
<td>(II)</td>
<td>LR</td>
<td>T/S</td>
</tr>
<tr>
<td>(III)</td>
<td>S</td>
<td>S</td>
</tr>
</tbody>
</table>

Table 7. Typical rotational states of light spheroidal particles of $r_p = 4$ in a Poiseuille flow with $Re_p \approx 0 - 150$.

means that the apparent viscosity will increase towards the wall. For oblate spheroids, there is instead no drift towards Log-rolling and the Tumbling state is believed to be stable instead. There will be a diverging period in region (I) and (II) of the Tumbling motion and thus decreasing with the distance from the center. In region (III), the particle will be in steady state and the viscosity will increase towards the wall.

6.3. Concluding remarks

This thesis has described the rotational behavior of spheroidal particles in a linear shear flow and the influence of both fluid and particle inertia. It has also been investigated how the particle motion affects the rheological properties of a dilute dispersion containing spheroidal particles. Given a certain flow problem, e.g., a fiber in a paper pulp suspension, an ice crystal in the atmosphere or a blood platelet in an artery, some valuable predictions can thus be made about the particle orientation distribution and dispersion rheology. It should be noted that for flow situations where $Re_p, St < O(1)$, the particles will be close to performing analytical orbits according to Jeffery (1922), and the orbit drift
induced by inertia will probably be negligible. For such cases, other effects such as e.g. Brownian diffusion, hydrodynamic interactions and particle-wall interactions will probably be more important. This thesis however provides the necessary foundation for physical understanding, and can be seen as one of the stepping stones towards full understanding of dispersed particle flows.
CHAPTER 7

Outlook

There are several different topics that are possible to investigate based on the presented results, some of which hopefully can be researched on in next few years. In this chapter, some of these will be presented.

7.1. Reduced model for the influence of fluid inertia

For large scale particle simulations in any practical application it is desired to look at the collective motion of many millions of particles. The approach here, with full interpolation of forces on the particle surface, will be impossible to employ. Instead, it is desired to use the flow statistics, such as local shear rates, in order to model the motion. The results of Jeffery (1922) has been successfully implemented in many large scale models since the angular velocity of the spheroid is a simple function of strain and vorticity.

Lundell & Carlsson (2010) used the torque from Jeffery (1922) and coupled with the full equation of motion of the particle. Even though it is much more expensive, in this way it is possible to get the instantaneous angular acceleration of the particle depending on strain and vorticity, and thus include particle inertia for the rotational motion.

Including fluid inertia however is much more difficult due to the many degrees of freedom in the flow. However, for prolate particles it was found that the competition of fluid and particle inertia was causing the particle to either behave like a Van der Pol-Duffing oscillator in the non-planar rotation or a damped driven pendulum in the planar rotation. It is thus believed that it should be possible to get a low order model, which can mimic the influence of fluid inertia on the rotation.

It was also seen that the local strength of the strain part of the flow could cause the bifurcations seen in the planar rotation. Using the model by Lundell & Carlsson (2010), we would find what the angular acceleration for a particle will be given a linear shear flow \( u = (V + D)x \), with \( V \) as the vorticity tensor and \( D \) as the strain tensor. If now fluid inertia has the effect that the strain flow is gaining strength, one can probably modify the input with a parameter \( \beta \) depending on the local \( \text{Re}_{\text{p}} \), such that \( u = (\beta V + (1 - \beta)D)x \). Initial results show that this type of model can be used for matching orbit drift, the subcritical Hopf bifurcation at \( \text{Re}_{\text{LR}} \) and the saddle-node bifurcation at \( \text{Re}_c \).
In principle this model will mimic a damped driven pendulum in the planar rotation but only a Van der Pol oscillator with non-linear damping in the non-planar motion. This model can thus not capture the Duffing part, i.e. the non-linear restoring forces, which must be included in some other way.

7.2. Stability of the Log-rolling prolate spheroid

In paper 1, it is found that the prolate spheroidal particle behaves like a Van der Pol-Duffing oscillator in the non-planar rotation. This leads to the belief that the Log-rolling prolate spheroid has a double-zero eigenvalue for a certain choice of \( Re_p \) and \( St \). Since the particle is rotating with constant angular velocity around its symmetry axis in the Log-rolling motion, a rotating grid is not necessary since the fluid assumes a steady state. One can instead set velocity boundary conditions on the particle surface to match this steady state, where the torque on the particle equals to zero. With an eigenvalue solver in Comsol, one can find the dominant eigenvalues for this rotation at different \( Re_p \) and \( St \). It should then be found that the Log-rolling solution has complex eigenvalues with negative real part for low \( Re_p \) with a transition to positive real part at the Hopf bifurcation at \( Re_{LR} \). Similarly, the pitchfork bifurcation at \( Re_{PF} \) should be found by seeing that we get a real positive eigenvalue above this point and the Log-rolling becomes a saddle. By tracking these two bifurcations, it should be possible to find the double-zero eigenvalue, which then will prove the existence of the set of bifurcations described in this work.

7.3. Experiments

In the numerical world, a lot of conditions are far too ideal compared to the real world. For example, any influence of gravity any type of Brownian motion of the particles or surrounding turbulence was neglected. However, it should still be possible to test some of the assumptions about particle rotation, which was revealed from the present numerical results.

7.3.1. Neutrally buoyant particles

In order to check any three-dimensional rotation of the spheroidal particles, they must be carefully made in order to match the density of the fluid. Otherwise, they will sediment and eventually hit the boundary of the experiment, and it will be hard to determine if the rotational behavior is caused through interaction with walls etc. However, if this is managed, one should be able to put such particles in a linear Couette flow, and by just observing the rotation we should be able to see a certain sequence of transitions with increasing shear rate. There is still at least one crucial factor that must be managed. The flow does probably not remain stable for those channel Reynolds numbers \( Re_H = \kappa^{-2} Re_p \) that were investigated in this numerical work. One way of reaching higher \( Re_H \) is to add a system rotation to the Couette flow (Tsukahara
et al. 2010), where Coriolis forces stabilize the flow and delay the transition to turbulence. However, in order to have a certain $Re_p$ of $> O(10)$, one must probably increase the confinement, and the domain size independent critical Reynolds numbers can thus probably not be found experimentally. For the oblate spheroid it would also be of interest to actually modify the confinement and observe if an Inclined rolling solution will stabilize/destabilize.

### 7.3.2. Heavy particles

The problem of heavy particles, is the fact that they will sediment in the direction of gravity. The study of the rotation of heavy particles is particularly interesting for prolate spheroids, since there are more interesting transitions depending on $St$ and it has a bigger impact on dispersion rheology. For these particles, due to particle inertia, it is probable that they end up in a planar motion, and therefore it is only of interest how it behaves when they rotate around the minor axis. One should thus be able to place a fixed axis in the flow, e.g. a wire, aligned in the vorticity direction, on which a prolate spheroid is free to rotate around its minor axis. One should in this way be able to observe the driven damped pendulum mechanism and perhaps experimentally pinpoint $Re_c$. Confinement will of course be an issue for this experiment as well. More discussion on how experiments with heavy particles can be performed is found in the work by Lundell & Carlsson (2010).

### 7.4. Investigation of other types of particles

The particles investigated in the present work all have rotational symmetry and a range of $r_p = 2 - 6$ was investigated. Even though this range of particles are enough to state many things about the dynamics, the results can be explored further for other types of particles.

#### 7.4.1. Low aspect ratio particles

The reason why no particles below $r_p = 2$ have been presented in this thesis, is because the dynamical behavior is much more complex than the typical bifurcations encountered here, especially for prolate spheroids.

Firstly, it was seen that the critical Reynolds numbers were exponentially decreasing with $r_p$ and the transitions thus occur at much higher $Re_p$ for $r_p < 2$. It was therefore not possible to find certain transitions since the maximum $Re_p$ was limited to $Re_p = 300$ for the flow to remain stable.

Secondly, the higher aspect ratio particles had a clear separation between fluid inertia domination in the non-planar rotation and particle inertia domination in the planar rotation. When the particle had low aspect ratio ($r_p < 2$), particle inertia started to influence the dynamical behavior also in the non-planar motion causing seemingly chaotic rotational states (described in paper 2).
Thirdly, for the low \( r_p \) particles in a Tumbling motion at high \( Re_p \), it seems the particle starts interacting with its own wake, leading to a Tumbling motion, which might counteract the particle inertial drift towards rotation in the flow-gradient plane. Consequently, we can find that the Tumbling motion, i.e. rotation around the minor axis, might actually not be in the flow-gradient plane.

The investigation of low aspect ratio particles will require a lot of extra attention in order to fully understand the dynamics and might be a topic for the future.

7.4.2. High aspect ratio particles

The reason why no particles above \( r_p = 6 \) have been investigated was purely due to computational effort. Since the results were restricted to \( \kappa = 0.2 \) and the minor axis was restricted to be \( \geq 3 \), the domain must be increased in order to simulate a high aspect ratio particle. For example, a particle of \( r_p = 8 \) must be simulated in a domain of \( N = 240 \), which will be eight times as computationally expensive as the simulation of the particle with \( r_p = 4 \). Another problem with a larger domain is that if the same time resolution, i.e. shear rate \( G \), should be used, the Mach number at the walls might be too large since it is defined as \( Ma_w = U_w/c_s = GN/(2c_s) \), with \( c_s = \sqrt{1/3} \) as the constant lattice sound speed.

In order to further investigate the behavior of high aspect ratio particles, it might be necessary to look at other computational methods.

7.4.3. Light particles

This work was restricted to having solid-to-fluid density ratio \( \alpha \geq 1 (St \geq Re_p) \) due to the fluid-structure interaction in the LB-EBF formulation. It is however believed that a lot of things will change for lighter particles, which can be predicted from the present results. For example, if particle inertia is much less important than fluid inertia (\( St \ll Re_p \)), it is believed in the prolate case, that all rotational states where the symmetry axis is non-stationary will cease to be stable. This means that the particle will go from Log-rolling (following Jeffery’s hypothesis) at low \( Re_p \) to Inclined rolling at higher \( Re_p \) and eventually Steady state at \( Re_p > Re_c \).

This, however, requires a thorough investigation and must be investigated with other ways of modeling the fluid-structure interaction.

7.4.4. Tri-axial ellipsoidal particles

All the particles in this thesis were spheroids, i.e. they have perfect rotational symmetry. This is however not commonly found in the applications talked about in the introduction. As soon as the prolate spheroid has a slight asymmetry and is defined as a tri-axial ellipsoid, its rotation can become unstable
resulting in a chaotic motion (Yarin et al. 1997). It was seen later by Lundell (2011b) that particle inertia can stabilize this chaotic behavior. However, it is still unknown what the effect of fluid inertia will be on the rotation of tri-axial ellipsoids. In principle, investigating this behavior numerically is an easy but time-consuming task with the present method since we add a second aspect ratio parameter to the study. Some initial results seems to show that fluid inertia also has a stabilizing effect on the particle motion.

7.4.5. Arbitrary shapes
Of course, even the tri-axial ellipsoid is a quite ideal form of a non-spherical particle. It might thus be interesting to see how well an arbitrary shaped particle can be approximated by the motion of an ellipsoid. For example, how well is the motion of a blood cell captured by an oblate spheroid? Or how well is a cylindrical fiber captured by a prolate spheroid?

7.4.6. Deformable particles
Within biological applications, rigid particles are rarely encountered, e.g. the motion of different biological cells. These are rather better captured by making the particle as a liquid capsule enclosed by an elastic membrane. Models for this are already used for simulating blood cells, for example by Reasor et al. (2013). It would be interesting to see how the particle behavior changes as we go from a capsule with practically inelastic membrane containing extremely viscosity fluid (i.e. essentially a rigid particle) to a capsule with low elasticity and viscosity.

7.5. Other flow cases
So far, only the behavior in a constant linear shear flow has been studied and any other forces, e.g. gravity, have been neglected. The flow situation can also be altered to build up knowledge about particle behavior in an arbitrary flow.

7.5.1. Oscillating shear flow
The shear flow in this thesis has always had constant shear rate $G$. In many practical applications, e.g. the flow of blood from the heart or the flow after a pump, often has a pulsatile behavior and the shear rate is a function of time $G(t)$. The planar motion of prolate spheroids with particle inertia in a creeping oscillating shear flow ($G = \cos \omega t$) was studied by Nilsen & Andersson (2013). It was found that the oscillating motion of the spheroids could be chaotic for certain $r_p$ and $St$. It still remains unknown what the influence of fluid inertia will be on this behavior. Initial results by Berg (2013) has showed that chaos still seems to be present at higher $Re_p$, but there were no conclusive results and additional research on this topic must be done.
7.5.2. Relative velocity to the fluid

When an external force is acting on the fluid-particle system, e.g., gravity, there will be a sedimentation process if the particle is not exactly density matched with the fluid. The consequence is that the particle gains a relative velocity to the fluid and a wake might start to form behind the particle. A translating spherical particle can experience a force due to a relative motion to the fluid in a linear shear flow, called a Saffman force, which acts in the direction of the velocity gradient Crowe et al. (2012). The particle can be affected by an extra force, called a Magnus force if the particle is also rotating relative to the fluid due to differences in pressure since the surface is moving towards the flow on one side of the particle, and away from the flow on the other side. The lift force on the spheroidal particle in this thesis can be investigated by adding a constant velocity to the flow and keeping the particle steady in the middle. Initial results seem to suggest that this relative velocity alters the rotational behavior of a neutrally buoyant prolate spheroidal particle significantly and we obtain lift forces in the velocity gradient direction that decreases with increasing \( Re_p \).

7.5.3. Particle-particle interaction

So far, only one single particle is considered in all the suggested cases in this chapter. In most practical applications, the particles are so close together that particle-particle interaction can’t be neglected. As a first step it would be interesting to see what happens if two particles that can rotate independently are placed beside one another with a certain distance in a shear flow. Presumably there is a critical distance where the particles stop behaving like individual particles, and that the flow between them act in a way so that the rotation is synchronized. This was already seen some first indications of this Tumbling prolate spheroids in paper 1 and that \( Re_c \) was changing depending on the distance between them. It will however be even more interesting to see when they are allowed to translate, if they attract or repel one another.

7.6. Improvements of numerical model

As was seen in chapter 4, there are several issues with the present numerical model that need to be addressed in order to get quantitatively correct results from the simulations. Probably, the fluid-structure interaction can be improved in order to eliminate the dependence on temporal and spatial resolution. Another problem is the domain size, which must be very large in order to be able to neglect influence from walls and periodic boundary conditions. These boundary conditions are implemented due to simplicity, but probably a lot of time can be saved by implementing Lees-Edwards boundary conditions (Wagner & Pagonabarraga 2002). These are especially useful in order to investigate bulk systems where the influence of the simulation boundaries are desired to be eliminated.
CHAPTER 8

Papers & author contributions

Paper 1
*Effect of fluid inertia on the dynamics and scaling of neutrally buoyant particles in shear flow*
T. Rosén (TR), F. Lundell (FL) & C. K. Aidun (CKA)

The non-linear dynamics of a neutrally buoyant \((St = Re_p)\) prolate spheroidal particle of fixed aspect ratio \((r_p = 4)\) in a shear flow was studied numerically. TR performed the simulations for verification, validation and the non-planar rotation under the supervision of FL. The simulations to show the scaling of the infinite-period saddle-node bifurcation in the planar rotation was provided by CKA. TR characterized the bifurcations with input from CKA and the physical explanation of fluid and particle inertial effects was jointly described by TR and FL. The paper was written by TR with input from FL and CKA. Typographical errors in the published version have been corrected.

Paper 2
*The dynamical states of a prolate spheroidal particle suspended in shear flow as a consequence of particle and fluid inertia*
T. Rosén (TR), F. Lundell (FL), M. Do-Quang (MDQ) & C. K. Aidun (CKA)

The results from the first paper was extended into describing the non-linear dynamics of prolate spheroids in shear flow at \(St \geq Re_p\) and \(r_p = 2 - 6\). TR performed all the simulations under supervision of FL and MDQ. The non-linear dynamics was characterized by TR with input from CKA and FL. TR wrote the paper with input from FL, CKA and MDQ. Parts of these results have been published in:

*Equilibrium solutions of the rotational motion of a spheroidal particle in Couette flow*
T. Rosén, F. Lundell, M. Do-Quang & C. K. Aidun
8th Int. Conf. on Multiphase Flow
May 26 – May 31 2013, Jeju, South Korea
Paper 3
Effect of fluid and particle inertia on the rotation of an oblate spheroidal particle suspended in shear flow
T. Rosén (TR), F. Lundell (FL), M. Do-Quang (MDQ) & C. K. Aidun (CKA)

The non-linear dynamics of an oblate spheroidal particle in a linear shear flow was studied numerically at $St \geq Re_p$ and $r_p = 2 - 5$. TR performed all the simulations and analyzed the resulting dynamics and bifurcations with input from FL, MDQ and CKA. The paper was written by TR with input from FL, CKA and MDQ.
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Tomas Rosén
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