Control of inertial microfluidics

vorgelegt von
Diplom-Physiker

Christopher Prohm
geboren in Wuppertal

von der Fakultät II - Mathematik und Naturwissenschaften
der Technischen Universität Berlin
zur Erlangung des akademischen Grades
Doktor der Naturwissenschaften (Dr. rer. nat.)

genehmigte

Dissertation

Promotionsausschuss:

Vorsitzender: Prof. Dr. rer. nat. Martin Oestreich
Erster Gutachter: Prof. Dr. rer. nat. Holger Stark
Zweiter Gutachter: Prof. Dr. rer. nat. Roland Netz

Tag der wissenschaftlichen Aussprache: 20. 10. 2014

Berlin 2015

D83
## Contents

1. **Introduction** .......................................................... 7

2. **Basics of inertial microfluidics** .................................. 11
   2.1. Review of inertial microfluidics ................................... 12
       2.1.1. Device design .................................................. 14
       2.1.2. Theoretical analysis of inertial focusing .................. 16
   2.2. Hydrodynamics ..................................................... 17
       2.2.1. The continuity equation and the Navier-Stokes equations 17
       2.2.2. Incompressibility ............................................. 19
       2.2.3. Importance of inertia ........................................ 19
       2.2.4. The Stokes equations ........................................ 20
       2.2.5. The no-slip condition ........................................ 21
   2.3. Poiseuille flow ................................................... 22
   2.4. Colloidal particles ............................................... 25
       2.4.1. Movement in a viscous fluid ................................ 26
       2.4.2. Hydrodynamics in two dimensions and Stokes paradox .... 28
       2.4.3. No lift force at zero Reynolds number .................... 29
       2.4.4. Matched asymptotic expansion for inertial migration ..... 31
       2.4.5. Dynamic pressure model for inertial migration ........... 33
       2.4.6. Thermal Motion ................................................ 35

3. **Mesoscopic simulations of fluid dynamics** ..................... 41
   3.1. Computational fluid dynamics .................................... 41
       3.1.1. Direct discretization of the Navier-Stokes equations .... 41
       3.1.2. Mesoscopic simulation methods ................................ 42
   3.2. Multi-particle collision dynamics ................................ 43
       3.2.1. Main algorithm .................................................. 44
       3.2.2. Transport coefficients ........................................ 47
       3.2.3. Boundary conditions .......................................... 49
       3.2.4. Colloidal particles ............................................ 50
       3.2.5. Choice of parameters .......................................... 51
       3.2.6. Validation ....................................................... 53
   3.3. The lattice Boltzmann method .................................... 55
       3.3.1. Lattice Bhatnagar-Gross-Krook ................................ 55
       3.3.2. Chapman-Enskog expansion .................................... 58
       3.3.3. Lattice aligned boundaries .................................... 61
       3.3.4. The immersed boundary method ................................ 62
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3.5. Choice of parameters</td>
<td>65</td>
</tr>
<tr>
<td>3.3.6. Validation</td>
<td>65</td>
</tr>
<tr>
<td>3.4. Measuring inertial lift forces</td>
<td>67</td>
</tr>
<tr>
<td>3.5. Software used</td>
<td>68</td>
</tr>
<tr>
<td>4. Channel geometry and inertial focusing</td>
<td>69</td>
</tr>
<tr>
<td>4.1. Circular channel cross sections</td>
<td>69</td>
</tr>
<tr>
<td>4.1.1. Probability distributions</td>
<td>69</td>
</tr>
<tr>
<td>4.1.2. Radial lift forces and axial velocity</td>
<td>73</td>
</tr>
<tr>
<td>4.2. Rectangular channel cross sections</td>
<td>77</td>
</tr>
<tr>
<td>4.2.1. Square channel cross sections</td>
<td>78</td>
</tr>
<tr>
<td>4.2.2. Rectangular channel cross sections</td>
<td>81</td>
</tr>
<tr>
<td>4.3. Conclusions</td>
<td>84</td>
</tr>
<tr>
<td>5. Control of inertial lift forces</td>
<td>87</td>
</tr>
<tr>
<td>5.1. Axial control forces</td>
<td>88</td>
</tr>
<tr>
<td>5.2. Axial feedback control</td>
<td>93</td>
</tr>
<tr>
<td>5.3. Control by rotational motion</td>
<td>95</td>
</tr>
<tr>
<td>5.3.1. Uncontrolled motion</td>
<td>95</td>
</tr>
<tr>
<td>5.3.2. Control by torque</td>
<td>96</td>
</tr>
<tr>
<td>5.3.3. Control by angular velocity</td>
<td>98</td>
</tr>
<tr>
<td>5.4. Conclusions</td>
<td>101</td>
</tr>
<tr>
<td>6. Optimal control of particle separation</td>
<td>103</td>
</tr>
<tr>
<td>6.1. System</td>
<td>103</td>
</tr>
<tr>
<td>6.2. Optimal control theory</td>
<td>106</td>
</tr>
<tr>
<td>6.2.1. Particle steering</td>
<td>106</td>
</tr>
<tr>
<td>6.2.2. Particle separation</td>
<td>109</td>
</tr>
<tr>
<td>6.2.3. Numerical solution</td>
<td>110</td>
</tr>
<tr>
<td>6.2.4. Comparison with related optimal control problems</td>
<td>112</td>
</tr>
<tr>
<td>6.3. Optimal particle steering</td>
<td>113</td>
</tr>
<tr>
<td>6.4. Optimal particle separation by size</td>
<td>115</td>
</tr>
<tr>
<td>6.5. Conclusions</td>
<td>119</td>
</tr>
<tr>
<td>7. Conclusions</td>
<td>121</td>
</tr>
<tr>
<td>A. Notation</td>
<td>125</td>
</tr>
<tr>
<td>B. Kernel density estimates</td>
<td>127</td>
</tr>
<tr>
<td>C. Optimal control with Lagrange multipliers</td>
<td>129</td>
</tr>
<tr>
<td>C.1. Optimal particle steering</td>
<td>129</td>
</tr>
</tbody>
</table>
## Contents

C.2. Optimal particle separation ............................................. 132

D. Numerical methods for stochastic systems 135
   D.1. Euler method for the Langevin equation .......................... 135
   D.2. Markov chain approximation methods .............................. 135
       D.2.1. Adjoint equation and state equation ....................... 135
       D.2.2. Optimal control equation .................................... 138

E. Parameters ................................................................. 141
Manipulation and handling of fluids are an important part of many established fields including chemistry, biology and medicine. Today, automatization and parallelization in these fields rely on robotics and large scale apparatus [1, 2]. In future, fully automated devices are hoped to operate on micrometer length scales, treating fluids in the microfluidic regime. The additional miniaturization, akin to the revolution in electronics, promises a number of economic advantages [1–3]. The drastically reduced size decreases the required sample volumes to mere nano liters [1–4]. It further renders the devices more portable such that analyses can be performed wherever samples arise [2] and reduces analysis times, thereby increasing efficiency [2]. Many components in microfluidics have been developed over the last years and integrating these components promises the miniaturization of whole laboratories to so-called labs on a chip [1, 2, 4].

Besides economic advantages, microfluidics and, more recently, nanofluidics introduce novel physical effects and phenomena due to the small length scales involved [3, 5]. In microfluidic systems, flow velocities are often small. Then, friction dominates and fluid inertia loses its significance. As one consequence, the forces exerted on particles in flows are strongly restricted [6]. In particular, spherical particles in channels do not experience any deterministic force perpendicular to the flow direction and the only cause for lateral migration of single particles is diffusion.

How fluid inertia gives rise to migration across streamlines, has first been discussed by Segré and Silberberg in 1961 [7–9]. They investigated experimentally particle suspensions in circular pipes at varying flow speeds. The particles order on a circular annulus irrespective of their initial distribution. The system is situated between the limiting cases of highly inertial, turbulent flows and non-inertial flows. Flows are still laminar, but lift forces associated with fluid inertia cause particles to migrate across streamlines.

Recently, experiments and theory started to explore inertial migration in the field of microfluidics [10, 11]. For increasing flow velocity, fluid inertia becomes significant even on micrometer scales. Various devices with different biomedical applications have been demonstrated over the last years (for example [12–18]). These devices rely on a self-organized order of the embedded particles mediated by inertial lift forces. The features of the emergent order strongly depend on the channel geometry and particle shape. In particular, the number, placement, and stability of the equilibrium positions of particles across the channel depend crucially on the channel cross section. In steady state, the observed patterns of particles range from the annulus in circular cross sections to discrete points in rectangular cross sections. In addition, the particle size strongly influences the magnitude of the lift forces, such that larger particles experience much stronger lift forces.
Lastly, hydrodynamic interactions in particle suspensions introduce an additional axial order in the form of complex microfluidic crystals [19] or triangular streaming lattices [12, 19].

Inertial focusing has proved resistant to analytic investigation. The nonlinear inertial term in the Navier-Stokes equations allows to find only approximate results. Semianalytic studies of inertial migration commonly employ the method of matched asymptotic expansion [20, 21]. However, they are only partially applicable as they assume particles to be small compared to the channel dimensions and do not take the channel geometry into account [22]. To overcome these limitations, numerical methods have to be used [22].

Devices in inertial microfluidics rely in different ways on inertial lift forces and the self-organized order between particles. In channels with rectangular cross sections, particles order in a single plane and the emergence of streaming lattices results in clear separation of particles. If combined with optical microscopes, this features enables the identification and counting of different cell types [12]. Once cells assume their well defined equilibrium positions, the mechanical properties of these cells can be probed by external sheath flows, for example, to detect cancer [14]. Further, the sensitivity of inertial lift forces to particle size has been utilized in different arrangements to separate particles by size. In channels with rectangular cross section, the size dependence of the magnitude of the lift forces has been used to separate red blood cells from bacteria [15]. In channels with trapezoidal cross section, a sudden switch of stability depending on particle size allowed to separate polystyrene beads by size [16]. Finally, the controlled placement of cylindrical obstacles in channels enhances the focusing of particles [17] and has recently been explored for the design of fluid flow with possible applications to particle separation [18]. This wide range of applications leads to a growing interest in commercializing inertial microfluidic devices [10].

In microfluidics, often external control methods are utilized, in particular electric and magnetic fields [23]. Over the years, focused laser beams, called optical tweezers, have proved to be a versatile control method [24–30]. They can create tailored optical potential landscapes for colloidal particles either as scanning optical tweezers [25–27] or holographic optical tweezers [28–30]. In particular, the latter have been used to create optical lattices for cell sorting [31]. Further, magnetic fields exert both forces and torques on particles. They are able to create microscale pumps [32, 33] and separate cells with magnetic markers [29].

Most devices in inertial microfluidics do not use external control methods and rely exclusively on the order induced by inertial lift forces. However, the advantages of external control mechanisms in the context of inertial microfluidics have recently been demonstrated. In Ref. [14], the mechanical properties of cells were probed with external sheath flows. In Ref. [34], magnetic fields and inertial microfluidics have been combined to filter circulating tumor cells from blood.

The mathematical field of control theory addresses the question, how to understand
and design control mechanisms \cite{35,36}. Control methods are generally classified by whether they take the current system state into account or not. This distinction separates open loop control from feedback control \cite{36}. In open loop control, the control law is determined as a function of time beforehand and not altered, regardless of the actual system behavior. Feedback control, on the other hand, adapts the control while it takes the current system state into account. A classic example is the thermostat of a house \cite{36}. With open-loop control, we compile a fixed list of thermostat settings beforehand. In contrast, feedback control does not rely on a precompiled list of thermostat settings, but rather specifies a rule how to determine the thermostat setting from the current temperature. Clearly, this scheme is much better at dealing with unforeseen events. In general, feedback control is often more robust against model uncertainties and system noise \cite{36}. However, it may increase the system complexity and introduce new instabilities if not designed carefully \cite{36}.

The design of control laws, both open loop and feedback, is addressed by optimal control theory \cite{35}. This field offers general methods, which have been applied to problems ranging from rocket flight \cite{37} to financial investment strategies \cite{38}. Optimal control theory specifies a control target and determines control laws by optimizing this target. Rooted in variational calculus and classical mechanics, the field emerged in the 1950s, when it was first applied to optimize the trajectories of missiles and rockets \cite{37}. Its stochastic generalization is utilized in fields as diverse as artificial intelligence and finance. In the former, optimal control theory is closely connected to reinforcement learning, where an agent aims to maximize its rewards \cite{39}. For example, applied to the game of Backgammon, it beat expert players and discovered previously unknown play strategies \cite{40}. In finance, stochastic optimal control is used to maximize profits \cite{38}. As a noteworthy example, Merton’s portfolio problem deals with investment decisions under an uncertain stock market \cite{41}.

In this thesis, we follow a threefold aim. First, we investigate the fundamental properties of inertial focusing. Second, we study the effects of external fields on the inertial lift forces. Finally, we explore how inertial microfluidics benefits from (optimal) control theory. We employ mesoscopic simulation methods to solve the Navier-Stokes equations and to investigate the features of inertial focusing. In particular, we analyze the dependence of the inertial lift force profiles on system parameters, such as particle size and flow velocity. We further investigate how external electric and magnetic fields influence inertial focusing. The electric fields slow down the particles and thereby change the inertial lift force profiles. Further, the electric fields enhance particle throughput, when combined with hysteretic feedback control. Magnetic fields influence the rotational motion of particles and, thereby, are able to control inertial focusing. Finally, we apply optimal control theory to design control force profiles for steering single particles and for separating particles by size at the channel outlet.

The remainder of this work is structured as follows:
Chapter 2 We discuss previous experimental and theoretical studies in inertial microfluidics. In particular, we discuss popular device designs and their applications. We continue by reviewing the concepts of hydrodynamics required in the following chapters. Further, we stress the origin of the inertial lift forces and discuss existing (analytic) models describing inertial migration.

Chapter 3 Here, we present numerical methods applicable to fluid dynamics with a special emphasis on mesoscopic simulation methods. We discuss in detail the methods used in this work, multi-particle collision dynamics and the lattice Boltzmann method. For both, we describe how to treat inertial focusing starting from a bulk fluid.

Chapter 4 We investigate the basics of inertial migration without external control. We focus on how the channel geometry influences inertial migration. In particular, we discuss the qualitative changes associated with going from circular, over square, to general rectangular cross sections.

Chapter 5 Next, we investigate how external electric and magnetic fields control inertial focusing. Here, we consider control methods that critically rely on fluid inertia and have no effect at low Reynolds number. Further, we show how an electric field combined with a feedback scheme enhances particle throughput in the system.

Chapter 6 We use optimal control theory to design control force profiles to steer and separate particles in inertial microfluidics. We develop the necessary formalism and contrast it to related approaches. Then, we apply it to steer particles towards a given target interval at the channel outlet. Furthermore, we demonstrate the separation of particles based on their size, where the underlying mechanism is extremely robust against noise.

Chapter 7 Finally, we conclude this work with a summary of the main results. Further, we emphasize the questions still left unanswered and point out possible avenues for further research.
Basics of inertial microfluidics

Microfluidics, applying fluid flow on micrometer scales, has many applications in biology or medicine and devices have been demonstrated for a diverse set of tasks. Commonly, fluid inertia is assumed to be negligible in microfluidics as flow speeds are small. However, recent experiments observed that particles assume a self-organized order as the flow rate increases. This dynamic order is now understood as the result of inertial lift forces. The analysis of the associated processes is a challenging problem: The Navier-Stokes equations describing the motion of Newtonian fluids are strongly nonlinear and obtaining explicit solutions is unfeasible for most problems. In this chapter, we survey experimental and theoretical studies applied to inertial migration in general and to inertial microfluidics in particular. Furthermore, we review the theoretical foundations necessary to understand inertial focusing. We discuss the Navier-Stokes equations in the context of inertial migration and the importance of fluid inertia to observe cross streamline migration.

Microfluidics applies fluids on micrometer scales with a particular emphasis on biomedical applications [3, 42]. Whereas typical pipes used in everyday life show diameters in the range of centimeters, microfluidic devices transport fluid in channels with typical dimensions of mere micrometers. Often, microfluidic devices are used in the field of life sciences as biological cells have micrometer sizes, too. However, chemical fabrication and even energy problems benefit also from microfluidics [43]. Microfluidic devices promise a number of advantages over large scale devices. Mainly, they operate on sample volumes as low as pico-liters, which simplifies sample analysis [1]. Furthermore, they are compatible with existing micro manufacturing processes and can be built in mass production [2]. Finally, their small sizes simplify their transport, such that samples can be analyzed wherever they arise [2]. However, fluids on micrometer scales behave very differently from fluids on macroscopic scales [3]. Most importantly, viscous forces become more dominant on small scales and, therefore, inertia becomes negligible in many instances. The Reynolds number quantifies the importance of fluid inertia, with low Reynolds numbers implying the absence of fluid inertia. Then, a number of counterintuitive effects emerge. Bacteria require swimming strategies different from those humans rely on, otherwise the greatly increased friction prevents them from swimming [44]. Mixing two fluids becomes a difficult problem at micrometer scales [3]. On large length scales, turbulence constantly mixes fluids. On micrometer scales, merely diffusive motion is available, which is much less efficient [3]. Here, devices have been designed that show chaotic advection, where fluids mix even without turbulence [3]. Finally, the forces the fluid exerts on
rigid particles are strongly restricted at low Reynolds number. While a spinning ball on macroscopic scales moves on a curved trajectory, it goes straight ahead at low Reynolds numbers \[45\]. Similarly, spherical particles in a microfluidic channel do not experience any force perpendicular to the channel axis at low Reynolds numbers \[6\], as we discuss in Sect. 2.4.3.

In microfluidics, the typical Reynolds numbers are \( \text{Re} = \frac{l_{\text{typ}} u_{\text{typ}}}{\nu} \sim 10^{-3} \) for channel dimensions \( l_{\text{typ}} \sim 10 \mu m \), flow velocities \( u_{\text{typ}} \sim 100 \mu m/s \), and kinematic viscosity \( \nu = 10^{-6} m^2/s \) \[3\]. Therefore, it is commonly assumed that Reynolds numbers in microfluidic flows are small. For example, Squires and Quake note \[3\]:

"Ironically, it [the Reynolds number] may also be the least interesting number for microfluidics: after all, almost without exception, microfluidic devices employ fluids with Reynolds numbers that are small enough for inertial effects to be irrelevant."

However, recent experiments demonstrated that fluid inertia does become important in microfluidics for increased flow velocities \[11, 46–48\]. These experiments reach typical flow velocities \( u_{\text{typ}} \sim 1 m/s \) and Reynolds numbers \( \text{Re} \sim 10 \). Then, a spontaneous order of embedded particles arises, driven by fluid inertia. This order has enabled applications as diverse as counting cells \[12\], separation of bacteria from red blood cells \[15\], and probing mechanical properties of cells \[14\].

2.1. Review of inertial microfluidics

While inertial microfluidics is a young field, first investigated in the late 2000s, inertial migration was first described in the early sixties. Segré and Silberberg \[7\] reported in 1961 the experimental observation of the formation of an annulus for particles flowing through centimeter pipes. Initially uniformly distributed particles reorganized themselves by moving across streamlines and collected on a circular annulus. Segré and Silberberg followed up with a detailed study the year after \[8, 9\]. In their experiments, they determined the particle distributions for different parameters at varying downstream positions. The distributions collapse onto a single master curve when the downstream position is scaled with the Reynolds number \[7\]. Thereby, Segré and Silberberg conclude that the lift force experienced by the particles is caused by fluid inertia \[7\]. Importantly, the Reynolds numbers in these experiments \( \text{Re} \leq 520 \) is below the onset of turbulence in channel flows (\( \text{Re}_c = 2000, \ [49] \)) and the flows in these systems are still laminar.

Interest in inertial migration renewed in the early 2000s, when it was observed that moderate Reynolds numbers cannot only be reached in tubes with centimeter radii, but also in microfluidic devices \[10, 11\]. For example, experiments in channels with micrometer widths commonly reach flow velocities of meters per second and, thereby, Reynolds numbers far above unity \[10, 12\]. The first reported experiments used inertial
2.1. Review of inertial microfluidics

Figure 2.1.: (a) A typical inertial lift force profile. The channel center is an unstable equilibrium position and particles migrate towards the channel walls. The strong repulsive wall lift forces drive particles back to the channel center and they collect at stable equilibrium positions halfway between channel center and channel walls. (b) Illustration of streaming lattices observed in particle suspensions. In lateral direction, particles collect at the stable equilibrium positions shown in (a). Along flow direction, hydrodynamic interactions result in additional order. The resulting streaming lattices resemble those of the experiments reported in Refs. [12, 19].

migration in curved microchannels to separate particles by size [46–48]. Importantly, shear stresses are still small enough to prevent cell damage even at these high flow velocities [50].

Most devices in inertial microfluidics rely on self-organized order between particles to perform their function. Whereas particles are randomly dispersed at low Reynolds numbers, they order on an annulus halfway between channel centerline and channel walls in channels with circular cross section [7, A] or on microfluidic crystals in channels with rectangular cross section [12, 19]. Particle migration and the emergent order of particles result from inertial lift forces. The exact shape and form of the lift force profile depend strongly on the channel geometry as we discuss in chapter [4]. Here, we show a typical lift force profile in Fig. 2.1a. It shows both stable and unstable equilibrium positions which determine how particles order in a channel. As a general feature of inertial lift forces, the channel center is an unstable equilibrium position and the particles migrate towards the channel walls. Close to the walls, strong wall lift forces arise and push particles back to the channel center. Both force contributions cancel about halfway between channel center and channel wall, stabilizing intermediate equilibrium positions. In channels with circular cross section, the symmetry of the system results in the formation of a circular annulus, where the radius of the annulus corresponds to the stable equilibrium position of the lift forces [7, A]. So far, we only described the particle motion in the channel cross section. Hydrodynamic interactions between particles result in an additional order in flow direction [19]. In experiments using channels with rectangular cross section, particles order on streaming lattices similar to those illustrated in Fig. 2.1b [12, 19]. For Reynolds numbers far above 100, also particle trains start to form [51, 53]. In this
2. Basics of inertial microfluidics

Figure 2.2.: Schematic of different channel cross sections used in inertial microfluidics. We indicate the equilibrium positions occupied for small (blue) and large particles (red). In channels with circular cross sections (a), the equilibrium position is degenerate and particles collect at the Segré-Silberberg annulus [7]. For channels with rectangular cross sections of low aspect ratio (c), both small and large particles collect at equilibrium positions on the short channel axis.

work however, we focus on single particles and restrict ourselves to Reynolds numbers below 100. In addition to inducing self-organized order between particles, the high flow velocities in inertial microfluidics naturally result in high throughput devices [10].

2.1.1. Device design

Microfluidic devices require careful design to harness inertial lift forces for applications. In the following, we review some popular design choices for experimental devices in inertial microfluidics with their corresponding applications.

One important design criterion is the geometry of the channel cross section as it strongly influences particle equilibrium positions. We show typical channel cross sections and the equilibrium positions of particles in Fig. 2.2. For circular cross sections (Fig. 2.2a), particles collect on an annulus about halfway between channel center and channel wall consistent with the symmetry of the system [7–9]. Channels with rectangular cross section break this symmetry and reduce the stable annulus to a set of discrete equilibrium positions. For square cross sections (Fig. 2.2b), four equilibrium positions remain. Experiments show stable equilibrium positions exclusively on the main axes [22, 54]. Theoretical studies observe stable equilibrium positions also on the diagonals [53, 55, C]. The number of equilibrium positions further reduces to two in channels with channels of low aspect ratio [12, 13, 56, B, C].

In curved channels, centrifugal forces cause secondary flows, so-called Dean flows [57]. Fig. 2.3a shows a typical example of a spiral microchannel similar to the one reported in Ref. [46]. The Dean flows further restrict the particle to a single stable equilibrium position [16, 16, 48, 58]. In curved channels with trapezoidal cross sections (Fig. 2.2d), particles occupy different equilibrium positions depending on their size and can be sep-
2.1. Review of inertial microfluidics

Figure 2.3.: Schematics of different device designs used to induced secondary flows. (a) In spiral microchannels, centrifugal forces reduce the number of equilibrium positions to one. (b) Extrusions of the channel walls create microscale vortices able to trap particles based on their size. (c) By carefully placing pillars in a channel, fluid flow is designed to steer particles.

arated by this mechanism \[16\].

In channels with rectangular cross sections of low aspect ratio (Fig. 2.2c), particles are restricted to move in the center plane and collect at two stable equilibrium positions. For optical instruments, this plane acts as the focal plane such that particles are always in focus and are easily detected and manipulated. As a direct application, the reduced number of equilibrium positions has been used for cell counting \[12, 58\]. The restricted equilibrium positions further allow to transfer particles across laminar streamlines \[13\]. Once particles are positioned on well defined equilibrium points, sheath flows can probe the mechanical cell properties ("mechanical phenotyping") \[14\] and separate bacteria from red blood cells by differences in stiffness \[59\]. Devices using the restricted number of equilibrium positions and the strong dependence of the magnitude of the lift force on particle size were able to separate particle based on their size \[15, 60\]. In particular, curved channels are extensively used for particle separation \[46, 47, 56, 61–64\]. Here, careful design of the channel cross section increases the efficiency of the separation process by making the stability of equilibrium positions strongly dependent on particle size \[16, 64, 65\].

Furthermore, geometrical features along the flow direction induce additional secondary flows. Channels using these features have been termed "structured channels" \[10\]. Channels with regular extrusions (Fig. 2.3b) have been used for particle focusing \[66, 67\], to construct "microscale centrifuges" \[68, 69\], or for the continuous separation of particles by size \[70, 71\]. Ref. \[18\] proposed to place pillars in a channel to induce secondary flows, similar to Fig. 2.3c. Thereby, the pillars modify the fluid flow profile and the trajectories of particles. The goal is to design flow fields separating particles by careful placement of the pillars.

As a reference, we list a selection of typical experimental parameters in table \[2.1\]. In this thesis, we consider problems with similar parameters.
2. Basics of inertial microfluidics

Table 2.1: A selection of typical parameters used in representative experiments using channels with rectangular cross sections. The flow velocity is given as the maximum flow velocity \( u_{\text{max}} \) at the channel center. The Reynolds number is defined as \( \text{Re} = \frac{2wu_{\text{max}}}{\nu} \), where we introduced the channel width \( 2w \) and kinematic viscosity \( \nu = 10^{-6} \text{m}^2/\text{s} \).

<table>
<thead>
<tr>
<th>Channel width ( \times ) height</th>
<th>Particle diameter</th>
<th>Flow velocity ( u_{\text{max}} )</th>
<th>Reynolds number</th>
<th>Ref.</th>
</tr>
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<tr>
<td>( 50 \mu\text{m} \times 50 \mu\text{m} )</td>
<td>( 4.2 \mu\text{m} )</td>
<td>( 0.02 \text{m/s} - 2\text{m/s} )</td>
<td>( 1 - 100 )</td>
<td>50</td>
</tr>
<tr>
<td>( 20 \mu\text{m} \times 50 \mu\text{m} )</td>
<td>( 1.9 \mu\text{m} )</td>
<td>( 0.05 \text{m/s} - 2\text{m/s} )</td>
<td>( 1 - 40 )</td>
<td>50</td>
</tr>
<tr>
<td>( 20 \mu\text{m} \times 20 \mu\text{m} )</td>
<td>( 1.9 \mu\text{m} )</td>
<td>( 1\text{m/s} )</td>
<td>( 20 )</td>
<td>50</td>
</tr>
<tr>
<td>( 16 \mu\text{m} \times 37 \mu\text{m} )</td>
<td>( 9.9 \mu\text{m} )</td>
<td>( 0.04 \text{m/s} - 0.8 \text{m/s} )</td>
<td>( 1 - 12 )</td>
<td>12</td>
</tr>
<tr>
<td>( 20 \mu\text{m} \times 20 \mu\text{m} )</td>
<td>( 4 \mu\text{m} - 16 \mu\text{m} )</td>
<td>( 1\text{m/s} )</td>
<td>( 20 )</td>
<td>22</td>
</tr>
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</table>

2.1.2. Theoretical analysis of inertial focusing

The nonlinear terms in the Navier-Stokes equations render the theoretical analysis of inertial focusing difficult. Hence, only limited analytic results are available and most theoretical investigations focus on numerical methods.

One semianalytic avenue available is the method of matched asymptotic expansion (MAE). It is a perturbation method useful for multi-scale problems. In case of the Navier-Stokes equations, fluid inertia is negligible close to the surface of small particles, and, only away from the surface, fluid inertia becomes important. The MAE has been repeatedly applied to the problem of inertial migration [20, 21, 72–74]. Saffman found that a particle, slowed down compared to an external shear flow, moves against the shear gradient towards higher velocities [74]. However, this result is not directly applicable for channel flow. While particles lag the external flow due to the presence of the channel walls, the result of Saffman predicts the same migration direction regardless of the particle position. Saffman already noted that higher order terms explain this discrepancy [74]. Subsequent studies used a semianalytic approach [20, 21, 72, 73], in which they determined the higher order terms numerically. In Sect. 2.4.4, we discuss this form of the MAE following the analysis of Schonberg and Hinch [72]. While the shape of the lift force profiles found by MAE agrees with lift force profile predicted by numerical simulations, the MAE is only partially applicable to the problem of inertial microfluidics. Assumptions used in the MAE are often violated in microfluidic systems. All studies using the method of matched asymptotic expansion assume that the particle radius is much smaller than the channel diameter [20, 21, 72, 73]. This assumption is routinely broken in microfluidic devices where particle sizes are similar to channel dimension (table 2.1). Furthermore, studies using the method of matched asymptotic expansion typically assume planar Poiseuille flow which is also of limited applicability in experimental systems, where other channel geometries are used.

To overcome the assumptions of MAE, one is ultimately forced to resort to numerical methods - a strategy which we employ in this work. There have been a limited number
of studies for three-dimensional systems. Di Carlo et al. investigated the equilibrium positions and the scaling of the lift forces in a channel with square cross section using the finite-element method [22]. They further explored the effect of different constraints on the lift force. Finally, Di Carlo et al. analyzed the importance of shear gradients for the lift force by using a channel with rectangular cross section [22]. Another finite-element study investigated correlations between slip velocities and lift forces in a channel with circular cross section [75]. The authors of Ref. [76] used the finite-element method with the immersed boundary method to investigate the migration of spherical particles in circular tubes. In particular, they investigated both the equilibrium position and migration velocity. Chun and Ladd studied the motion of rigid particles using the lattice Boltzmann method in channels with square cross section [53]. They investigated the equilibrium position for different Reynolds numbers and explored the collective behavior of the particles. For Reynolds numbers above 100, they observed the formation of particle trains. Another lattice Boltzmann study investigated the migration and deformation of drops in channels with square cross sections [55]. The authors in particular focused on the interplay between deformability and fluid inertia.

There have also been some numerical investigations for two-dimensional systems. Feng et al. investigated the migration trajectories of spherical particles at different Reynolds numbers using the finite-element method [77]. In particular, they investigated the distribution of pressure around the particle and compared it with the dynamic pressure model (Sect. 2.4.5). With the same method, Joseph et al. investigated correlations between slip velocity and lift force [78]. They further compared their results with a simple empirical model and obtained qualitative agreement. Sun et al. used a finite-difference model to investigate the migration and equilibrium positions of spherical particles in oscillatory and non-oscillatory Poiseuille flows [79]. Recently, Chen et al. used finite-element simulations to investigate the migration of elliptical particles with an emphasis on the time resolved rotational motion [80].

We further comment on the results obtained in these studies in later chapters. In particular, we focus on the novel aspects of our work in the context of prior research.

2.2. Hydrodynamics

2.2.1. The continuity equation and the Navier-Stokes equations

Commonly, fluid flow is described by using continuum equations [81, 82]. In contrast to microscopic models, the continuum description of fluid mechanics does not describe individual particles, but the macroscopic conservation laws for mass, momentum, and, depending on the application, energy. The continuum equations describe fluids as continuous densities of mass, momentum, and energy with their dynamics described by balance equations. This continuum description of fluids hinges on the assumption that dynam-
ics on the level of molecules is not observed. In microfluidic flows, this assumption is commonly valid, however, molecular details may become important to correctly describe fluids close to solid surfaces [3].

In a given volume in space, only an influx or outflux of particles changes the mass in this volume. For an infinitesimal volume, we express the conservation of mass by the continuity equation for the mass density $\rho(x, t)$ [81, 82]

$$\frac{\partial}{\partial t} \rho + \nabla \cdot [\rho u] = 0,$$

where we introduced the local fluid velocity $u(x, t)$. The product $\rho u$ of mass density and fluid velocity has two physical interpretations: it gives both the mass flux and the momentum density.

For an incompressible fluid, the continuity equation reduces to the condition for the flow field [81, 82]

$$\nabla \cdot u = 0.$$  \hspace{1cm} (2.2)

For the systems discussed in this thesis, water is incompressible and its density is constant both in time and space. Here, we use the value $\rho = 0.9982 \times 10^3 \text{kg/m}^3$ for a temperature $T = 20^\circ\text{C}$ tabulated in Ref. [81]. We further discuss the validity of the incompressibility assumption in Sect. 2.2.2.

The temporal change of momentum density $\rho u$ is governed by the Navier-Stokes equations [81, 82]. The local momentum in a volume only changes due to two processes: Either there is a net momentum flux through the surface or external forces change the local momentum. We write this statement as the balance equation [81, 82]

$$\frac{\partial}{\partial t} [\rho u] + \nabla \cdot \Pi = g,$$

where we introduced the total momentum flux $\Pi(x, t)$ and the body forces $g(x, t)$. Possible sources for the body forces are for example gravity or electric fields in the case of charged liquids. We express the total momentum flux as [81, 82]

$$\Pi_{ij} = \rho u_i u_j + p \delta_{ij} - \sigma_{ij}.$$  \hspace{1cm} (2.3)

Here, the convective term $\rho u_i u_j$ includes momentum transport by fluid flow. The internal pressure $p$ balances density differences and results in the incompressibility of water as discussed in Sect. 2.2.2.

The viscous stress tensor $\sigma_{ij}$ balances momentum differences. Water is a Newtonian fluid and its stress tensor is linear in the velocity gradients [81, 82]. Further, it is symmetric as there is no viscous stress in fluids rotating with constant angular velocity [82]. The components of the viscous stress tensor read [81, 82]

$$\sigma_{ij} = \eta \left( \frac{\partial}{\partial x_i} u_j + \frac{\partial}{\partial x_j} u_i \right),$$  \hspace{1cm} (2.5)
where we assumed $\nabla \cdot \mathbf{u} = 0$ and introduced the dynamic shear viscosity $\eta$ as the constant of proportionality. In water, it is approximately $\eta = 1.002 \times 10^{-3}$ kg/ms at temperature $T = 20^\circ$C [81]. In the following, we also repeatedly use the kinematic viscosity $\nu = \eta/\rho$.

The stress tensor $\tau$ is the sum of pressure and viscous stress tensor,

$$\tau_{ij} = -p\delta_{ij} + \sigma_{ij}, \quad (2.6)$$

and gives the forces the fluid exerts per unit area [83]. The pressure term corresponds to isotropic compression, while the viscous stress results in shear forces [83].

In summary, we describe the fluid by the incompressible Navier-Stokes equations and the statement of incompressibility. The relevant equations are often written as [81, 82]

$$\rho \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u} + \mathbf{g}, \quad (2.7)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (2.8)$$

### 2.2.2. Incompressibility

As described in the previous section, we assume water to be incompressible. Then, the divergence of the vector field of the fluid velocity has to vanish, $\nabla \cdot \mathbf{u} = 0$. This assumption does hold in particular if the density is constant in space and time. The variations of density crucially depend on the relative magnitude of typical velocities $u_0$ compared to the speed of sound $c_s$. Specifically, the relative change of the density approximately follows [82]

$$\frac{\Delta \rho}{\rho} \approx \left( \frac{u_0}{c_s} \right)^2 = Ma^2, \quad (2.9)$$

where we defined the Mach number $Ma = u_0/c_s$. The high speed of sound in water ($c_s = 1470$ m/s at $15^\circ$C [81]) typically results in small Mach numbers. For microfluidic flows investigated here the typical velocities are on the order of m/s, and the Mach number satisfies $Ma \lesssim 10^{-3}$. Hence, we neglect compressibility in the following. However, in the mesoscopic simulations schemes we describe in chapter 3 the speed of sound is comparably small. We further discuss the implications there.

### 2.2.3. Importance of inertia

As stated in the beginning of this chapter, fluid inertia is typically neglected in microfluidics [3]. We estimate the importance of inertial forces compared to viscous forces by performing the following dimensional analysis. We compare all lengths to a typical length $l_0$, all velocities to a typical velocity $u_0$ and finally all times to a typical time scale $t_0$. We rescale the Navier-Stokes equations by writing all quantities as the product of their
typical value and a numerical factor. For example, we express the velocity as \( u = u_0 u' \).

The Navier-Stokes equations read in their rescaled form \[81\]

\[
\frac{1}{\text{St}} \frac{\partial}{\partial t'} u' + \nabla' \cdot (u' \otimes u') = -\frac{p_0}{l_0 u_0 \rho} \nabla' p' + \frac{1}{\text{Re}} (\nabla')^2 u',
\]

(2.10)

where we introduced the Strouhal number \( \text{St} = u_0 t_0 / l_0 \) and the Reynolds number \( \text{Re} = l_0 u_0 / \nu \). The Strouhal number characterizes how fast the flow field reacts to perturbations. Without external driving, the fluid dynamics determines the time scale \[81, 82\] and we set \( \text{St} = 1 \). The pressure \( p \) balances both inertial and viscous forces such that the fluid remains incompressible \[81\].

The Reynolds number represents the ratio \[81, 82\]

\[
\text{Re} = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{l_0 u_0}{\nu}.
\]

(2.11)

Since typical scales depend on the concrete problem, there are several ways to define the Reynolds number. For channel flow, we use the channel width \( 2w \) as the typical length scale and the maximum velocity \( u_{\text{max}} \) as the typical velocity. The corresponding channel Reynolds number reads

\[
\text{Re} = \frac{2wu_{\text{max}}}{\nu}.
\]

(2.12)

Another choice of length scale is the diameter \( 2a \) of a colloidal particle. Then, the particle Reynolds number reads

\[
\text{Re}_p = \frac{2au_{\text{max}}}{\nu}.
\]

(2.13)

\subsection*{2.2.4. The Stokes equations}

In the limit of small Reynolds numbers, fluid inertia is negligible and the Navier-Stokes equations \[2.8\] simplify considerably. Then, we recover the Stokes equation

\[
\eta \nabla^2 u - \nabla p = -g,
\]

(2.14)

where we assumed steady flow and kept the body force \( g \). The Stokes equation is linear and shows a peculiar symmetry called kinematic reversibility. Here, kinematic reversibility implies that for reversed pressure gradient \( -\nabla p \) and reversed body force \( -g \), the Stokes equation is solved by the fluid velocity \( -u \). We discuss the consequences for the lateral migration of colloidal particles in Sect. \[2.4.3\].

As the Stokes equation is linear, it can be solved with Green functions \[83, 81\]. In particular, a point force \( g(x) = g_0 \delta(x) \) creates the flow field, called stokeslet, \[83\]

\[
u(x) = G(x)g_0.
\]

(2.15)
2.2. Hydrodynamics

Figure 2.4.: The flow field for two fundamental solutions of the Stokes equation. The stokeslet (2.16) is the flow field for a point force (a). The stresslet (2.17) is the flow field for a pure straining motion (b). It is equivalent to four point forces with infinitesimal displacement.

Here, we introduced the Oseen tensor

\[ G(x) = \frac{1}{8\pi\eta} \left( \frac{1}{|x|} + \frac{x \otimes x}{|x|^3} \right). \]  

(2.16)

We plot the stokeslet in Fig. 2.4a. At large distances, the flow field behaves like \( \frac{1}{|x|} \). It is also the far field of a sphere dragged through a quiescent fluid \[83\], as can be seen by comparing with Fig. 2.7a.

The stokeslet is the first fundamental solution in a multipole expansion of general body force distributions. The next higher order term is a force dipole, also called stresslet. It results from the first derivative of the stokeslet. In particular, the stresslet corresponding to the derivative

\[ \left[ \hat{e}_z \frac{\partial}{\partial z} + \hat{e}_x \frac{\partial}{\partial x} \right] G(r) = -\frac{3}{4\pi\eta} \frac{xz}{|x|^5} x, \]  

(2.17)

characterizes the far field of the disturbance flow caused by a sphere in shear flow \[72\] \[81\]. We plot the stresslet in Fig. 2.4b.

2.2.5. The no-slip condition

Up to now, we considered bulk fluids without any boundaries. To describe bounded flows, we have to supply a suitable boundary condition for the Navier-Stokes equations (2.8). In the following, we consider a surface with normal \( \hat{n} \). The fluid velocity normal to the surface \( u_\perp = \hat{n} \cdot (\hat{n} \cdot u) \) has to vanish,

\[ u_\perp = 0, \]  

(2.18)
2. Basics of inertial microfluidics

Figure 2.5.: Geometries considered in this work. The planar channel has no bounding walls along the \( y \) direction. The blue dot shows the origin of the coordinate system for all geometries. In chapters \[4\] and \[5\] we determine the lift forces for channels with rectangular cross sections. There, we restrict ourselves to positions inside the red area. The full cross section results from symmetry operations.

as the fluid does not flow through the boundary \[82\]. For the parallel component \( u_\parallel = u - u_\perp \), Navier and Maxwell proposed \[85\] that it is proportional to the local shear rate. The complete boundary condition reads \[85\]

\[
\mathbf{u}|_{\text{wall}} = \lambda (\hat{n} \cdot \nabla) u_\parallel,
\]

with the slip length \( \lambda \). For Newtonian fluids, typical slip lengths are of the order of nanometers \[85\]. Only if the length scales of the flow are close to molecular scales, nonzero slip becomes important \[3, 81\]. Therefore, for the microfluidic devices considered in this work, we assume \( \lambda = 0 \). Then, the boundary condition close to solid walls reduces to the no-slip boundary condition \[4, 81\]

\[
\mathbf{u}|_{\text{wall}} = 0.
\]

For moving boundaries, for example the surface of colloidal particles, the fluid velocity has to be equal to the local surface velocity. For a rigid body with center of mass \( \mathbf{r}_c \), moving with velocity \( \mathbf{v} \), and rotating with an angular velocity \( \mathbf{\Omega} \), the no-slip condition at the boundary reduces to \[81\]

\[
\mathbf{u}(\mathbf{r})|_{\text{surface}} = \mathbf{v} + \mathbf{\Omega} \times (\mathbf{r} - \mathbf{r}_c).
\]

2.3. Poiseuille flow

In inertial microfluidics, the fundamental building blocks for many applications are microchannels with straight walls but different cross sections. In this section, we review the
2.3. Poiseuille flow

flow fields for the specific geometries discussed in this thesis and illustrated in Fig. 2.5. Specifically, we discuss planar channels and channels with circular or rectangular cross section. To move the fluid through a channel with length $L$ we apply a pressure difference $\Delta p$. After a characteristic time, the steady Poiseuille flow profile establishes. In the following, we only consider steady and fully developed flows. Furthermore, we restrict ourselves to channels with straight walls, so the velocity always points along the channel axis. Then, the pressure gradient $\nabla p = (\Delta p/L) \hat{e}_z$ is constant \[86\]. We choose the coordinate system such that the $z$ axis points along the channel axis. The $x, y$ axes span the channel cross section. For rectangular or planar channels we choose the coordinate system such that the axes align with the symmetry axes of the cross section. We further call the direction along the channel axis the axial direction, while we call the remaining directions the lateral directions.

In general, the Navier-Stokes equations (2.8) for channel flow with straight walls reduce to the following partial differential equation for the axial velocity $u_z$ \[86\]

$$
\nu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u_z(x, y) = \frac{\Delta p}{L}, \tag{2.22}
$$

$$
u u_z(x, y)_{\text{boundary}} = 0, \tag{2.23}
$$

where the channel boundary specifies the geometry.

The channel walls are located at $x = \pm w$ in a planar channel with infinite plate geometry. Here, we choose the origin ($x = 0$) to coincide with the center of the cross section of the channel (blue dot in Fig. 2.5). In steady state, the flow field develops the parabolic profile \[86\]

$$
-u_z(x) = \frac{w^2 \Delta p}{2 \eta L} \left[ \left( \frac{x}{w} \right)^2 - 1 \right] \tag{2.24}
$$

In the case of a channel with circular cross section and radius $R$, the flow profile

$$
u u_z(r) = \frac{R^2 \Delta p}{4 \eta L} \left( 1 - \left( \frac{r}{R} \right)^2 \right) \tag{2.25}
$$

is again a parabolic function of the radial position $r = \sqrt{x^2 + y^2}$ \[86\].

For a channel with rectangular cross section, a solution based on a series expansion is available. We choose the origin ($x = 0, y = 0$) to coincide with the center of the cross section of the channel (blue dot in Fig. 2.5). To include the boundary condition, we expand the axial velocity field into a product of hyperbolic and trigonometric functions similar to problems encountered in classical electrostatics \[87\]. The series expansion results in the flow profile \[86\]

$$
u u_z(x, y) = \frac{4h^2 \Delta p}{\pi^3 \eta L} \sum_{n, \text{odd}}^{\infty} \frac{1}{n^3} (-1)^{n-1} \left[ 1 - \frac{\cosh(n\pi \frac{y}{2h})}{\cosh(n\pi \frac{w}{2h})} \right] \cos \left( \frac{n\pi x}{2h} \right), \tag{2.26}
$$

where the channel has height $2h$ and width $2w$. We plot this flow field in Fig. 2.6.
Figure 2.6: Poiseuille flow profile $u_z(x, y)$ in a channel with rectangular cross section. The channel has height $2h$ and width $2w$. The flow profile in a channel with aspect ratio $w/h = 0.5$ (a). The plots (b) and (c) show the flow profile along the white dashed lines for different aspect ratios $w/h$. When varying the aspect ratio the velocity profile along the shorter channel dimension does change little (b), along the longer channel dimension the flow profile develops a blunted shape (c).
2.4. Colloidal particles

In this thesis, we investigate the inertial migration of colloidal particles in flow. Graham introduced the name “colloid” in 1861 [83], when he investigated the transport of solute particles across membranes. He called those particles that could not cross the membrane colloids after the Greek work for glue (kolla) [83]. Today, particles immersed in a fluid with nanometer to micrometer dimensions are commonly classified as colloids [83]. Their large size allows them to be analyzed and manipulated with optical methods [28–30]. Furthermore, colloidal particles can be created with high precision in size and shape. Their properties make them an important class of model systems to study fundamental properties of matter [88–90].

In this spirit, we focus on spherical, neutrally buoyant, hard particles as a reference system, since they allow to investigate the fundamental properties of inertial migration. Where deformability or shape of the particles become important, the particles experience additional lift forces not related to fluid inertia. Particles with radius \( a \) have a mass \( M = \frac{4}{3} \pi a^3 \rho \) and moment of inertia \( I = \frac{2}{5} a^2 M \). As we consider rigid particles, their state is fully described by their position \( \mathbf{x} \), velocity \( \mathbf{v} \), and angular velocity \( \Omega \). Here, we do not consider the orientation of the particles, since it does not influence their dynamics. Without noise, the particle motion obeys Newton’s equations of motion [91]

\[
\begin{align*}
\frac{d}{dt} \mathbf{r} &= \mathbf{v}, \\
M \frac{d}{dt} \mathbf{v} &= \mathbf{f}_{\text{fluid}} + \mathbf{f}_{\text{ext}}, \\
I \frac{d}{dt} \Omega &= \mathbf{T}_{\text{fluid}} + \mathbf{T}_{\text{ext}},
\end{align*}
\]

where we introduced the force exerted on the particle by the fluid \( \mathbf{f}_{\text{fluid}} \) and external forces \( \mathbf{f}_{\text{ext}} \). Similarly, the fluid exerts a torque \( \mathbf{T}_{\text{fluid}} \), and there may be further external torques \( \mathbf{T}_{\text{ext}} \). For example, we consider forces generated by electric fields in Sect. 5.2 and torques generated by magnetic fields in Sect. 5.3.

From the definition of the stress tensor (2.6), we can determine the force exerted by the fluid by the surface integral [82]

\[
\mathbf{f}_{\text{fluid}} = \int dS \, \hat{n} \cdot (-p \mathbb{I} + \mathbf{\sigma}).
\]

Similarly, the fluid exerts the torque [82]

\[
\mathbf{T}_{\text{fluid}} = \int dS \, \hat{n} \times (-p \mathbb{I} + \mathbf{\sigma}).
\]
2. Basics of inertial microfluidics

2.4.1. Movement in a viscous fluid

For the motion of colloidal particles in fluids, only a limited subset of problems can be solved analytically. In this section, we focus on those problems, which are instructive in analyzing the results for inertial focusing presented in later chapters.

First, we consider a particle dragged with force \( f_{\text{ext}} \) through an otherwise quiescent fluid. In steady state the fluid exerts a force on the particle such that it balances the external force. Initially, we assume that the particle velocity is small enough that we can neglect fluid inertia. Then, the fluid is described by the Stokes equation (2.14).

At infinity, the fluid velocity has to vanish. At the particle surface, the fluid velocity has to satisfy the no-slip boundary condition (2.21) and, therefore, be equal to the particle velocity. In steady state, the particle experiences a drag force from the fluid proportional to its velocity

\[
\mathbf{f}_{\text{fluid}} = -\mathbf{f}_{\text{ext}} = -\xi \mathbf{v},
\]

(2.30)

with Stokes’ friction coefficient

\[
\xi = 6\pi \eta a
\]

(2.31)
as the constant of proportionality. We plot the flow field in Fig. 2.7a. It decays like \( a/|x| \) for large distances, where it behaves like the stokeslet (2.16). Another solvable problem is the flow field \( \mathbf{u} \) of a sphere in shear flow \( \mathbf{u}_0 = \gamma y \mathbf{e}_x \).

When we apply an external torque \( \mathbf{T}_{\text{ext}} \) as opposed to an external force, the particle rotates. Again, the fluid resists the particles rotation and exerts a torque onto the particle proportional to its steady-state angular velocity

\[
\mathbf{T}_{\text{fluid}} = -\mathbf{T}_{\text{ext}} = \xi \Omega,
\]

(2.32)
2.4. Colloidal particles

with rotational friction coefficient $\zeta_r = 8\pi \eta a^3$. When the particle experiences both forces and torques, the linearity of the Stokes equation allows to superimpose both effects.

So far, we discussed the motion in a quiescent fluid. Faxén calculated the velocity of a sphere dragged through a fluid with flow field $u_0(x)$, which satisfies the Stokes equation without sphere. The sphere assumes the velocity

$$v = \left(1 + \frac{a^2}{6} \nabla^2\right) u_0(x_c) + \frac{1}{\zeta} f_{\text{ext}}, \quad (2.33)$$

where $x_c$ is the center of mass of the particle. This result is exact and holds for arbitrary velocity fields $u_0(x)$ in an unbounded fluid. Further, the fluid vorticity $\Omega_0(x) = \frac{1}{2} \nabla \times u_0(x)$ determines the angular velocity of the particle by

$$\Omega = \Omega_0(x_c) + \frac{1}{\zeta_r} T_{\text{ext}}. \quad (2.34)$$

In the case of a channel, we cannot merely use the flow fields derived in Sect. 2.3 with Faxén’s law. While channel flows do satisfy the no-slip boundary condition at the channel walls, the disturbance flow created by the particle does not generally satisfy the boundary condition. However, as the flow fields decay with $(a/r)^2$, we can approximately use Faxén’s laws if the particle is small and the distance to the channel wall is large. In fact, we use this insight in chapter 3 to validate our simulations.

Previously, we assumed small Reynolds numbers and used the Stokes equation to describe the motion of a sphere in a quiescent fluid. Oseen showed that the flow field of the sphere is inconsistent with the assumption of small Reynolds number at distances far away from the sphere \[82\]. At those distances, we cannot neglect the nonlinear terms in the Navier-Stokes equations. In the Oseen approximation, the Navier-Stokes equations are linearized in the disturbance flow $u' = u - v$ and the nonlinear term becomes $(u \cdot \nabla)u \approx (v \cdot \nabla)u'$. Thereby, the sphere experiences the drag force \[82\]

$$f = \zeta v \left(1 + \frac{3}{8} \text{Re}_p\right). \quad (2.35)$$

Here, the drag force is not linear in particle velocity, but an additional term including the particle Reynolds number $\text{Re}_p = a|v|/\nu$ enters. This result only represents the first order in an expansion in particle Reynolds number and higher order terms appear in the full solution \[82\].

Finally, we discuss how to include the disturbance flow generated by a particle in the presence of bounding walls. As the flow velocity has to be zero at solid walls, the fluid is slowed down and the particle experiences a higher friction. In general, the problem cannot be solved exactly. However, approximate solutions for specific geometries exist in the limit of zero Reynolds number and small particle size. They are based on the method of mirror images introduced by Lorentz \[93\]. It works similar to the method of mirror
2. Basics of inertial microfluidics

Charges in electrodynamics, where the boundary condition is successively approximated by using the method of reflections. As the flow fields decay to zero with increasing distance from the boundary, we expect the approximation to become better and better with higher number of iterations. Even this approximate scheme is not solvable in closed form for most problems. In the following, we try to gain insights by two special cases for which approximate solutions in first order of the inverse distance exists. For a particle moving in front of a single wall, the friction coefficient depends on the direction of motion. A particle moving with velocity \( \mathbf{v} \) at a distance \( d \) from the wall experiences the drag force

\[
\mathbf{f}_{\text{drag}} = \xi \left( 1 + \frac{9}{8} \frac{a}{d} \right) \mathbf{v}_\perp + \xi \left( 1 + \frac{9}{16} \frac{a}{d} \right) \mathbf{v}_\parallel + \mathcal{O}\left( \frac{(a/d)^2}{d} \right). \tag{2.36}
\]

Here, \( \mathbf{v}_\perp \) is the velocity perpendicular to the normal and \( \mathbf{v}_\parallel \) the velocity parallel to the normal of the surface. Another solvable case is the motion of a particle in a channel with circular cross section and radius \( R \), where the particle translates along the central axis in a quiescent fluid. Ladenburg found that it experiences the drag force

\[
\mathbf{f}_{\text{drag}} = \xi \left( 1 + C \frac{a}{R} \right) \mathbf{v} + \mathcal{O}\left( \frac{(a/R)^2}{d} \right), \tag{2.37}
\]

where \( C \approx 2.4 \). For both cases, the friction coefficient strongly increases with decreasing distance between particle and channel wall.

2.4.2. Hydrodynamics in two dimensions and Stokes paradox

In contrast to the motion of spherical particles in three dimensions, there is no solution for a translating particle in a quiescent fluid on the level of the Stokes equation in two dimensions [82]. Mathematically, the stokeslet in two dimensions depends logarithmically on the position in contrast to the \( 1/|\mathbf{x}| \) dependence of the stokeslet in three dimensions (2.16). Since the logarithm does not decay to zero, we cannot satisfy the boundary condition that the fluid velocity is zero at infinity.

The Oseen approximation introduced in the previous section remedies this problem. Oseen found that a spherical particle moving with velocity \( \mathbf{u} \) through a quiescent two-dimensional fluid at nonzero Reynolds number experiences the drag force [82]

\[
\mathbf{f} = \frac{4\pi \eta}{2 - \gamma - \log(8\text{Re}_p)} \mathbf{u}. \tag{2.38}
\]

Here, we introduced Euler’s constant \( \gamma \approx 0.577 \). Similar to the three-dimensional case, the particle Reynolds number (2.13) enters the denominator and the friction coefficient depends on the velocity. In the limit of \( \text{Re}_p \to 0 \), however, the friction coefficient diverges.
2.4. Colloidal particles

Bretherton showed in 1962 by symmetry arguments that only fluid inertia can explain lateral migration of spherical particles in channel flows [6]. By using the kinematic reversibility of the Stokes equation and mirror symmetry along the channel axis, Bretherton found that only particle trajectories without lateral motion are free of contradiction [6]. In this section, we follow the discussion of Bretherton [6] for the system shown in Fig. 2.8a. Concretely, we consider a spherical colloid with radius $a$ placed inside a channel filled with a viscous fluid. The channel has arbitrary cross section and we only require that the channel walls are straight. By applying the pressure gradient $\nabla p$, we generate the Poiseuille flow profile $u$ as discussed in Sect. 2.3. The colloidal particle moves in this flow with velocity $v$. We also include the possibility that external control methods act on the particle. In particular, we assume that the colloid experiences an external control force $f_{\text{ctl}}$ and an external control torque $T_{\text{ctl}}$. We choose the coordinate

\begin{align}
\xi_{\text{rot}} &= 4\pi \eta a^2, \\
(2.39)
\end{align}

in two dimensions. To our surprise, the rotation is exactly described by Faxén’s law (2.34) with the constant rotational friction coefficient

\begin{align}
\xi_{\text{rot}} &= 4\pi \eta a^2, \\
(2.39)
\end{align}

for arbitrary Reynolds number [94].

2.4.3. No lift force at zero Reynolds number

Bretherton showed in 1962 by symmetry arguments that only fluid inertia can explain lateral migration of spherical particles in channel flows [6]. By using the kinematic reversibility of the Stokes equation and mirror symmetry along the channel axis, Bretherton found that only particle trajectories without lateral motion are free of contradiction [6]. In this section, we follow the discussion of Bretherton [6] for the system shown in Fig. 2.8a. Concretely, we consider a spherical colloid with radius $a$ placed inside a channel filled with a viscous fluid. The channel has arbitrary cross section and we only require that the channel walls are straight. By applying the pressure gradient $\nabla p$, we generate the Poiseuille flow profile $u$ as discussed in Sect. 2.3. The colloidal particle moves in this flow with velocity $v$. We also include the possibility that external control methods act on the particle. In particular, we assume that the colloid experiences an external control force $f_{\text{ctl}}$ and an external control torque $T_{\text{ctl}}$. We choose the coordinate

\begin{align}
\xi_{\text{rot}} &= 4\pi \eta a^2, \\
(2.39)
\end{align}

in two dimensions. To our surprise, the rotation is exactly described by Faxén’s law (2.34) with the constant rotational friction coefficient

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\end{align}

for arbitrary Reynolds number [94].
2. Basics of inertial microfluidics

system such that the channel axis coincides with \( \hat{e}_z \) and that \( z = 0 \) coincides with the current particle position. We further use the notation \( \mathbf{v}_\perp = \mathbf{v} - \hat{e}_z (\hat{e}_z \cdot \mathbf{v}) \) to denote the lateral components.

In the following, we restrict the external fields such that pressure gradient and control force are strictly parallel to the channel axis and that the control torque is strictly parallel to the channel walls. We express these requirements by

\[
\nabla_\perp p = 0, \quad f_{\text{ctl,} \perp} = 0, \quad T_{\text{ctl,} z} = 0. \tag{2.40}
\]

For given external fields \( \nabla p, f_{\text{ctl}}, T_{\text{ctl}} \), the Stokes equation determines the fluid velocity \( \mathbf{u} \), the colloid velocity \( \mathbf{v} \), and the colloid angular velocity \( \Omega \).

We continue by using the kinematic reversibility of the Stokes equation (Fig. 2.8b). It implies that for reversed external fields, \( \nabla p' = -\nabla p, \ f_{\text{ctl}}' = -f_{\text{ctl}}, \ T_{\text{ctl}}' = -T_{\text{ctl}} \), the new fluid velocity and colloid velocities satisfy

\[
\mathbf{u}'(\mathbf{x}) = -\mathbf{u}(\mathbf{x}), \tag{2.41}
\]

\[
\mathbf{v}' = -\mathbf{v}, \tag{2.42}
\]

\[
\Omega' = -\Omega. \tag{2.43}
\]

We can easily verify that this is indeed a valid solution by inserting the transformed quantities into Eqs. (2.14), (2.21), (2.27b), (2.27c), (2.28), and (2.29).

Next, we mirror the system on the \( z = 0 \) plane (Fig. 2.8c). Thereby, the \( z \) component of a vector \( \mathbf{v}' \) reverses sign \( v'_z = -v'_z \), while the lateral components stay the same \( \mathbf{v}'_\perp = \mathbf{v}'_\perp \). The angular velocity \( \Omega \) and the torque \( T_{\text{ctl}} \) are pseudovectors. Upon mirror transformations, they gain an additional factor \(-1\). Concretely, the angular velocity transforms as \( \Omega_z' = \Omega'_z \) and \( \Omega'_\perp = -\Omega'_\perp \). Thereby, the cross product of \( \Omega \) with an arbitrary vector transforms as a vector [87].

We chose the external fields in Eq. (2.40) such that they transform into their original values

\[
\nabla p'' = \nabla p, \quad f_{\text{ctl}}'' = f_{\text{ext}}, \quad T_{\text{ctl}}'' = T_{\text{ctl}}. \tag{2.44}
\]

Furthermore, the colloid does not change under the mirror transformation, as the origin coincides with its position.

The velocities, however, do not transform into their original values. For the fluid velocity, we find

\[
\mathbf{u}'_\perp(\mathbf{x}_\perp, -z) = \mathbf{u}_\perp(\mathbf{x}_\perp, z), \quad u'_z(\mathbf{x}_\perp, -z) = -u_z(\mathbf{x}_\perp, z). \tag{2.45}
\]

The velocity of the particle transforms into

\[
\mathbf{v}'_\perp = -\mathbf{v}_\perp, \quad v'_z = v_z \tag{2.46}
\]
and the angular velocity transforms into
\[ \Omega''_\perp = \Omega, \quad \Omega''_z = -\Omega_z. \] (2.47)

Since the external fields \( p, f_{\text{ctl}}, T_{\text{ctl}} \) and the geometry are the same, the Stokes equation is solved by the original flow velocity \( u \), velocity of the particle \( v \), and angular velocity of the particle \( \Omega \). However, the transformed fields also have to be a solution of the Stokes equation as the symmetry operations leave the system unchanged. Only when they are equal, do these two solutions not contradict. Therefore, the velocity of the particle has to satisfy
\[ v_\perp = 0 \] (2.48)
and there cannot be any lateral migration without fluid inertia.

### 2.4.4. Matched asymptotic expansion for inertial migration

If the Reynolds number is on the order of one, where fluid inertia does become important, lateral migration occurs. One semi-analytic method to analyze this behavior is the method of matched asymptotic expansion \[20, 21, 72–74\]. Common to all investigations of inertial migration using matched asymptotic expansion is the assumption that two distinct dynamic regions, called inner and outer region, exist. In the inner region close to the particle surface, inertia is negligible, as the fluid and particle move with similar velocity. Hence, close to the particle, we describe the fluid by the linear Stokes equation, where we assume that the flow generated by the particle vanishes at infinity. In the outer region or far away from the particle, we assume that the disturbance flow generated by the particle is small and we linearize the Navier-Stokes equations in the disturbance flow (Oseen approximation, Sect. 2.4.1). To obtain a consistent solution, we require both solutions in the outer region and the inner region to match asymptotically. Specifically, the inner solution has to converge to the outer solution as we approach the channel wall and the outer solution has to converge to the inner solution as we approach the particle. In the following, we discuss the features of the asymptotic expansion following the discussion by Schönberg and Hinch \[72\].

We consider a colloidal particle with radius \( a \) inside a planar channel with width \( 2w \) (Fig. 2.9a). The channel is filled by a Newtonian fluid, which exhibits the flow profile \( u \). Without particle, the undisturbed flow profile is given by the Poiseuille flow \( u_0 \) (Sect. 2.3) with channel Reynolds number \( \text{Re} \). However, by its presence, the particle introduces the disturbance flow \( u' = u - u_0 \). We choose the coordinate system such that \( e_z \) coincides with the channel axis and the \( x \) coordinate describes the lateral position. We place the origin of the coordinate system at the center of mass of the colloid.

We assume \( a/w \ll 1 \) and, therefore, can approximate the flow field close to the particle by a linear shear flow \( u_{\text{shear}}(x) = u_0(x_c) + \dot{\gamma} x \hat{e}_z \) with shear rate \( \dot{\gamma} = \partial u_{0,z}/\partial x \). To
2. Basics of inertial microfluidics

Figure 2.9.: (a) Schematic of the matched asymptotic expansion for a spherical particle with diameter $2a$ in a planar channel with width $2w$. Close to the particle (inner region), we approximate the undisturbed flow field by a linear shear flow. (b) The lateral migration velocity predicted by the matched-asymptotic-expansion study of Schonberg and Hinch and LBM simulations presented in chapter 4. We extracted the data for the matched asymptotic expansion from Fig. 2 of [72].

estimate the importance of inertia close to the particle surface, we use the flow velocity difference $\Delta u$ on either side of the particle. We approximate the shear rate by $\dot{\gamma} \approx u_{\text{max}}/w$ and obtain $\Delta u \approx 2au_{\text{max}}/w$. Finally, we calculate the shear particle Reynolds number $Re_{sp} = 2a^2 u_{\text{max}}/w\nu = (a/w)^2 Re$. In the following, we assume that the shear particle Reynolds number is small, $Re_{sp} \ll 1$. However, we do not assume that the channel Reynolds number $Re$ itself is small.

With these assumptions, the Stokes equation is valid close to the particle surface. Furthermore, since the particle is small compared to the channel dimensions, we approximate the flow field close to the particle by an unbounded shear flow and include the channel walls only on the level of the outer solution. The flow field can be found explicitly [81]. However, to connect it to the outer solution only the far field is required. At large distances from the particle, the disturbance flow is given by [72, 81]

$$-\frac{5\dot{\gamma}a^3}{2} \frac{xz}{|x|^5} x$$

and decays to zero with increasing distance. Therefore, the inner solution is consistent with the surrounding flow field in the outer region.

In the outer domain, we neglect the extent of the particle and consider only the far field of the disturbance flow. Then, the particle behaves as a point source with the flow field (2.49), which is reproduced by the stresslet (2.17). Since, the stresslet is the first derivative of the stokeslet (2.16), we can model the particle by including the singularity

$$-\frac{10\pi \eta \dot{\gamma}a^3}{3} \left( \hat{e}_x \frac{\partial}{\partial z} + \hat{e}_z \frac{\partial}{\partial x} \right) \delta(x)$$

and...
as a body force in the Navier-Stokes equations \[ \text{(2.51)} \]. To include inertial effects, we apply the Oseen approximation (Sect. 2.4.1) and linearize the equation in the disturbance flow. Then, the Navier-Stokes equations in steady-state reduce to \[ \text{(2.51)} \]

\[
(u_0 \cdot \nabla) u' + (u' \cdot \nabla) u_0 =
- \frac{1}{\rho} \nabla p' + \nu \nabla^2 u' - \frac{10 \pi \gamma a^3}{3} (\hat{e}_x \frac{\partial}{\partial z} + \hat{e}_z \frac{\partial}{\partial x}) \delta(x).
\]

Close to the sphere, the disturbance flow \( u' \) reproduces the stresslet and, therefore, the far field behavior of the inner solution. These equations cannot be solved analytically, but have to be solved numerically \[ 21, 72, 73 \].

We show the lateral migration velocity determined by Schonberg and Hinch \[ 72 \] in Fig. 2.9b. We also include the lift force determined in our lattice Boltzmann simulations suitably scaled (Sect. 4.2). While both curves differ, they agree on the qualitative behavior. The disagreement between the full numerical methods and the method of MAE can be mainly attributed to the finite particle size. As Table 2.1 shows, the particle sizes in inertial microfluidics are often comparable to the channel width.

The lift forces determined by the MAE show a strong dependence on particle size and Reynolds number. Asmolov summarized the dependence in the scaling relation \[ 21 \]

\[
f_{\text{lift}} = \text{Re}^2 \left( \frac{a}{w} \right)^m \rho \nu^2 f(x/w),
\]

with an exponent \( m = 4 \). The lift coefficient \( f(x/w) \) depends only on the relative position. As we discuss in chapter 4, a similar scaling law is also applicable for inertial microfluidics. However, the exponent is different and a weak dependence of the lift coefficient on particle size and Reynolds number exists.

Historically, one of the first approaches to inertial migration was the study of Saffman for the lateral migration of a particle in the shear flow \( u = \gamma x \hat{e}_z \) \[ 74 \]. He found that a particle lagging the flow with a velocity \( \Delta v = v_z - u_z \) experiences the lift force

\[
f_{\text{lift}} = 6 \pi a K \Delta v \text{Re}_{\text{shear}}^{1/2} \hat{e}_x,
\]

with the shear Reynolds number \( \text{Re}_{\text{shear}} = a^2 \gamma / \nu \). Numerical evaluation gives \( K \approx 81.2 \). We discuss the application of the Saffman lift force to the control of inertial focusing in Sect. 5.1.

### 2.4.5. Dynamic pressure model for inertial migration

Even though the MAE uses strong assumptions to simplify the equations, it can only be solved numerically in most cases. Hence, it is hard to get an intuitive understanding of the physical effects. Similarly, numerical studies are always tied to a specific value of the parameters and it can be hard to extrapolate outside the considered parameter range.
2. Basics of inertial microfluidics

Figure 2.10.: Schematic of the dynamic pressure model for three characteristic situations: If the velocity of the is equal to the velocity of the undisturbed flow at its center (a), if the particle lags the Poiseuille flow with velocity $\Delta v$ (b), and if the particle has an additional angular velocity $\Omega$ (c). The blue line shows the undisturbed flow profile $u_z$, while the gray dashed lines show the velocity $v_z$ of the particle. The arrows indicate the relative velocity between flow and particle surface, which causes the inertial lift force $f_{\text{lift}}$.

An alternative to obtain an intuitive understanding of inertial focusing is to consider the relative velocities between the undisturbed flow profile and the particle surface [20, 95]. Importantly, we use the unperturbed flow profile to gain an intuition of the resulting lift forces, even though the flow field is certainly disturbed in the actual system.

Consider the situation shown in Fig. 2.10a. The curvature in the flow profile causes a difference in relative velocity between particle (gray, dashed line) and the undisturbed flow profile (blue) across the particle. According to Bernoulli’s principle [82], the higher relative velocity on the wall side causes a dynamic pressure pulling the particle towards the wall [20, 95]. Close to the wall, the fluid velocity between particle surface and wall goes to zero, as it has to obey the no-slip boundary condition at both surfaces. Then, only a contribution on the center side remains and the particle migrates back to the channel center. Both effects cancel at about halfway between channel center and channel wall and a stable equilibrium position arises.

With this argument, we are further able predict how external control methods influences inertial focusing. If we slow down the particle, the difference in particle velocity to fluid velocity dominates at some point the curvature of the flow profile. We show this situation in Fig. 2.10b. Now, the relative velocity on the center side is more pronounced and the particle migrates towards the channel center. We show how to use this Saffman force to control inertial focusing in Sect. 5.1.

Finally, consider the case when we change the angular velocity of the particle as shown in Fig. 2.10c. If the rotation has the same sign as the vorticity of the Poiseuille flow, the inertial lift force increases. Similarly, if the rotation acts against the vorticity of the Poiseuille flow, the lift force is reduced. We investigate how to control the equilibrium
positions in inertial microfluidics using the rotational motion of the particle in Sect. 5.3.

2.4.6. Thermal Motion

We close this chapter by discussing how to include thermal noise in inertial microfluidics. For most systems in inertial microfluidics, noise plays a secondary role compared to deterministic motion as we discuss below. However, it is still fruitful to include. First, stochastic fluctuations become important close to equilibrium positions where the deterministic force vanishes. In particular, we include thermal noise in the description of feedback control in Sect. 5.2 to be able to observe the instability of the channel center. Furthermore, even though thermal noise is a secondary effect it still is real in all physical systems. Finally, the method of multi-particle collisions dynamics, introduced in the next chapter, includes thermal noise. To interpret the simulation results, we have to understand thermal effects.

The forces the fluid exerts on colloidal particles originate from countless microscopic collisions between fluid molecules and the particles. In addition to the forces described by the continuum equations, the collisions manifest themselves in an erratic motion of the colloid first described by Brown. As we discuss below, the velocities in lateral and axial direction differ one to two orders in magnitude. We take this fact into account by including the thermal noise only in lateral direction. Therefore, we first consider exclusively the lateral coordinates \( \mathbf{x}_\perp = (x, y) \) with gradient \( \nabla_\perp = (\partial/\partial x, \partial/\partial y) \) and comment on the axial coordinate \( z \) at the end of this section.

To include thermal noise, we add a stochastic force \( \eta(t) \) to the equation of motion (2.27) for the particle. The corresponding equation of motion, known as Langevin equation, reads

\[
M \frac{d^2 \mathbf{x}_\perp}{dt^2} + \xi \frac{d \mathbf{x}_\perp}{dt} = \mathbf{f}_{\text{ext}} + \eta(t),
\]

where we inserted the Stokes drag force \( \xi \mathbf{v}_\perp \) on the left hand side. We demand that the random noise has zero mean \( \langle \eta_i(t) \rangle = 0 \) and is uncorrelated for different components and at different times, \( \langle \eta_i(t) \eta_j(t') \rangle = 2k_B T \delta_{ij} \delta(t - t') \). The prefactor \( 2k_B T \xi \) follows from the fluctuation dissipation theorem, discussed below. In a time interval \( \Delta t \), thermal noise changes the particle momentum by \( \Delta \mathbf{p} \). The increments \( \Delta \mathbf{p} \) are independent Gaussian random variables with zero mean and variance \( 2k_B T \xi \Delta t \). We expect this form for many independent collisions with solvent molecules.

Similar to the reduction of the Navier-Stokes equations to the Stokes equation, the equation of motion for the colloid simplifies considerably in the friction-dominated regime. If friction is large, the Langevin equation reduces to the overdamped Langevin equation

\[
\xi \frac{d \mathbf{x}_\perp}{dt} = \mathbf{f}_{\text{ext}} + \eta(t).
\]
2. Basics of inertial microfluidics

To better understand the consequences of the stochastic force, we consider a free particle without external control forces \( f_{\text{ext}} = 0 \) in the overdamped limit. In particular, we consider its displacement \( \Delta x_\perp(t) = x_\perp(t) - x_\perp(0) \) after time \( t \). Since the stochastic force does not produce a mean drift, the ensemble average of the displacement vanishes \[83, 96\]

\[
\langle \Delta x_\perp(t) \rangle = 0. \tag{2.56}
\]

On the other hand, the average of the squared displacement does not vanish. The correlations between displacements satisfy \[83, 96\]

\[
\langle \Delta x_\perp(t) \otimes \Delta x_\perp(t) \rangle = 2Dt \mathbf{1}, \tag{2.57}
\]

where we introduced the diffusion constant \( D \). The displacements in different directions are uncorrelated. Therefore, the trace of this expression is often considered, which results in \( \langle |\Delta x_\perp(t)|^2 \rangle = 2dDt \), where \( d \) gives the number of lateral dimensions. For the Langevin equation, there exists a typical time scale \( M/\xi \) separating deterministic from diffusive motion \[83\]. For times \( t \ll M/\xi \), the particle moves with its initial velocity. For times \( t \gg M/\xi \), the particle loses the memory of its initial velocity and diffuses \[83\].

The temperature and the translational friction coefficient determine the diffusion constant via the Einstein relation \[83\]

\[
D = \frac{k_B T}{\xi}. \tag{2.58}
\]

The Einstein relation is an example of the so-called fluctuation-dissipation theorem, which relates the equilibrium fluctuations (diffusion) to the response of the system to small forces (friction) \[96, 97\].

To estimate the relative importance of stochastic and deterministic forces, we introduce the Péclet number as the ratio of potential energy to thermal energy. For inertial microfluidics, we estimate the potential energy by the product of inertial lift force \( f_{\text{lift}} \) and channel width \( 2w \). Then, the Péclet number takes the form

\[
\text{Pe} = \frac{\text{potential energy}}{\text{thermal energy}} = \frac{2wf_{\text{lift}}}{k_B T}. \tag{2.59}
\]

In this thesis, the inertial lift force assumes typical values \( f_{\text{lift}} \approx 1\text{nN} \). For room temperature and a channel with width \( 2w = 20\mu\text{m} \), the Péclet number assumes typical values \( \text{Pe} \approx 10^6 \). Hence, thermal noise plays only a role, when the inertial lift forces are small, for example, close to equilibrium positions.

In the analysis so far, we restricted ourselves to the first two moments of position in the case of free diffusion. To gain further insight, we have to consider the full probability
density $P(\mathbf{x}_\perp, t)$ to find a particle at position $\mathbf{x}_\perp$ at time $t$. The probability density obeys the continuity equation \[96, 97\]

$$\frac{\partial}{\partial t} P(\mathbf{x}_\perp, t) + \nabla_\perp \cdot \mathbf{j}(\mathbf{x}_\perp, t) = 0,$$

(2.60)

with probability flux $\mathbf{j}(\mathbf{x}, t)$. The probability flux has two contributions: external forces result in deterministic motion, whereas random collisions result in diffusive motion. We write the total probability flux as \[97\]

$$\mathbf{j}(\mathbf{x}, t) = (\xi^{-1} \mathbf{f}_{\text{ext}} - D \nabla_\perp) P(\mathbf{x}_\perp, t).$$

(2.61)

The continuity equation with this form for the probability flux is also known as Smoluchowski equation \[96\].

Alternatively, we interpret the divergence of the probability flux as the action of an operator $\mathcal{L}_\perp$ acting on the probability distribution \[96\]

$$\frac{\partial}{\partial t} P(\mathbf{x}_\perp, t) = \mathcal{L}_\perp P(\mathbf{x}_\perp, t),$$

(2.62)

where we defined the Smoluchowski operator

$$\mathcal{L}_\perp = -\nabla_\perp \cdot (\xi^{-1} \mathbf{f}_{\text{ext}} - D \nabla_\perp).$$

(2.63)

For conservative forces, we express the force in terms of a potential, $\mathbf{f}_{\text{ext}} = -\nabla_\perp V$. Then, the position in steady state follows the Boltzmann distribution \[96\]

$$P(\mathbf{x}_\perp) = \frac{1}{Z} \exp \left[ -\frac{1}{k_B T} V(\mathbf{x}_\perp) \right].$$

(2.64)

Here, the partition function $Z$ ensures that the distribution is normalized. A potential can always be constructed in one-dimensional systems or systems with radial symmetry. When inertia is important, the Smoluchowski equation has to be extended to the Kramers equation. The steady-state distribution of the Kramers equation factorizes into position and velocity distributions. The position is distributed as before, whereas the velocity is distributed according to a Maxwell-Boltzmann distribution. The complete steady-state distribution of the Kramers equation reads \[96\]

$$P(\mathbf{x}_\perp, \mathbf{v}_\perp) = \frac{1}{Z} \exp \left[ -\frac{1}{2 k_B T} \frac{m}{2} |\mathbf{v}_\perp|^2 \right] \exp \left[ -\frac{1}{k_B T} V(\mathbf{x}_\perp) \right].$$

(2.65)

For bounded systems, we require boundary conditions for the Smoluchowski equation. Here, we demand that the current through the boundary vanishes, $\hat{\mathbf{n}} \cdot \mathbf{j} = 0$, where $\hat{\mathbf{n}}$ is the normal to the boundary.
2. Basics of inertial microfluidics

Up to now, we discussed the Smoluchowski equation for a density evolving from an initial distribution. When we choose the initial distribution as a Dirac delta, the density becomes the probability \( P(x_\perp, x'_\perp | t) \) for the particle to move from its current position \( x'_\perp \) to position \( x_\perp \) in time \( t \). The transition probability satisfies a Smoluchowski equation too [96],

\[
\frac{\partial}{\partial t} P(x, x'| t) = \mathcal{L} P(x, x'| t),
\]

where all spatial derivatives in \( \mathcal{L} \) act on \( x \). Since the particle was at position \( x'_\perp \) at \( t = 0 \) with certainty, the transition probability has to satisfy \( P(x_\perp, x'_\perp | t = 0) = \delta(x_\perp - x'_\perp) \). The no-flux boundary condition for the density translates into

\[
\hat{n} \cdot [\xi^{-1} f_{ext} - D \nabla_\perp] P(x, x'| t) = 0 \quad \text{at the boundary.}
\]

We express the probability to find a particle at \( x_\perp \) at time \( t \) in terms of the transition probability and the distribution at \( t = 0 \) as

\[
P(x_\perp, t) = \int dx'_\perp P(x_\perp, x'_\perp | t) P(x'_\perp, 0).
\]

We further use the transition probability to describe the evolution of expectation values in time. In particular, we consider the expectation value \( K(x_\perp, t) \) of a function \( k(x_\perp) \) at time \( t \), when the particle starts at position \( x_\perp(0) \). We express it as

\[
K(x_\perp, t) = \int dx'_\perp P(x_\perp, x'_\perp | t) k(x'_\perp),
\]

where, we exchanged the primed and unprimed variable in the transition probability. The time evolution of \( K(x, t) \) obeys the Kolmogorov backward equation [96, 98]

\[
\frac{\partial}{\partial t} K(x_\perp, t) = \mathcal{L}^+ K(x_\perp, t),
\]

where we introduced the adjoint operator

\[
\mathcal{L}^+ = (\xi^{-1} f_{ext} + D \nabla_\perp) \cdot \nabla_\perp.
\]

At the boundary the normal gradient of the expectation value \( K \) has to vanish and we find [96]

\[
\hat{n} \cdot \nabla_\perp K(x, t) = 0 \quad \text{at the boundary.}
\]

In the discussion up to this point, we only considered the lateral dimensions. We quantify the importance of thermal noise for the axial motion by the axial Péclet number
2.4. Colloidal particles

Pe\textsubscript{z}. Here, we use the drag force \( f_{\text{drag}} = \xi v \) instead of the lift forces in Eq. (2.59). For typical velocities \( v \approx 1 \text{m/s} \) and typical particle radii \( a \approx 5 \mu\text{m} \) in inertial microfluidics, we find \( \text{Pe}_{\text{z}} \approx 10^2 \text{Pe} \). Therefore, the axial motion is much less influenced by thermal noise and we assume the movement in axial direction to be deterministic. In microchannels, the particle translates with a velocity \( v_z(x_{\perp}) \) along the axial direction and the Langevin equation has to be supplemented by the equation

\[
\frac{d}{dt} z = v_z(x_{\perp}).
\] (2.73)

We include the axial motion in the Smoluchowski operator by adding a drift term along the axial direction. Then, the total Smoluchowski operator becomes

\[
\mathcal{L} = \mathcal{L}_{\perp} - \frac{\partial}{\partial z} v_z = -\nabla_{\perp} \cdot (\xi^{-1} f_{\text{ext}} - D \nabla_{\perp}) - \frac{\partial}{\partial z} v_z,
\] (2.74)

with its adjoint

\[
\mathcal{L}^+ = \mathcal{L}_{\perp}^+ + v_z \frac{\partial}{\partial z} = (\xi^{-1} f_{\text{ext}} + D \nabla_{\perp}) \cdot \nabla_{\perp} + v_z \frac{\partial}{\partial z}.
\] (2.75)
To correctly describe inertial migration, we have to solve the full Navier-Stokes equations. Due their nonlinearity and the added complexity of moving boundaries from the colloidal particles, we choose to solve them numerically. In this chapter, we discuss the simulation methods used. First, we compare different methods to model fluid flow with a particular emphasis on mesoscopic simulation methods. Then, we describe the two particle-based mesoscopic methods used in this work: multi-particle collision dynamics and the lattice Boltzmann method. For both, we explain the algorithm for a bulk fluid and discuss necessary steps to correctly describe inertial focusing.

3.1. Computational fluid dynamics

The numerical treatment of the Navier-Stokes equations has a long history, since only few analytic results are available. The nonlinearities of the underlying equations and the complex, possibly moving, boundaries pose a great challenge. Over the years, methods with different areas of application and with different properties have been proposed. Especially for flows at low Reynolds number, a number of highly specialized and, therefore, efficient methods are available. Examples are the multipole expansion [99], the boundary element method [100], and the use of mobilities in Stokesian dynamics [101]. However, all these methods rely on the linearity of the Stokes equation and are no longer applicable for inertial microfluidics. Hence, we focus on general Navier-Stokes solvers which account for the full nonlinearity. In the following discussion, we do not order methods chronologically, but rather by similarity.

3.1.1. Direct discretization of the Navier-Stokes equations

A huge class of numerical methods start from the Navier-Stokes equations (2.8) and discretize the velocity field and the differential operators.

The finite-difference approximation is a particularly popular method to discretize partial differential equations, such as the Navier-Stokes equations [102]. It describes the solution on a regular lattice and discretizes the differential operators on this lattice using differences of function values between different lattice positions. While conceptually simple, ensuring stability and convergence can be difficult. Furthermore, the regular lattice structure makes it difficult to include boundaries which do not conform to this lattice.
An alternative method is the finite-element method which divides the computational domain into simple elements such as tetrahedra \[102\]. Importantly, the subdivision of space called mesh can adapt to the geometry of the problem. The differential equations are approximated on each element separately by projecting them onto a set of basis functions. Different elements are coupled by enforcing continuity of the solution across elements. This scheme results in a set of coupled nonlinear equations which have to be solved. The coupling between different elements often prevents the exact inversion of the operators and iterative schemes are used to approximately invert the operators. This fact complicates the time integration, as it typically requires inversion of the operators \[103\].

The Navier-Stokes equations together with the continuity equation describes the conservation of mass and momentum. For many discretization schemes, these conservation laws are not fulfilled numerically. Finite-volume methods \[104\] address this problem by constructing a scheme which explicitly enforces the conservation laws. Finite-volume methods also work on geometry conforming meshes similar to finite-element methods, but describe the evolution of average quantities in each element. Different elements are coupled by a numerical flux, which models the physical flux through the element boundary. To achieve high accuracy, finite-volume methods require fine meshes, which increases runtime and memory requirements. A possible solution are hybrid models such as discontinuous Galerkin methods \[103\], which combine features from both finite-element and finite-volume methods to retain their respective advantages.

All methods mentioned rely on a fixed discretization of space and, therefore, have difficulty when dealing with moving boundaries. In particular for mesh-based methods, the mesh needs to be constantly adapted to the moving boundaries. A possible solution is to use the immersed boundary method \[105\], which we explain in connection with the lattice Boltzmann method in Sect. 3.3.4.

### 3.1.2. Mesoscopic simulation methods

An alternative to the approximation of the exact differential equations are mesoscopic methods. Even though not a mesoscopic simulation method itself, molecular dynamics (MD) \[106\] provides the concepts and tools fundamental to mesoscopic algorithms. MD describes molecular details in terms of classical potential between individuals atoms. Since it uses an atomistic description, it is only feasible to describe small systems \[107\]. This observation prompted the invention of mesoscopic methods, which simplify the microscopic dynamics to allow for larger systems, while sacrificing physical fidelity. Mesoscopic simulation methods place a special emphasis on conservation laws and symmetries. Therefore, they reproduce the correct macroscopic dynamics \[108\]. The resulting methods are very efficient and are able to deal with effects on different time and length scales \[108\]. Furthermore, as they are based on simplified micro-dynamics, they often are easily extended to complex systems such as mixtures of different fluids or colloidal particles in
flows. The different mesoscopic methods are often similar in features and behavior as noted by Dünnweg [109].

“Different [mesoscopic] methods [...] have been invented and implemented, and in author’s opinion they are all very similar both in terms of philosophy and (probably) computational efficiency.”

One popular mesoscopic method is dissipative particle dynamics (DPD) [110]. DPD describes the fluid by individual particles, similar to MD, but replaces the detailed interaction potentials by simpler ones. A common choice is a repulsive harmonic potential with a cutoff [110]. As the potential is rather soft, it permits time-steps much larger than those found in MD simulations. DPD uses a thermostat and hence includes stochastic fluctuations. Both the thermostat and the interactions locally conserve linear and angular momentum [110]. Thereby, DPD is able to correctly describe hydrodynamics on length scales larger than the potential cutoff [111].

In DPD, most simulation time is spent to calculate the pairwise interaction between fluid particles. The method of multi-particle collision dynamics further simplifies the interactions. It divides the system into a grid of cubic cells. At discrete time-steps all fluid particles in a cell exchange momentum by a set of collision rules designed to locally conserve momentum. These multi-particle interactions are the only interactions in the system and the particles move independently in between. MPCD borrows this interaction model from direct simulation Monte Carlo (DSMC) [112], which uses Monte-Carlo sampling to perform pairwise collisions in each cell. In MPCD, however, the collisions are collective between all fluid particles in each cell and as such increase the performance.

The lattice Boltzmann method (LBM) [113–115] follows the idea of particle-based fluid simulations, but restricts the dynamics to a regular lattice. In contrast to lattice gas automata, which also follow this path, LBM describes the dynamics by distributions functions not individual particles. Therefore, LBM does not include stochastic fluctuations related to thermal noise.

In this work we investigate inertial focusing with multi-particle collision dynamics [116, 117] and the lattice Boltzmann method [113–115]. In the following, we introduce both methods and discuss their application to the simulation of colloidal particles in microfluidic channel flows. We also comment on the choice of parameters and the challenges, but also advantages, of using mesoscopic simulation methods.

3.2. Multi-particle collision dynamics

Malevanets and Kapral introduced the original version of multi-particle collision dynamics called stochastic rotation dynamics (SRD) in [118]. It is similar in spirit to DSMC [112], in that it describes fluid flow by pointlike particles and it introduces a grid
3. Mesoscopic simulations of fluid dynamics

of regular cells for the interactions, where fluid particles in the same cell interact. However, it replaces the Monte-Carlo sampling used in DSMC to describe the interactions by collective interactions between all fluid particles in a cell [116, 117]. The interactions between fluid particles are designed such that they locally conserve momentum and energy [116, 117]. The name SRD reflects the interaction rule for which the velocities of fluid particles in a cell are rotated around a randomly chosen axis relative to the mean velocity in this cell. By using a multi-scale Chapman-Enskog expansion, Ihle showed that, on length scales larger than the collision cells and time scales larger than the collision time, SRD solves the Navier-Stokes equations [119]. In this work, we do not use SRD, but rather a variant called MPCD-AT+a which ensures constant temperature and locally conserves angular momentum [120]. Here, we restrict the discussion to this specific variant. For thorough reviews of alternative variants and models, we refer to Refs. [116, 117].

Multi-particle collision dynamics is a versatile simulation technique and is able to describe a large range of different systems. It has been used to describe the settling and hydrodynamic interaction in dense suspensions of colloids [108, 121]. Other studies considered the motion of model microswimmers [122–124] and also such diverse biological systems as the parasite African Trypanosome [125], red blood cells in flow [126], and swimming fish at moderate Reynolds number [127, 128].

3.2.1. Main algorithm

MPCD describes the fluid by point particles which undergo two distinct steps, the streaming and the collision step. In the streaming step, fluid particles move under the action of external forces for a fixed time interval, however, without any mutual interactions. In the collision step, a grid of cubic cells is superimposed and fluid particles in the same cell interact via a set of effective collision rules. We illustrate the algorithm in Fig. 3.1.

We continue by describing the individual steps, starting with the streaming step. The fluid particles have mass $m_f$, positions $\mathbf{r}_i$, and velocities $\mathbf{v}_i$. The duration of the streaming step is called the collision time $\Delta t_c$, as it gives the interval between collisions. The number of fluid particles is typically specified as the average number of particles $n$ per collision cell, introduced below. For cells with edge length $l_c$, the number of particles determines the average mass density $\rho = m_f n / l_c^d$, where $d$ is the number of dimensions. We determine the new position and velocities after the streaming step by using the velocity Verlet algorithm [106]. Its integration error is proportional to $(\Delta t_c)^2$ [106]. Here, further dividing the streaming step decreases the integration error. If we split the streaming step into $N_{MD}$ molecular dynamics steps, time advances in steps of $\Delta t_{MD} = \Delta t_c / N_{MD}$. In the streaming step, the fluid particles move without mutual interaction and experience a constant acceleration $\mathbf{a}$. Then, the velocity Verlet algorithm for a single molecular
3.2. Multi-particle collision dynamics

Figure 3.1.: Overview of the MPCD algorithm. (a) It divides the time evolution into two distinct steps. (b) First, particles perform free streaming for a time $\Delta t_c$. To increase numerical accuracy, we further divide the time interval into $N_{\text{MD}}$ molecular dynamics steps with length $\Delta t_{\text{MD}} = \Delta t_c/N_{\text{MD}}$. (c) Then, all particles in one cell instantaneously collide with each other.

The streaming step updates the fluid particles by

\begin{align}
\mathbf{r}_i(t + \Delta t_{\text{MD}}) &= \mathbf{r}_i(t) + \Delta t_{\text{MD}} \mathbf{v}_i(t) + \frac{1}{2} \left( \Delta t_{\text{MD}} \right)^2 \mathbf{a}, \\
\mathbf{v}_i(t + \Delta t_{\text{MD}}) &= \mathbf{v}_i(t) + \Delta t_{\text{MD}} \mathbf{a}.
\end{align}

With the acceleration $\mathbf{a}$, we model a body force $\mathbf{g} = \rho \mathbf{a}$, with which we implement the Poiseuille flow as discussed in Sect. 2.3. Here, we already used that the body force is constant and does not depend on position. For non-constant body forces, the velocity Verlet algorithm has a different form \[106\].

The streaming step is followed by the collision step, in which fluid particles exchange momentum in instantaneous collisions. We sort the fluid particles into cubic cells with edge length $l_c$ as illustrated in Fig. 3.1c. In each cell, we find $N_c$ particles. This number is Poissonian distributed in uniform systems, with the mean value $n = < N_c >$. The collisions update the particle velocities according to the rule \[120\]

\begin{equation}
\mathbf{v}_i \rightarrow \mathbf{v}'_i = \mathbf{v}_{\text{cell}} + \mathbf{v}_{\text{therm},i} + \mathbf{v}_{\text{corr},-p,i} + \mathbf{v}_{\text{corr},-l,i}.
\end{equation}

Here, we defined the mean of the particle velocities in the cell $\mathbf{v}_{\text{cell}} = \frac{1}{N_c} \sum_{i \in \text{cell}} \mathbf{v}_i$. The thermal velocity $\mathbf{v}_{\text{therm},i}$ introduces stochastic fluctuations into the system and is distributed according to the Maxwell-Boltzmann distribution for temperature $T$

\begin{equation}
P(\mathbf{v}_{\text{therm},i}) = \left( \frac{m_f}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{1}{2} \frac{m_f |\mathbf{v}_{\text{therm},i}|^2}{k_B T} \right].
\end{equation}

The correction terms $\mathbf{v}_{\text{corr},-p,i}$, $\mathbf{v}_{\text{corr},-l,i}$ ensure the conservation of linear and angular momentum in each cell.
Without explicit corrections, the thermal velocities \( v_{\text{therm},i} \) change the momentum of the collision cell. As we draw only \( N_c \) samples of thermal velocities, they generally do not sum to zero as we expect for an infinite number. We correct this sampling effect by explicitly subtracting the gained momentum and set

\[
v_{\text{corr} - p, i} = -\frac{1}{N_c} \sum_{i \in \text{cell}} v_{\text{therm}, i}.
\]  

(3.5)

To ensure angular momentum conservation, we modify the particle velocity such that the change in angular momentum is exactly canceled. We determine the correction velocity by assuming that the collision cell is a rigid body. We make the ansatz for the correction of angular momentum as

\[
v_{\text{corr} - l, i} = -\omega_{\text{corr}} \times (r_i - r_c),
\]  

(3.6)

where we defined the cell center of mass \( r_c = \frac{1}{N_c} \sum_{i \in \text{cell}} r_i \) and introduced the angular velocity \( \omega_{\text{corr}} \). This ansatz does not change the linear momentum of the cell. Without the correction term, the angular momentum changes as

\[
\Delta L = m \sum_{i=1}^{N_c} r_i \times [v_{\text{cell}} + v_{\text{therm},i} + v_{\text{corr} - p, i} - v_i].
\]  

(3.7)

Demanding that \( \Delta L + \sum_i v_{\text{corr} - l, i} \times r_i = 0 \), we derive the angular velocity

\[
\omega_{\text{corr}} = \theta^{-1} \Delta L,
\]  

(3.8)

where we introduced the moment of inertia tensor of the collision cell

\[
\theta = m \sum_i \left[ |r_i - r_c|^2 - (r_i - r_c) \otimes (r_i - r_c) \right].
\]  

(3.9)

The MPCD algorithm with a fixed arrangement of collision cells does not preserve Galilean invariance \[129\]. When the mean free path \( l_{mf} \) is smaller than the cell edge length \( l_c \), the same fluid particles collide in subsequent collision steps. However, when the whole systems moves with a constant velocity, the collision partners do change in subsequent collisions. To ensure that both the moving and stationary system behave the same, we shift the grid of collision cells by a random vector \( \Delta r \in [-l_c/2, +l_c/2]^d \) in each time step \[129\]. This way, we remove the fixed grid structure and restore Galilean invariance.

Finally, we discuss how the MPCD fluid relates to the Navier-Stokes equations. We determine the mass density and flow velocity in a volume \( V(x) \) by averaging over the individual fluid particles. Concretely, we calculate the mass density by

\[
\rho(x, t) = \sum_{i \in V(x)} \frac{m_f}{V(x)}
\]  

(3.10)
3.2. Multi-particle collision dynamics

and the flow velocity by

\[ u(x, t) = \frac{1}{\rho(x)} \sum_{i \in V(x)} \frac{m_f v_i}{V(x)}. \]  \hspace{1cm} (3.11)

3.2.2. Transport coefficients

The MPCD algorithm can be viewed as a stochastic solver of the Navier-Stokes equations. This can be verified by a multi-scale Chapman-Enskog expansion. For the SRD variant, this calculation has been explicitly performed by Ihle \[119\]. He derived the Navier-Stokes equations and obtained expressions for the macroscopic transport coefficients in terms of the parameters of the micro dynamics. The calculation follows similar steps as the Chapman-Enskog expansion of the LBM equation explained in Sect. 3.3.2. However, the number of particles in each cell is Poissonian distributed and the calculation is more involved. Noguchi and Gompper proposed an alternative method to determine the transport coefficients in MPCD \[130\]. They considered the mass and momentum transport in a linear shear flow. By assuming the validity of the viscous stress tensor (2.5) for a Newtonian fluid, they derived explicit expressions of the transport coefficients. We perform two-dimensional and three-dimensional simulations in this thesis and hence present the transport coefficients for both dimensions, \(d = 2\) and \(d = 3\).

Between collisions fluid particles move for a time \(\Delta t_c\) with a typical velocity \(v_0 = \sqrt{k_B T/m}\). The typical distance traveled by particles between collisions is the mean free path \[108\]

\[ l_{mf} = \sqrt{k_B T/m \Delta t_c}. \]  \hspace{1cm} (3.12)

The stochastic collisions cause fluid particles to quickly lose memory of their initial velocity and to move diffusively on large time scales. We expect that the diffusion constant depends on the mean free path and the collision time like \(l_{mf}^2/\Delta t_c\). The analytic expression confirms this assumption \[130\]:

\[ D = \frac{l_{mf}^2}{\Delta t_c} \left( \frac{1}{s_m(n)} - \frac{1}{2} \right), \]  \hspace{1cm} (3.13)

\[ s_m(n) = 1 - \frac{d + 1}{2n} + \frac{1}{2} e^{-n} \left( \frac{(d-1)(d-2)n}{2d} + d - 1 \right), \]  \hspace{1cm} (3.14)

where the factor \(s_m(n)\) includes the effect of correlations between particles. As the mean free path is linear in the collision time, the diffusion satisfies \(D \propto \Delta t_c\). The diffusive motion of the particles also causes the internal pressure of the MPCD fluid and the equilibration of density gradients. The MPCD fluid behaves thermodynamically like an ideal gas with a speed of sound \(c_s = \sqrt{5k_B T/3m}\) \[116\].
3. Mesoscopic simulations of fluid dynamics

Figure 3.2.: (a) Analytic prediction for the kinematic viscosity versus collision time step for different numbers of particles per cell. The squares show the viscosity for $n = 10$ measured from simulations of the Poiseuille flow and comparison of the analytic formula. The red square shows the default parameters ($\Delta t_c = 0.1$, $n = 10$) used in this work. (b) The factors of Eqs. (3.14), (3.16), and (3.17) plotted versus the number of particles per cell $n$.

The viscosity in the Navier-Stokes equations describes momentum transport. In the MPCD fluid, momentum is transported by two physical processes. First, particles carry their own momentum with them and we expect a kinetic contribution to the kinematic viscosity proportional to $l^2mf/\Delta t_c$. Second, collisions distribute momentum randomly over the collision cell and we expect a contribution proportional to $l^2c/\Delta t_c$. The total kinematic viscosity calculated in [130] combines both contributions and takes the form

$$\nu = \frac{l^2mf}{\Delta t_c} \left( \frac{1}{c_m(n)} - \frac{1}{2} \right) + \frac{l^2_c}{\Delta t_c} \frac{d_m(n)}{24}, \quad (3.15)$$

with the additional correction factors

$$c_m(n) = 1 - e^{-n}(1 + n) + \left(1 + \frac{1}{d}\right) \frac{ne^{-n}}{d + 2} + \left(2 - d\right) \frac{1 - e^{-n}(1 + n + n^2/2)}{2n} \quad (3.16)$$

$$d_m(n) = 1 - \frac{7}{5n} + \frac{e^{-n}}{n} \left( \frac{7}{5} + \frac{2n}{5} + n^2 \left( \frac{1}{d} - \frac{3}{10} \right) \right) \quad (3.17)$$

to account for correlations between particles.

We plot the kinematic viscosity $\nu$ for different particle numbers as a function of collision time in Fig. 3.2a. The squares show the viscosity for $n = 10$ measured from simulations of Poiseuille flow in a channel with circular cross section. Specifically, we apply a constant body force to the fluid and determine the maximum flow velocity in the channel center. With the analytic formula for the flow field (2.25), we calculate the viscosity.

The correction factors account for correlations between fluid particles introduced by the constraints of the conservation laws. As we increase the particle number and with it
3.2. Multi-particle collision dynamics

Figure 3.3.: (a) Schematic of the approximate bounce-back rule by [Padding et al. 131] described in the main text. (b) Typical arrangement of the fluid (blue) and ghost particles (red) for a spherical colloid in front of a wall. The gray dashed lines show the boundaries of the collision cells.

the degrees of freedoms, the constraints become less dominant and we find

\[
\lim_{n \to \infty} s_m(n) = 1, \quad \lim_{n \to \infty} d_m(n) = 1, \quad \lim_{n \to \infty} c_m(n) = 1. \tag{3.18}
\]

We plot the factors versus the numbers of particles per cell in Fig. 3.2b. In practice for \( n \geq 10 \), these factors do not differ more than 20 % for different values of the particle number. In particular, the viscosity \( \nu \) does hardly change for \( \Delta t_c \leq 0.2 \) (Fig. 3.2a).

3.2.3. Boundary conditions

In the previous sections, we discussed the MPCD method for a bulk fluid without boundaries. We discuss how to modify the MPCD method to include boundaries in this section. Here, we only consider boundaries of solid bodies such that the boundaries always enclose a finite volume. As discussed in Sect. 2.2.5, close to a boundary the fluid assumes the surface velocity of this boundary. To model this no-slip boundary condition accurately with MPCD, we have to modify both streaming and collision step.

When a fluid particle collides with a surface at point \( r_s \) in the streaming step, we apply the bounce-back rule to enforce the no-slip condition [132]. We choose the velocity after the collision such that the average velocity before and after the collision is equal to the surface velocity

\[
\frac{1}{2} [v_{\text{before}}(r_s) + v_{\text{after}}(r_s)] = v_{\text{surface}}(r_s). \tag{3.19}
\]

The name “bounce-back” stresses that for an immobile surface, \( v_{\text{surface}} = 0 \), the particle velocity changes sign upon collision with the surface, \( v_{\text{after}} = -v_{\text{before}} \). Accurately resolving the instance of collision drastically reduces the efficiency of the simulation algorithm.
Padding et al. proposed the following alternative \[131\]: First, we perform the molecular dynamics step without checking for collisions and fluid particles move freely for a time $\Delta t_{\text{MD}}$. Second, for any fluid particle we find inside a solid body after the molecular dynamics step, we apply the steps illustrated in Fig. 3.3a. First, we move the particle back for $\Delta t_{\text{MD}}/2$ and place it on the closest point at the surface. Then, we apply the bounce-back rule and let the particle continue for $\Delta t_{\text{MD}}/2$ with its new velocity.

In the collision step, the collision cell may overlap with a solid boundary, similar to the situation show in Fig. 3.3b. Collision cells which intersect with boundaries are only partially filled by fluid particles. We fill up all solid bodies with so-called ghost particles to ensure equal average particle density on both sides of the boundary \[132\]. In each collision step, we uniformly distribute the ghost particles in any solid volume with the density of the fluid $\rho$. In practice, we fill the solid bodies up to a depth of $\sqrt{3}l_c$, as only cells which overlap with the fluid domain contribute to the physical dynamics. We assign each ghost particle the velocity

$$v_g = v_{\text{solid}}(r_g) + v_{\text{thermal}}, \quad (3.20)$$

where $v_{\text{solid}}(r_g)$ is the velocity of the solid body at the position of the ghost particle and the thermal velocity $v_{\text{thermal}}$ is distributed according to the Maxwell-Boltzmann distribution \[3.4\]. This way, all solid bodies in contact with the fluid act as further thermostats. For a fixed wall, $v_{\text{solid}}(r_g) = 0$ and the velocity of ghost particles only has a thermal component. We explain the implementation of colloidal particles in the next section.

In both the streaming and collision step, the presence of solid bodies changes the momentum of the fluid particles. In the streaming step, the bounce-back rule exchanges momentum between fluid and boundaries. In the collision step, momentum is transferred between the fluid particles and the ghost particles inside the solid.

### 3.2.4. Colloidal particles

We model a colloidal particle as a hard sphere. It moves according to Newton’s equations \[2.27\], which we solve by the Euler integrator \[133\]. We couple the colloidal particle to the MPCD fluid by the bounce-back rule in the streaming step and fill it with ghost particles in the collision step, as explained in the previous section. Here, we describe the surface of the colloidal particle by analytic expressions. A ghost particle at position $r_g$ has the solid body velocity

$$v_{\text{solid}}(r_g) = v + \Omega \times (r_g - r), \quad (3.21)$$

where the colloidal particle has position $r$, velocity $v$, and angular velocity $\Omega$. To apply the bounce-back rule \[3.19\], we need to determine the surface velocity at the position of the fluid particle. The velocity follows from Eq. \[3.21\] setting $r_g$ equal to the
surface position $r_s$. In both streaming and collision step, interactions with solid particles change linear and angular momentum of the fluid. To restore overall conservation of both quantities, we transfer the change in linear and angular momentum to the colloidal particle.

### 3.2.5. Choice of parameters

A collection of dimensionless numbers characterizes the physical properties of the MPCD fluid [108]. As we discuss below, algorithmic and runtime constraints do not allow to match all fluid properties with these dimensionless numbers. Luckily for many systems, the dimensionless numbers do not need to match exactly, but rather fulfill certain bounds. Padding discussed this problem and the implications for the MPCD algorithm in detail in Ref. [108]. We follow [108] but adapt the discussion to the problem of inertial microfluidics. Specifically, we consider a colloidal particle with radius $a$ inside a channel with circular cross section and radius $R$. To correctly describe inertial focusing, we need to reproduce the Reynolds number and the ratio of particle radius to channel radius exactly. Therefore, we always consider a fixed Reynolds number $Re$ and a fixed ratio of particle to channel radius $a/R$. The remaining physical properties of the fluid depend only on two parameters, the Knudsen number

$$Kn = \frac{l_{mf}}{R},$$  \hspace{1cm} (3.22)

and the number of collision cells per channel radius $N_R = R/l_c$.

The Knudsen number quantifies how important the individual particles are to the overall dynamics. In particular, it is directly related to the validity of the no-slip boundary condition as we demonstrate in Sect. 3.2.6. Padding [108] proposed that the Knudsen number should satisfy $Kn < 0.05a/R$. For particle sizes $a/R \geq 0.2$, this translates into the bound $Kn < 0.01$, which we always satisfy for the systems considered here.

Next, we consider the Schmidt number $Sc = \nu/D$. It compares momentum transport characterized by viscosity to mass transport characterized by the diffusion constant. Using the analytic expressions of Eqs. (3.13) and (3.15), we express it as

$$Sc = \frac{\nu}{D} = \frac{d(n)}{24Kn^2N_R^2} + \frac{2/c(n) - 1}{2/s(n) - 1}. \hspace{1cm} (3.23)$$

In fluids, momentum transport dominates mass transport with typical bounds of $Sc > 5$ [108].

As we discussed in the previous chapter, there are two important dimensionless number for continuum fluid dynamics, the Reynolds number and the Mach number (Sect. 2.2.2). Using the analytic expressions of the transport coefficients (Sect. 3.2.2), we express the
3. Mesoscopic simulations of fluid dynamics

Figure 3.4.: (a) The maximum Reynolds number attainable as a function of the number of collision cells per radius $N_R$ and Knudsen number Kn such that $Ma < 0.3$. (b) Péclet number as a function of $N_R$ and Kn. The gray lines show the constraints for fixed Reynolds numbers. They correspond to the isocontours of (a). In both plots, the gray area shows the region where the Schmidt number violates the bound $Sc \geq 5$.

Typical bounds for incompressible fluids are $Ma < 0.3^{108}$. We translate this bound into a maximum Reynolds number achievable for given Kn and $N_R$. We plot it in Fig. 3.4a, where we show the bound for the Schmidt number as the gray shaded area. To increase the Reynolds number, we have to necessarily increase the number of collision cells per radius. Thereby, we also increase the runtime and memory consumption.

Finally, we quantify the importance of stochastic fluctuations in the MPCD method by the Péclet number $Pe$ (2.59). It compares the potential energy associated with inertial lift forces to thermal energy. The fluid properties change the magnitude of the inertial lift forces by the factor $\rho v^2$ (Sect. 2.4.4). Therefore, we estimate the Péclet number by

$$Pe = \frac{R \rho v^2}{k_B T}.$$  

(3.25)

Using the analytic expressions for the transport coefficients (Sect. 3.2.2), we express it as

$$Pe = nN^3 R \left[ \frac{Kn}{c(n)} - \frac{1}{2} + \frac{d(n)}{24KnN^2_R} \right]^2,$$

(3.26)

$$= nN^3 R \left( \frac{Ma}{Re} \right)^2.$$  

(3.27)
3.2. Multi-particle collision dynamics

Figure 3.5.: (a) The parabolic Poiseuille flow profile observed by applying a constant body force. The inset shows the observed slip. (b) Axial velocity $v_z$ of a sphere with radius $a = 4$ plotted versus radial position at $Re = 1$. The dashed line shows the analytic prediction from Faxén’s law (2.33).

We plot the Péclet number in Fig. 3.4b with the bound for the Schmidt number shown as the gray shaded area. For an experimental setup with $R = 20\mu m$ at temperate $T = 300K$, we find $Pe \approx 5 \times 10^6$. If we compare with the Péclet number shown in Fig. 3.4b, we observe that reaching physical Péclet numbers is infeasible. Therefore, the stochastic fluctuations in MPCD are artificially high compared to physical systems. Indeed, the parameters used (Appendix E) satisfy the bound for Schmidt number and Mach number, but show an artificially increased temperature. We discuss the implications for inertial focusing in Sect. 4.1.2.1.

3.2.6. Validation

We implement the no-slip boundary condition as explained in Sect. 3.2.3 for both the channel walls and embedded particles. To test the boundary conditions, we simulate the flow through a channel with circular cross section and radius $R = 25l_c$. For the MPCD fluid, we use parameters $P_1$ given in appendix E. The MPCD boundary condition does not reproduce the no-slip boundary condition exactly. At the channel wall, we observe a small nonzero velocity, called slip velocity. To determine the slip velocity, we determine the flow field according to Eq. (3.11) and fit it to the Poiseuille flow (2.25) with the slip velocity as an additional offset,

$$u_{z,fit}(r) = u_{\text{max}} \left( 1 - \frac{r^2}{R^2} \right) + u_{\text{slip}}.$$ (3.28)

Following Eq. (2.19), the slip velocity determines the slip length $\lambda$ by

$$\frac{\lambda}{R} = \frac{u_{\text{slip}}}{2u_{\text{max}}}.$$ (3.29)
3. Mesoscopic simulations of fluid dynamics

We plot the flow profile and the fit in Fig. 3.5a. We are able to reproduce the parabolic flow profile with a small slip length, which we show for different Reynolds numbers in the inset. The slip lengths are close to $\lambda = 1.15l_{mf}$, the value expected for a dilute gas.

For small colloidal particles at low Reynolds numbers, we use Faxén’s law (2.33) to describe approximately the velocity of the particle inside a channel flow. We plot the results for $Re = 1$ in Fig. 3.5b and observe that the colloidal velocity follows the expected profile. Here, we use parameters $P_1$ for the MPCD fluid given in appendix E.

Finally, we analyze the thermal motion of a spherical colloidal particle by considering the probability distribution for its translational and rotational velocity. The particle has a radius $a = 3$, mass $m = 1131$, and moment of inertia $I = 4071$. For the fluid, we choose the parameters $P_1$ given in appendix E. We expect that the translation velocity is distributed according to

$$P(v) = \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{1}{2} \frac{m|v|^2}{k_B T} \right],$$

(3.30)

and the angular velocity according to

$$P(\Omega) = \left( \frac{I}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{1}{2} \frac{I|\Omega|^2}{k_B T} \right].$$

(3.31)

In Fig. 3.6, we demonstrate that the colloidal velocities follow the expected distributions.
3.3. The lattice Boltzmann method

As we discussed in Sect. 3.2.5, the stochastic nature of MPCD results in artificially high fluctuations. Here, the lattice Boltzmann method (LBM) offers an alternative. The LBM describes the fluid as a gas with added interactions similar in spirit to MPCD. However, in contrast to MPCD, it describes the fluid state by distribution functions and, therefore, the hydrodynamic fields do not fluctuate. Furthermore, the LBM uses a regular lattice and solves the Navier-Stokes equations efficiently. The LBM has a strong footing in the field of soft-matter research [113]. Examples include the motion of red blood cells [135], deformable drops [55], and multiphase fluids [136]. This wide range of applications is indicative of the flexibility of the LBM. Historically, the LBM developed from lattice gas automata, which track individual particles moving on a lattice and therefore are also susceptible to high fluctuations [115]. The LBM was developed as an averaged lattice gas automaton to sidestep this problem. Another route to motivate the LBM is to discretize the Boltzmann equation on a lattice [137]. In the following, we describe only the variant of LBM used in this work. For a detailed discussion, we refer to the reviews [113, 114] or the book [115].

3.3.1. Lattice Bhatnagar-Gross-Krook

The LBM describes the fluid by particles moving on a regular cubic lattice with spacing $\Delta x$. The particle velocities $c_i$ are constrained such that after each time step $\Delta t$ the particle positions lie again on the lattice. We discuss the choice of allowed particle velocities at the end of this section. The local distribution functions $f_i(x, t)$ give the number of particles on each lattice site $x$ with velocity $c_i$ at time $t$. The velocity moments of the distribution functions determine the macroscopic fluid variables. In particular, the zeroth moment gives the mass density

$$\rho(x, t) = \sum_i f_i(x, t),$$

and the first moment determines the fluid velocity

$$u(x, t) = \frac{1}{\rho(x, t)} \sum_i f_i(x, t) c_i.$$  

The second moment gives the momentum flux tensor $\Pi(x, t) = \sum_i f_i(x, t) c_i \otimes c_i$ necessary to correctly describe hydrodynamic behavior, as we discuss in Sect. 3.3.2.

The LBM describes the evolution of the distribution functions in two consecutive steps, a collision step followed by a streaming step. We model the collisions with the Bhatnagar-Gross-Krook (BGK) approximation [113, 115, 138]. It was first introduced to describe the collisions in high density plasmas using the Boltzmann equation [138]. While the
authors of Ref. [138] introduced also a nonlinear collision term, we follow the common
convention for LB methods and only retain the linear term. In the BGK approximation,
the distribution function relaxes towards the local equilibrium distribution \( f_i^{\text{eq}}(x, t) \) with
a single relaxation time \( \tau \). The collisions are instantaneous and result in distribution functions
\[
f_i^+(x, t) = f_i(x, t) + \frac{\Delta t}{\tau} [f_i^{\text{eq}}(\rho(x, t), \mathbf{u}(x, t)) - f_i(x, t)].
\]
(3.34)

Here, the local equilibrium populations \( f_i^{\text{eq}} \) depend only on the local density and velocity. Following common convention, we choose the local equilibrium \( f_i^{\text{eq}} \) as the expansion of the Maxwell-Boltzmann distribution up to second order in velocity [137]
\[
f_i^{\text{eq}}(\rho, \mathbf{u}) = w_i \rho \left(1 + \frac{c_i \cdot \mathbf{u}}{c_s^2} + \frac{1}{2} c_i Q_i : (\mathbf{u} \otimes \mathbf{u})\right),
\]
(3.35)
where \( c_s = \sqrt{k_B T/m} \) is the speed of sound and the weights \( w_i \) ensure that the first
three moments correctly reproduce the hydrodynamic variables [113]. We also define the tensor
\[
Q_i = c_i \otimes c_i - c_s^2 \mathbb{1}.
\]
(3.36)

To determine the weights \( w_i \), we require that the first three moments of the lattice distribution agree with fluid density, fluid velocity, and momentum flux tensor respectively. Furthermore, the weights have to be invariant under the discrete coordinate transformations that leave the lattice invariant. In particular, the weights for those directions that transform into each other under discrete rotations have to be equal. Then, the weights \( w_i \), lattice velocities \( c_i \), and the tensors \( Q_i \) show the following properties [113]
\[
\sum_i w_i = 1, \quad \sum_i w_i c_i = 0, \quad \sum_i w_i c_i \otimes c_i = c_s^2 \mathbb{1},
\]
(3.37a)
\[
\sum_i w_i Q_i = 0, \quad \sum_i w_i c_i \otimes Q_i = 0, \quad \sum_i w_i c_i \otimes c_i (Q_i : A) = c_s^4 (A + A^T),
\]
(3.37b)
for an arbitrary matrix \( A \). For the D3Q19 lattice introduced below, we insert the velocities \( c_i \) into these conditions and determine the weights \( w_i \). With these conditions the zeroth moment of the equilibrium distribution gives the density
\[
\sum_i f_i^{\text{eq}} = \rho,
\]
(3.38)
the first moment gives the current
\[
\sum_i f_i^{\text{eq}} c_i = \rho \mathbf{u},
\]
(3.39)
and finally, the second moment gives the Euler pressure tensor \[113\]
\[\sum_i f_i^{eq} c_i \otimes c_i = \rho c_s^2 + \rho u \otimes u. \tag{3.40}\]

The temperature is not associated with thermal fluctuations of the hydrodynamic fields as we consider the evolution of distribution functions. Only the speed of sound \(c_s\), as a measure of compressibility is important. Since the local equilibrium distributions are chosen to reproduce mass and momentum density, the collision rule conserves both mass and momentum. The combination of the BGK approximation with LBM, is also called the lattice Bhatnagar-Gross-Krook model.

After the collision, particles stream with their respective velocities to the adjacent lattice positions and we update the distribution functions as

\[f_i(x + c_i \Delta t, t + \Delta t) = f_i^*(x, t). \tag{3.41}\]

When we insert the distribution functions after the collision step (3.34) into Eq. (3.41), we arrive at the lattice Boltzmann equation

\[f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = \frac{\Delta t}{\tau} [f_i^{eq}(\rho(x, t), u(x, t)) - f_i(x, t)]. \tag{3.42}\]

The LBM as introduced, describes a force-free fluid. We include body forces \(g = \rho a\) in the LBM by modifying the velocity used to calculate equilibrium populations \[136, 139\]. Specifically, we center the equilibrium distribution around the velocity

\[u'(x, t) = u(x, t) + \tau a(x, t), \tag{3.43}\]

instead of the local fluid velocity \(u(x, t)\). We can understand this rule as follows: After inserting the modified equilibrium velocity (3.43) into Eq. (3.34), we obtain the post-collisional distributions

\[f_i^*(x, t) = \left(1 - \frac{\Delta t}{\tau}\right) f_i(x, t) + \frac{\Delta t}{\tau} f_i^{eq}(\rho(x, t), u'(x, t)). \tag{3.44}\]

Thereby, the fluid velocity after the collision, \(u^* = \sum_i f_i^* c_i\), is accelerated by \(a(x, t)\):

\[u^*(x, t) = \left(1 - \frac{\Delta t}{\tau}\right) u(x, t) + \frac{\Delta t}{\tau} u'(x, t), \tag{3.45}\]

\[= u(x, t) + \Delta t a(x, t). \tag{3.46}\]

In Ref. [136], this rule was used to drive the Poiseuille flow and to provide the interactions between two demixing fluids. Here, we implement the Poiseuille flow and the immersed boundaries described in Sect. [3.3.4] with this rule.
3. Mesoscopic simulations of fluid dynamics

Figure 3.7.: The D3Q19 lattice. Particles either move to the nearest neighbors (green) and next nearest neighbors (blue). Transitions to next next nearest neighbors (white) are not allowed.

To fully specify the LBM model, we also have to choose a discrete set of velocities. We require enough degrees of freedom to satisfy the conditions (3.37) [115, 140]. To correctly model the Navier-Stokes equations, we require the moments up to second order: density, velocity and the momentum flux tensor, in total 10 = 1 + 3 + 6 degrees of freedom. In a three-dimensional model where particles only move to the nearest neighbors we only have 7 degrees of freedom and hence are unable to correctly model hydrodynamics. By including next-nearest neighbors, we arrive at a total of 19 degrees of freedom, which can express all tensors up to second order. For moments of higher order however, the tensorial components are no longer independent. It is common to denote the choice of lattice by $D_dQ_q$, where $d$ denotes the dimensions of space and $q$ the degrees of freedom.

In this work we use the D3Q19 lattice with nearest and next-nearest neighbor connections illustrated in Fig. 3.7. The weights are given by $w_0 = 1/3$ for the rest particles, $w_{1-6} = 1/18$ for nearest neighbor jumps, and $w_{7-18} = 1/36$ for next-nearest neighbor jumps [113]. Furthermore, the speed of sound is also restricted by the lattice and is given by $c_s = \sqrt{1/3 \Delta x/\Delta t}$.

3.3.2. Chapman-Enskog expansion

The Chapman-Enskog (CE) expansion is a method to derive hydrodynamic equations from the microscopic dynamics of an interacting gas [141]. Since mesoscopic simulation methods are often based on microscopic gas dynamics, the CE expansion is a common tool to derive hydrodynamic equations for these methods [113, 119]. In this section, we discuss the derivation of the Navier-Stokes equations from the LBM equations, where we follow the discussion in Ref. [113].

The basic assumption underlying the CE expansion is that there is a separation between microscopic and macroscopic scales. For example, microscopic lengths $l$ appear much smaller when viewed from macroscopic scales (Fig. 3.8). To quantify this scale
3.3. The lattice Boltzmann method

Figure 3.8.: Schematic of the relationship between microscopic and macroscopic scales in the Chapman-Enskog expansion. On microscopic scales, molecular details are visible, whereas the system appears continuous on macroscopic scales. Similar, the microscopic length \( l \) appears much smaller when viewed from macroscopic scales. Therefore, we introduce the macroscopic length \( l_1 = \epsilon l \) with \( \epsilon \ll 1 \).

separation, we introduce the macroscopic lengths \( l_1 = \epsilon l \) with \( \epsilon \ll 1 \). Similar, we relate microscopic spatial positions \( x \) to macroscopic positions by \( x_1 = \epsilon x \). We also distinguish between microscopic and macroscopic time scales. However, we make the different macroscopic time scales associated with sound propagation and momentum diffusion explicit by introducing two macroscopic times scales. We describe sound propagation by the macroscopic time variable \( t_1 = \epsilon t \), whereas we describe momentum diffusion, as a much slower process, by the macroscopic time variable \( t_2 = \epsilon^2 t \). We interpret the distribution function of the LBM as a function of the macroscopic scales and write \( f_i(x_1, t_1, t_2) \). Here, we assume that the different time variables \( t_1, t_2 \) are formally independent.

In a single time step \( \Delta t \), a fluid particle with velocity \( c_i \) moves to position \( x_1 + c_i \epsilon \Delta t \), whereas the times advance as \( t_1 + \epsilon \Delta t \) and \( t_2 + \epsilon^2 \Delta t \). Then, the streaming step (3.41) becomes

\[
\frac{\Delta t}{\tau} f_i(x_1 + \epsilon c_i \Delta t, t_1 + \epsilon \Delta t, t_2 + \epsilon^2 \Delta t) = \frac{\Delta t}{\tau} [f_i^{eq}(\rho, u) - f_i(x_1, t_1, t_2)].
\]

Similarly, the lattice Boltzmann equation (3.42) on macroscopic scales becomes

\[
f_i(x_1 + \epsilon c_i \Delta t, t_1 + \epsilon \Delta t, t_2 + \epsilon^2 \Delta t) - f_i(x_1, t_1, t_2) = \frac{\Delta t}{\tau} [f_i^{eq}(\rho, u) - f_i(x_1, t_1, t_2)].
\]

A Taylor expansion up to second order in \( \epsilon \) results in

\[
\left[ \epsilon \left( \frac{\partial}{\partial t_1} + c_i \cdot \mathbf{V}_1 \right) + \epsilon^2 \frac{\partial}{\partial t_2} + \frac{1}{2} \epsilon^2 \left( \frac{\partial}{\partial t_1} + c_i \cdot \mathbf{V}_1 \right)^2 \right] f_i(x_1, t_1, t_2) + \mathcal{O}(\epsilon^3) = \frac{\Delta t}{\tau} [f_i^{eq}(\rho, u) - f_i(x_1, t_1, t_2)].
\]

59
We also expand the distribution function $f_i$ into orders of $\epsilon$

$$f_i(x_1, t_1, t_2) = \sum_{n=0}^{\infty} \epsilon^n f_i^{(n)}(x_1, t_1, t_2). \tag{3.49}$$

Since the collision rule preserves mass and momentum, the different orders of the distribution function have to satisfy \[113\]

$$f_i^{(0)} = f_i^{eq}, \tag{3.50}$$

$$\sum_i f_i^{(n)} = 0, \text{ for } n > 0, \tag{3.51}$$

$$\sum_i c_i f_i^{(n)} = 0, \text{ for } n > 0. \tag{3.52}$$

To derive the continuity equation (2.1) and the Navier-Stokes equations (2.3), we continue by substituting the expansion of the distribution function into Eq. (3.48). First, we collect terms by orders in $\epsilon$ and then take moments with respect to the set of discrete velocities $c_i$ up to first order. This procedure results in the equations of motion for the conserved quantities on macroscopic scales.

First, we consider the evolution of the mass density $\rho = \sum_i f_i$. In order $\epsilon$, we find

$$\frac{\partial}{\partial t_1} \rho + \nabla_1 (\rho \mathbf{u}) = 0. \tag{3.53}$$

In order $\epsilon^2$, we find

$$\frac{\partial}{\partial t_2} \rho = 0. \tag{3.54}$$

To obtain the equation of motion on the original scales, we use that the macroscopic coordinates are functions of the microscopic coordinates, $x_1 = x_1(x)$, $t_1 = t_1(t)$, $t_2 = t_2(t)$. For the density $\rho(x_1(x), t_1(t), t_2(t))$, we express the derivatives with respect to the microscopic coordinates as

$$\nabla \rho = \epsilon \nabla_1 \rho, \tag{3.55}$$

$$\frac{\partial}{\partial t} \rho = \left( \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \right) \rho. \tag{3.56}$$

After we insert Eqs. (3.53) and (3.54) into Eq. (3.56), we recover the mass continuity equation

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{3.57}$$
For the momentum density \( \rho \mathbf{u} = \sum_i f_i \mathbf{c}_i \), we follow similar steps to obtain the conservation law for momentum:

\[
\frac{\partial}{\partial t} \rho \mathbf{u} + \nabla \cdot \Pi = 0,
\]

with the momentum flux tensor

\[
\Pi = \sum_i f_i^{(0)} \mathbf{c}_i \otimes \mathbf{c}_i + \left[ 1 - \frac{\Delta t}{2\tau} \right] \epsilon \sum_i f_i^{(1)} \mathbf{c}_i \otimes \mathbf{c}_i.
\]

The stress tensor \( \Pi^{(0)} \) only includes equilibrium contributions, since \( f_i^{(0)} = f_i^{eq} \), and simplifies to the Euler stress for an ideal gas (3.40)

\[
\Pi^{(0)}_{ij} = p \delta_{ij} + \rho u_i u_j,
\]

with internal pressure \( p = c_s^2 \rho \). This result justifies identifying \( c_s \) with the speed of sound. The stress tensor \( \Pi^{(0)} \) has no viscous contributions. They only enter at the level of the nonequilibrium stress tensor, which we express as

\[
\Pi^{(1)}_{ij} = -\tau c_s^2 \rho \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right],
\]

where we neglect terms of third order in \( \mathbf{u} \) as we assume low Mach numbers. Combining both equilibrium and nonequilibrium contributions, we reproduce the momentum flux of the Navier-Stokes equations (2.4)

\[
\Pi_{ij} = \rho u_i u_j + p \delta_{ij} - \eta \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right],
\]

where we define the dynamic shear viscosity as

\[
\eta = c_s^2 \rho \left( \tau - \frac{1}{2} \Delta t \right).
\]

### 3.3.3. Lattice aligned boundaries

The boundary conditions proposed for the LBM fall into two classes [142]: those for which the boundary node does not evolve according to the LBM, and those for which the boundary node does. A typical example for the first kind is the bounce-back rule, for which the boundary is located halfway between fluid node and boundary node [115]. In this work, we use the regularized boundary condition introduced by Latt et al. [142], an
example of the second kind. Here, the boundary node is updated according to Eq. (3.42) and the boundary is located directly on the node.

The distribution function at the boundary is a priori unknown and we have to determine it such that the macroscopic no-slip condition holds. The regularized boundary condition by Latt et al. splits the distribution function into an equilibrium $f_{bb,i}^{(0)}$ and off-equilibrium part $f_{bb,i}^{(1)}$, similar to the Chapman-Enskog expansion discussed in the previous section. After the distribution function at the boundary node has been set, it participates in both collision and streaming step.

We choose the zeroth order equal to the equilibrium distribution with the desired surface velocity $u_s$ and density $\rho_s$ [142]

$$f_{bb,i}^{(0)} = f^{(eq)}(u_s, \rho_s).$$

(3.64)

However, as discussed in the previous section the equilibrium contributions fail to produce viscous behavior. To correctly account for the viscous contributions at the boundary, we apply the off-equilibrium bounce-back rule [143]. It introduces an additional stress tensor

$$\Pi_{bb}^{(1)} = \sum_i f_{-i,i}^{(1)} c_i \otimes c_i,$$

(3.65)

where we defined the negative indices $-i$ such that $c_{-i} = -c_i$. The additional stress tensor defines the nonequilibrium contribution to the boundary condition via [142]

$$f_{bb,i}^{(1)} = \frac{u_i}{2c_s^2} Q_i \cdot \Pi_{bb}^{(1)}.$$  

(3.66)

With the properties of the tensor $Q_i$ (3.37), the distribution function $f_{bb,i}^{(1)}$ does not change the fluid density or velocity. Concretely, it obeys $\sum_i f_{bb,i}^{(1)} = 0$ and $\sum_i f_{bb,i}^{(1)} c_i = 0$. The full distribution function $f_{bb,i} = f_{bb,i}^{(0)} + f_{bb,i}^{(1)}$ correctly reproduces the no-slip condition as shown in [142] and verified in Sect. 3.3.6.

### 3.3.4. The immersed boundary method

As the LBM is a grid based method, the boundaries of colloidal particles never exactly align with the grid structure. Consider for example the situation shown in Fig. 3.9a. A possible solution is to discretize the boundary such that it always aligns with the lattice [144], with the disadvantage that the colloid surface gains unphysical edges. Here, we use the immersed boundary method (IBM) as an alternative to couple the colloidal particle to the LBM fluid [105, 145]. Originally developed for the finite-difference approximation of the Navier-Stokes equations [105], the immersed boundary method is compatible with different computational fluid dynamics methods [145]. We use a specific variant developed by [Inamuro] to model hard particles inside the LBM fluid [146]. The basic idea
3.3. The lattice Boltzmann method

behind the IBM is to smooth out the interface such that it has a finite width. Fig. 3.9a illustrates the smoothed interface. While the sharp interface does not overlap with the lattice, the smoothed interface overlaps with several lattice nodes at the same time.

We represent the interface of the colloidal particle by a triangular mesh, which we obtain by successive refinement of an icosahedron. In particular, we split each triangle into four new triangles until all triangles sides are smaller than the grid length. After each splitting, we move the vertices to the surface of the colloidal particle.

We couple the surface vertices to the lattice by using the smoothed delta function \( \delta_h(x) \) proposed by Peskin [105]. It is a product of individual delta functions for each coordinate direction, \( \delta_h(x) = \phi(x/\Delta x)\phi(y/\Delta x)\phi(z/\Delta x) \), where we define the one-dimensional smoothed delta function as

\[
\phi(x) = \begin{cases} 
\frac{1}{8} \left( 3 - 2|x| + \sqrt{1 + 4|x| - 4x^2} \right) & \text{if } 0 \leq |x| \leq 1, \\
\frac{1}{8} \left( 5 - 2|x| - \sqrt{-7 + 12|x| - 4x^2} \right) & \text{if } 1 \leq |x| \leq 2, \\
0 & \text{if } 2 \leq |x|.
\end{cases}
\]  

We plot the one-dimensional delta function \( \phi(x) \) in Fig. 3.9b. The specific form of \( \phi(x) \) is necessary to ensure stability if used with finite-difference methods [105]. While the restriction does not apply to the LBM, we choose to keep this form.

The IBM tries to update the fluid velocity such that it obeys the no-slip condition on the particle surface. To this end, we introduce a penalty force acting on the fluid and designed to ensure that fluid velocity and surface velocity are equal. We continue in three steps: First, we interpolate the fluid velocities to the mesh vertices. Then, we define the penalty force for each mesh vertex. Finally, we interpolate the penalty force to the fluid. We use the smoothed delta function introduced above to evaluate the fluid

Figure 3.9.: (a) Schematic of the coupling between the surface of the colloidal particle (red) and the underlying grid (black dots) in the IBM. (b) The one-dimensional smoothed delta function \( \phi(x) \) proposed by Peksin.
velocity at the mesh vertex \( x_i^m \) by interpolating it as

\[
u_i^m = \sum_j \delta_h(x_i^m - x_j)u_j.
\] (3.68)

In general, the velocities of the fluid \( u_i^m \) and of the mesh vertex \( v_i^s \) differ. We enforce the no-slip boundary condition (Sect. 2.2.5) with a penalty force acting on the fluid on the vertex \( x_i^m \)

\[
f_i^m = \frac{1}{\Delta t} (v_i^s - u_i^m).
\] (3.69)

The penalty forces \( f_i^m \) act on the fluid as the interpolated body forces

\[
f_i = \sum_j \delta_h(x_i - x_j^m)f_j^m.
\] (3.70)

This penalty force brings the vertex velocity exactly to the fluid velocity in a single time-step, if the mesh vertex and fluid node exactly overlap and the delta function had no finite width. However, the finite width of the delta function introduce spurious slip. To improve the no-slip condition, we iteratively refine the penalty forces. After we apply the penalty force onto the fluid, we start anew. After each application of the IBM rule, the slip velocity becomes smaller and the boundary condition improves. Here, we use in total five iterations as suggested by Inamuro [146]. Finally, we use the penalty forces and modify the equilibrium distribution in the collision step as in Eq. (3.43).

To conserve linear and angular momentum, the penalty forces exerted on the fluid have to affect the colloidal particle with equal magnitude but opposite sign. The sum of the vertex contribution over all IBM iterations results in force and torque experienced by the colloid. If we denote the penalty force at vertex \( i \) in iteration \( j \) by \( f_{i,j}^m \), the fluid exerts on the particle the force and torque

\[
\mathbf{f}_{\text{fluid}} = - \sum_{i,j} f_{i,j}^m,
\] (3.71)

\[
\mathbf{T}_{\text{fluid}} = - \sum_{i,j} (x_i^m - r_c) \times f_{i,j}^m.
\] (3.72)

Here, \( r_c \) is the center of mass of the colloid. The fluid force defined in terms of the penalty forces, has two contributions. We find fluid nodes both outside the particle but also inside the colloidal particle (Fig. 3.9a). The penalty forces contain contributions from both, the fluid outside and inside. To correct for the internal fluid, we use Feng’s rigid body approximation [147]. It assumes that the fluid inside the colloidal particle moves as a rigid body and introduces a force and a torque to match the change in particle
3.3. The lattice Boltzmann method

(angular) velocity,

\[
f_{\text{Feng}}(t) = \frac{M}{\Delta t} (v(t - \Delta t) - v(t)), \tag{3.73}
\]

\[
T_{\text{Feng}}(t) = \frac{I}{\Delta t} (\Omega(t - \Delta t) - \Omega(t)). \tag{3.74}
\]

For an incompressible fluid, the correction forces balance the forces from the internal fluid exactly. However, the torque is an approximation even for an incompressible fluid.

Finally, we update the colloid with the Euler scheme \[133\]

\[
r(t + \Delta t) = r(t) + \Delta t v(t), \tag{3.75}
\]

\[
v(t + \Delta t) = v(t) + \Delta t M^{-1} (f_{\text{fluid}} + f_{\text{Feng}} + f_{\text{ctl}}), \tag{3.76}
\]

\[
\Omega(t + \Delta t) = \Omega(t) + \Delta t I^{-1} (T_{\text{fluid}} + T_{\text{Feng}} + T_{\text{ctl}}), \tag{3.77}
\]

where we already introduced the control force \(f_{\text{ctl}}\) and control torque \(T_{\text{ctl}}\) used in later chapters.

3.3.5. Choice of parameters

Three parameters determine the properties of the combined LBM-IBM, the lattice spacing \(\Delta x\), the time step \(\Delta t\), and the relaxation time \(\tau\). We choose the lattice spacing to obtain the desired spatial resolution and the time step such that we reproduce the desired Mach number \(M_a\), defined in Sect. 2.2.2. For reasons of computational efficiency, we are not able to reach physical Mach numbers. However, we can certainly reach \(M_a \leq 0.1\).

Following the discussion in Sect. 2.2.2, we expect density variations of about 1 % for this Mach number. We choose the relaxation time such that we reproduce the correct Reynolds number. However, the combined LBM-IBM method is no longer accurate for \(\tau > \Delta t\) and additional slip occurs [148, 149]. We therefore lower the Mach number until \(\tau = \Delta t\). This procedure improves the incompressibility of the scheme and as such is beneficial. We give the exact parameters used in this work in Appendix E.

3.3.6. Validation

We verify that the proposed LBM method reproduces the correct Poiseuille flow profile for a channel with rectangular cross section in Fig. 3.10. We use the simulation parameters \[P4\] given in appendix E. For all aspect ratios, we observe excellent agreement between theory and simulation.

For a small colloidal particle, \(a = 0.1 w\), we verify Faxén’s law for the translational velocity (2.33) and the angular velocity (2.34). We simulate at channel Reynolds number \(Re = 10^{-3}\). We discretize the channel by \((126, 380, 126)\) lattice sites in \(x, y, z\) direction. We choose a Mach number \(M_a = 2.31 \times 10^{-6}\) and the relaxation time satisfies \(\tau = \Delta t\).
3. **Mesoscopic simulations of fluid dynamics**

![Image of axial fluid velocity for a rectangular Poiseuille flow along the x axis (a) and y axis (b). The solid lines show the analytic solution (2.26). The dots show the simulations results at selected points.](image1)

![Image of translational velocity (a) and angular velocity (b) of a colloidal particle with a/w = 0.1 in a rectangular Poiseuille flow at channel Reynolds number Re = 10^-3. The red lines show the expected value according to Faxén’s law.](image2)

Figure 3.10.: Axial fluid velocity for an rectangular Poiseuille flow along the x axis (a) and y axis (b). The solid lines show the analytic solution (2.26). The dots show the simulations results at selected points.

Figure 3.11.: The translational velocity (a) and angular velocity (b) of a colloidal particle with a/w = 0.1 in a rectangular Poiseuille flow at channel Reynolds number Re = 10^-3. The red lines show the expected value according to Faxén’s law.
We plot the results in Fig. 3.11, where we find excellent agreement between the expected and observed values. Deviations occur only close to the channel wall, where Faxén’s law loses its validity.

3.4. Measuring inertial lift forces

In the following chapters, we apply both MPCD and LBM to determine inertial lift forces. We describe how we measure the inertial lift forces for both methods in this section. In inertial focusing, the colloidal particle moves along the channel axis with axial velocity $v_z$ and migrates laterally under the influence of the inertial lift force $f_{\text{lift}}$. To measure the inertial lift force, we keep the particle at a fixed lateral position, while it moves unconstrained in axial direction. We then identify the lateral momentum transfer $\Delta p_\perp$ from the fluid to the colloid during time step $\Delta t$ with the lift force via

$$f_{\text{lift}} = \frac{\Delta p_\perp}{\Delta t}.$$  

(3.78)

When we also apply an axial control force as in Sects. 5.1 and 5.2, the momentum transfer in axial direction balances the applied control force. To account for all momentum transfer in MPCD, we include both the momentum transferred in the streaming step and the collision step as explained in Sect. 3.2.3. In LBM we identify the lift force with the lateral components of the penalty forces introduced in Sect. 3.3.4. A similar procedure to determine the lift forces has also been used in Ref. [22].

MPCD is a stochastic simulation method and all measurements carry an inherent uncertainty. We estimate the standard error of the lift force and axial velocity by averaging over $N_{\text{sim}}$ independent simulations. First, we calculate the mean lift force $f_{\text{lift},i}$ for simulation $i$. Then, we determine the lift force averaged over simulations $\bar{f}_{\text{lift}} = \frac{1}{N_{\text{sim}}-1} \sum_{i=1}^{N_{\text{sim}}} f_{\text{lift},i}$. Finally, we estimate the standard error as the square root of the variance

$$\sigma^2_{f_{\text{lift}}} = \frac{1}{N_{\text{sim}}-1} \sum_{i=1}^{N_{\text{sim}}} \left( f_{\text{lift},i} - \bar{f}_{\text{lift}} \right)^2.$$  

(3.79)

We estimate the standard error of the axial velocity in the same manner.

As we show in Sect. 4.1.2.1, we can determine the equilibrium position and approximate magnitude of the lift forces from the particle probability densities. We determine them in MPCD by collecting samples $x_i$ of the particle position while it moves freely. From the samples, we determine the probability density by using Kernel-Density estimates, explained in Appendix B.
3.5. Software used

For MPCD, we wrote our own C++ code. A noteworthy detail is the fact that the algorithm is mainly limited by memory access and the algorithm to generate Gaussian random numbers. Here, rewriting the algorithm to use as few memory traversals as possible is highly advantageous. Direct implementation of the MPCD-AT+a collision rule results in three iterations over the particles and three iterations over the collision cells. By rearranging the computations, we are able to perform the collision steps by iterating once over all particles, once over the collision cells and finally once more over the particles. We further improve the program performance by using the Ziggurat algorithm [150] [151] for the generation of Gaussian random numbers instead of the commonly used Box-Müller transform [133] [151]. Compared to the implementation with six iterations using the Box-Mueller algorithm, we achieve a speed up of about three times for the collision step alone and a speed up of about two times for the complete simulation.

For the LBM, we use the open source Palabos code [152] with minor modifications. The Palabos code is written in C++ and has a special emphasis on extendability and parallelizability. We supplement the Palabos code with custom modules to include the colloidal particles using the IBM. In particular, we added periodic boundary conditions of the immersed boundary method and implemented the Euler integrator for the colloidal equations of motion.
The features of inertial focusing strongly depend on the channel geometry. In this chapter, we investigate the profiles of inertial lift forces in straight channels with different cross sections. First, we investigate channels with circular cross sections using multi-particle collision dynamics. The high symmetry of the system allows us to focus on the basics of inertial migration. Second, we investigate channels with rectangular cross sections. The reduced symmetry of the system strongly modifies the inertial lift forces and we discuss the implications for the design of devices in inertial microfluidics.

The results presented in this chapter have been published for channels with circular cross section in [A], for channels with rectangular cross section in [C].

4.1. Circular channel cross sections

Microfluidic devices are commonly fabricated by optical lithography [4] and therefore often feature channels with rectangular cross sections [4, 153]. Still it is worthwhile to consider inertial microfluidics in channels with circular cross sections. First, the high symmetry of circular cross sections greatly reduces the complexity of the system and allows us to concentrate on the basics of inertial focusing. Second, early experiments in inertial migration [7–9] and experiments in non-inertial microfluidics [154–157] used channels with circular cross sections.

In the following, we consider a spherical colloidal particle with radius $a$ inside a channel with circular cross section (Fig. 4.1). The channel has radius $R$ and length $L$ with periodic boundary conditions applied along the direction of the channel axis. We choose a cylindrical coordinate system $(r, \phi, z)$ with the $z$ axis coinciding with the channel axis. The lateral distance from the channel axis gives the radial position $r$. The results were obtained from simulations with multi-particle collision dynamics (MPCD) (Sect. 3.2) using parameters [P1] given in appendix E.

4.1.1. Probability distributions

At low flow speeds, the Reynolds number becomes small and fluid inertia is negligible. Then, flow is described by the Stokes equation (2.14) and colloidal particles do not experience an inertial lift force (Sect. 2.4.3). In a deterministic system, the particles follow the
4. **Channel geometry and inertial focusing**

**Figure 4.1.** (a) Schematic of inertial focusing for colloidal particles in channels with circular cross sections. The channel has radius $R$ and is filled by a Newtonian fluid. (b) The plane spanned by the channel axis (dashed) and the colloidal particle. The particle has radius $a$ and radial distance $r$ from the channel center. It moves with velocity $v_z$ parallel to the streamlines and experiences the inertial lift force $f_{\text{lift}}$ perpendicular to streamlines.

**Figure 4.2.** Typical particle positions in the channel cross section for different Reynolds numbers $\text{Re}$ and particle sizes $a/R$. Each plot shows particle positions obtained from different independent runs at different time steps. In all plots particles order on a Segré-Silberberg annulus.
4.1. Circular channel cross sections

Figure 4.3.: Radial distribution function $P(r)$ as a function of radial position $r/R$, (a) for increasing Reynolds number at fixed particle sizes $a/R = 0.5$ and $a/R = 0.2$ (inset) and (b) for increasing particle size at fixed Reynolds numbers $Re = 40$ and $Re = 20$ (inset).

streamlines of the Poiseuille flow without lateral migration. With thermal fluctuations, we expect a flat uniform distribution in steady state. However, as flow speeds increase, we can no longer neglect fluid inertia and inertial lift forces cause the particle to migrate laterally \cite{10}. We plot the center of mass position of the colloidal particle for different times in Fig. 4.2. The distributions are markedly nonuniform and show the form of the Segré-Silberberg annulus \cite{7}. The shape of the distribution strongly depends on particle size and Reynolds number. In particular, the width of the distribution is remarkably sharp for particle radius $a/R = 0.5$ and Reynolds number $Re = 40$.

To analyze this dependence in detail, we exploit the symmetry of the system and plot the radial probability distribution $P(r)$ in Fig. 4.3. We estimate the radial probability distributions from the position of the particle with the method of kernel density estimates introduced in appendix \ref{b}. To accommodate for the different simulation parameters used, we normalize the radial probability distributions for $Re = 40$ by the Péclet number $Pe = \frac{\rho \nu^2 R}{k_B T}$. We first concentrate on a fixed particle size at different Reynolds numbers (Fig. 4.3a). The distribution changes from a flat distribution at Reynolds numbers $Re \leq 1$ towards a strongly peaked distribution at higher Reynolds numbers. At the same time, the peak of the distribution shifts towards the channel wall with increasing Reynolds number. In Fig. 4.3b, we analyze how the particle size influences the radial distribution function for fixed Reynolds number. The distribution becomes much narrower and its peak shifts towards the channel center for increasing particle size. We interpret the shift of the peak

\footnote{To reach Reynolds number $Re = 40$, we use parameters different from those used in the remaining simulations. We normalize the radial distributions $P_{40}(r)$ by the Péclet number $Pe = \frac{\rho \nu^2 R}{k_B T}$. The normalized distribution reads $\hat{P}_{40}(r) \propto P_{40}(r)^{Pe_{40}/Pe}$, where $Pe_{40}$ is the Péclet number for $Re = 40$ and $Pe$ is the Péclet number for the remaining simulations. We justify this procedure in Sect. 4.1.2.1.}
4. Channel geometry and inertial focusing

Figure 4.4.: (a) Main characteristics of the radial distribution functions $P(r)$ for two different Reynolds numbers $Re$. The main plots show, the half width at full maximum $b/R$ as a function of particle size $a/R$. The dashed line indicates the scaling with particle size. The inset shows the maximum of the distribution $r_{\text{max}}/R$ versus the particle size $a/R$. (b) Joint Probability distribution $P(r, v_z)$ for a particle size $a = 0.2R$ and Reynolds number $Re = 20$. The black lines show the isocontours of probability. The blue dashed line shows the axial velocity as determined in Sect. 4.1.2, while the red line shows the position dependent mean axial velocity determined from the distribution as described in Sect. 4.1.1.

as the interplay between excluded volume and increased hydrodynamic interactions with the channel wall.

The distributions are unimodal and strongly peaked for most parameters. Hence, they are well characterized by the peak position $r_{\text{max}}$ and the full width at half maximum $b$ around the peak. We define the full width at half maximum as the difference $b = |r_{+1/2} - r_{-1/2}|$, where we introduced the radial positions $r_{\pm 1/2}$ at which the probability density assumes half the value of its peak, $P(r_{\pm 1/2}) = P(r_{\text{max}})/2$. We plot both characteristics in Fig. 4.4a. The main plot show the full width at half maximum $b/R$ versus the particle size $a/R$, while the inset shows the peak position $r_{\text{max}}/R$ versus the particle size $a/R$. The width of the distribution follows the power law $b/R \propto (a/R)^{-1.75}Re^{-0.92}$. The exponents are in good agreement with the scaling properties of the lift force, as we discuss in Sect. 4.1.2.1. The peak of the distribution shifts towards the channel center in an approximately linear fashion. Here, the smallest particle with radius $a = 0.2R$ experiences the highest fluctuations and, therefore, the corresponding peak position deviates from the linear behavior. Further, the peak positions move slightly closer towards the channel wall with increasing Reynolds number.

Just like the position, the axial velocity of the colloidal particle too undergoes random fluctuations. In the same way, we estimated the radial distribution function from the radial position of the particle, we also estimate the joint probability distribution $P(r, v_z)$
4.1. Circular channel cross sections

Figure 4.5.: Radial lift force \( f_{\text{lift}} \) versus particle position \( x \) for different particle sizes \( a \) at Reynolds numbers \( \text{Re} = 40 \) (a) and \( \text{Re} = 20 \) (b). The filled background indicates the range of one standard error \( \sigma \) estimated by Eq. (3.79).

from the position and velocity of the particle. We plot \( P(r, v_z) \) in Fig. 4.4b for a particle size \( a = 0.2R \) and Reynolds number \( \text{Re} = 20 \). With help of the joint probability distribution, we can determine, for example, the mean axial particle velocity \( \bar{v}_z^P(r) \) at radial position \( r \) by the conditional average \( \bar{v}_z^P(r) = \int dv_z \, v_z \, P(r, v_z) \). We plot this position dependent mean value as the red line in Fig. 4.4b and compare it with the axial velocity determined in Sect. 4.1.2 plotted as the blue line. While both values agree well for this particular example, it is difficult to use for other parameters. For most parameters the radial probability distributions are highly peaked (Fig. 4.3), hence radial positions far away from the peak have a low number of samples. For this reason, estimating the velocity directly from the trajectories incurs a high variance. We remedy this problem in the following section by introducing additional constraints to improve the number of samples for a given position.

4.1.2. Radial lift forces and axial velocity

In this section, we measure the radial lift forces acting on the particle by keeping its position to a fixed radius, as described in Sect. 3.4. We discuss how to relate the radial probability distributions to the lift forces in the next section.

We plot the lift force as a function of radial position for different particle sizes at Reynolds number \( \text{Re} = 40 \) in Fig. 4.5a and at lower Reynolds number \( \text{Re} = 20 \) in Fig. 4.5b. The lift forces we measured agree qualitatively with lift forces reported in the literature. In particular, they show the same features as lift forces calculated for channels with square and rectangular cross sections in finite-element simulations [22, C] and the those obtained by a matched asymptotic expansion [20, 21]. The lift forces all result in the same basic dynamics: the channel center \((r = 0)\) is an unstable equilibrium position and
4. Channel geometry and inertial focusing

Figure 4.6.: (a) Radial lift force $f_{\text{lift}}$ versus particle positions $r$ normalized by the scaling factor introduced in the text. Shown are the lift forces for different particle sizes at Reynolds number $Re = 40$ (solid lines) and $Re = 20$ (dashed lines). We did not use the lift force values for $a/R = 0.2$, $Re = 20$ to determine the scaling coefficient. (b) Axial velocity $v_z$ normalized by the undisturbed flow profile $u_z$ versus the radial position $r$ for different particle sizes $a$ at Reynolds numbers $Re = 20$ (open symbols) and Reynolds number $Re = 40$ (closed symbols). As the standard error of the axial velocities is close to the symbol size, we do not plot it. The inset shows the difference between particle velocity and undisturbed flow velocity at the channel center. It scales with the particle size as $(a/R)^{1.68}$.

particles migrate towards the channel wall. However, close to the channel wall, the wall lift forces push particles back towards the channel center. Both lift force contributions cancel at the stable equilibrium position $r_{eq} \approx 0.5R$. Due to the continuous rotational symmetry, this stable equilibrium position in radial direction is degenerate in the full cross section. This degeneracy causes the formation of the Segré-Silberberg annulus in Fig. 4.2. The magnitude of the lift forces strongly increases with the Reynolds number and particle size. Experiments use this fact to perform particle separation [15, 60]. The stable equilibrium position shifts closer towards the channel center with increasing particle size and closer towards the channel walls with increasing Reynolds number. Previous studies of inertial migration in channels with rectangular cross sections [22] observe the shift with particle size too. The shift with Reynolds number has been observed in simulation [22, 53] and studies using the matched asymptotic expansion [21, 72].

For applications, it is important how the magnitude of inertial lift forces changes with particle size and Reynolds number. A common approach is to summarize this behavior in terms of scaling laws of the form $f_{\text{lift}} \propto Re^n (a/R)^m$ inspired by studies using the matched asymptotic expansion (Sect. 2.4.4). We use the lift force values shown in Fig. 4.5 up to a radial position $r = 0.2R$ to fit the scaling law. Since fluctuations for $a = 0.2R$, $Re = 20$ are large, we do not use it in the fitting procedure. We choose the scaling with Reynolds
number as \( n = 2 \), consistent with inertial lift forces. The exponent connected to the scaling with particle size takes a value of \( m \approx 3.13 \). When normalized by the scaling coefficient the lift forces collapse onto a single master curve close to the channel center (Fig. 4.6a). This is consistent with previous simulations by Di Carlo et al. [22], where they found an exponent \( m = 3.28 \) for circular channels.

We plot the axial velocity of the colloidal particle normalized by the undisturbed flow velocity in Fig. 4.6b. The values for both Reynolds numbers, \( \text{Re} = 20 \) and \( \text{Re} = 40 \), collapse. Close to the channel center, the graphs are almost horizontal, indicating that the axial velocity of the particle is close to a parabolic profile. However, the axial velocity is always lower than the undisturbed flow velocity. The axial velocity further decreases with increasing particle size and decreasing distance to the channel wall. We fit the velocity at the channel center to \( \bar{v}_z(0)/u_{\text{max}} \approx 1 - (a/R)^{1.68} \) (Fig. 4.6b inset), implying that Faxén’s law (2.33) does no longer describe the velocity. The breakdown of Faxén’s law is a consequence of the large particle size, for which the disturbance flow is significant.

4.1.2.1. From lift forces to radial distribution functions

Now, we have two different views on the same system. Without constraints, we obtain the radial distribution functions. With constraints, we are able to measure the radial lift forces. By interpreting the unconstrained particle motion in terms of diffusion in the radial potential connected to the inertial lift forces, we connect both views and show that they are indeed consistent. Further, we verify that the lift forces obtained by constraining the particle are able to describe the free particle motion.

If we assume that the particle motion is described by the Langevin equation (2.54), the radial position \( r \) and the lateral velocity \( v_\perp \) of the particle follow in steady state the distribution (2.65)

\[
P(r, v_\perp) = \frac{1}{Z} \exp \left[ -\frac{1}{2k_B T} |v_\perp|^2 \right] \exp \left[ -\frac{1}{k_B T} V(r) \right],
\]

where we obtain the potential \( V(r) \) connected to the radial lift force by the integral

\[
V(r) = - \int_0^r \text{d} r' f_{\text{lift}}(r').
\]

We evaluate the integral by the trapezoidal integration rule [133]. For particle suspensions, similar approaches were discussed in Refs. [20, 158].

We compare the radial probability distributions calculated from the lift forces and the probability distributions for the radial position in Fig. 4.7a and for the lateral velocity in Fig. 4.7b. Even though the lift force and axial velocity are only known at a moderate number of positions (indicated by the symbols), all curves agree well for the different particle sizes and Reynolds numbers. The form of the steady-state distributions hinges
4. Channel geometry and inertial focusing

Figure 4.7.: The probability distribution of radial position $P(r)$ (a) and of lateral velocity $P(v_{\perp})$ (b). The dashed line gives the distribution expected from the Maxwell-Boltzmann distribution, the solid line shows the result from simulations. We determined the lift forces at the positions indicated by markers.

on the Fluctuation-Dissipation theorem. Although, we consider a system driven out of equilibrium, this assumption yields excellent results.

With this relation of lift force to radial distribution function, we are able to discuss the connection between the scaling of the lift forces (previous section) and the width of the distribution (Sect. 4.1.2). If the distributions are sufficiently narrow, only the lift force close to the equilibrium position $r_{eq}$ is relevant, which we linearize as $f(r) \approx -f_0(r-r_{eq})/R$. The prefactor $f_0$ gives the overall magnitude and scales like the lift force. The linear lift force corresponds to a harmonic potential and the probability density in steady state reduces to

$$P(r, v_{\perp}) = \frac{1}{Z} \exp \left[ -\frac{1}{2} \frac{m}{k_B T} |v_{\perp}|^2 \right] \exp \left[ -\frac{1}{2} \frac{(r-r_{eq})^2 f_0 R}{R^2 k_B T} \right]. \quad (4.3)$$

Then, the radial position $r/R$ is Gaussian with mean $r_{eq}/R$ and variance $\sigma^2 = k_B T/f_0 R$. Given this form of the distribution and the fore scaling, $f_0 \propto \text{Re}^2 (a/L)^m$, the width of the distribution scales as $b/R \propto \text{Re}^{-1} (a/L)^{-m/2}$. In the previous sections, we found the scaling of the distribution width $b/R \propto (a/R)^{-1.75} \text{Re}^{-0.92}$ and the scaling of the lift force $f_0 \propto \text{Re}^2 (a/R)^{3.13}$. Both scaling behaviors agree nicely with only minor discrepancies. The most likely cause for the discrepancy is the difference in positions we determined the scaling at. For the scaling of the lift force, we used positions close to the channel center. For the scaling of the distribution width, we used positions close to the stable equilibrium position.

Finally, we explain how the MPCD parameters influence the distributions. We nondimensionalize the lift force by the factor $\rho \nu^2$. Then, it is independent of the fluid properties and only depends on the dimensionless quantities Reynolds number $\text{Re}$, relative particle
4.2. Rectangular channel cross sections

Devices in microfluidics often use channels with rectangular instead of circular cross sections [4, 10]. For inertial focusing, the loss of symmetry associated with going from circular to rectangular cross sections has a number of important implications. First, we no longer observe the Segré-Silberberg annulus connected to the degenerate stable equilibrium position. In contrast, the particle collects at a set of discrete equilibrium positions. Furthermore, the aspect ratio of the cross section strongly influences the placement and even the number of the equilibrium positions. In particular, for channels with a low aspect ratio, only two stable equilibrium positions remain. Many experiments exploit the reduction to only two stable equilibrium positions [12, 15, 60, 68].

In the following, we consider the profiles of inertial lift forces acting on a colloidal particle with radius $a$ inside a channel with rectangular cross section with width $2w$ and height $2h$ (Fig. 4.8). The maximum fluid velocity $u_{\text{max}}$ at the channel center determines the channel Reynolds number $\text{Re} = 2wu_{\text{max}}/\nu$. We restrict the discussion to upper right quadrant indicated by the red area in Fig. 4.8. The full lift force profile results from the symmetry of the problem. We choose the coordinate system such that the $z$ axis coincides with the channel axis and the origin ($x = 0, y = 0$) coincides with the center of the channel cross section. The results were obtained by lattice Boltzmann simulations, using the parameters given in appendix E if not otherwise stated.

In Fig. 4.9 we plot the lift forces for a particle with radius $a = 0.4w$ in a channel flow with Reynolds number $\text{Re} = 10$ for different channel cross sections. We discuss the relevant features for square and rectangular cross sections in the following sections.
4. Channel geometry and inertial focusing

Figure 4.8.: (a) Schematic of inertial focusing of colloidal particles in channels with rectangular cross section. The channel has width $2w$ and height $2h$. The origin of the coordinate system ($x = 0$, $y = 0$) coincides with the center of the cross section (green dot). The red area shows the part of the cross section in which we determine the inertial lift forces. (b) The $y = 0$ plane. The colloidal particle has radius $a$ and lateral position $x$. It moves with axial velocity $v_z$ parallel to the undisturbed stream lines and experiences the inertial lift force $f_{\text{lift}}$ perpendicular to the stream lines. Further, it rotates with angular velocity $\Omega$.

4.2.1. Square channel cross sections

In channels with square cross sections ($w/h = 1$), there is only a discrete rotational symmetry replacing the continuous symmetry of circular cross sections. Fig. 4.9a shows the inertial lift force profile for a particle with size $a = 0.4w$ at channel Reynolds number $Re = 10$. The main features of inertial focusing remain. The channel center is an unstable equilibrium position and the channel walls repel the particle. The equilibrium positions however mirror the loss of symmetry. In contrast to the continuous degeneracy of the circular cross section, we only observe a set of discrete equilibrium positions with different stabilities. In the complete cross section, obtained by mirroring the upper quadrant, we find one unstable equilibrium position in the channel center, four stable equilibrium positions on the diagonals and four equilibrium positions with saddle node stability on the main axes. We still observe an almost circular annulus in the form of the unstable manifold of the saddle nodes. The migration occurs in two steps. First, the particle quickly migrates to the unstable manifold. Then, it slowly approaches one of the stable equilibrium positions. Here, we observe stable equilibrium positions placed on the diagonals of the channel, which have not been observed in experiments [22, 54], but in numerical simulations [53, 55]. We further comment on this fact below.

We analyze the equilibrium positions by plotting their distance $d_{\text{eq}} = |x_{\perp,\text{eq}}|$ from the channel center together with their stability as a function of particle size for different Reynolds numbers in Fig. 4.10a. The symmetry of the system results in equilibrium positions on the main axes and the diagonals for all parameters. However, the distance
Figure 4.9.: Cross sectional lift force profiles for different aspect ratios. (a) $w/h = 1$, (b) $w/h = 1/2$, (c) $w/h = 1/3$ at Reynolds number $Re = 10$ and particle size $a = 0.4w$. The gray lines show the trajectories for an unconstrained particle. The white squares indicate positions where we do not show the lift forces, as they exceed $0.35\rho u^2$. We further show the equilibrium positions and their stability.
4. Channel geometry and inertial focusing

Figure 4.10.: (a) Distance \( d_{\text{eq}} = |x_{\perp,\text{eq}}| \) of the equilibrium positions from the channel center as a function of particle size \( a \) for a channel with square cross section at different Reynolds numbers \( \text{Re} \). We find equilibrium positions on the diagonal and the \( x \) axis. The symbols indicate the stability of the equilibrium positions. (b) Lateral probability density of the particle in a channel width square cross section for \( a = 0.5w \) and \( \text{Re} = 20 \) simulated with MPCD. The peaks of high probability density correspond to the stable equilibrium positions in (a).

from the channel center and the stability of the equilibrium positions depend on the respective parameters. In agreement with the results for circular cross sections, the equilibrium positions for smaller particles are closer to the channel walls. At the same time, increasing the Reynolds number too moves the equilibrium positions closer to the channel wall. Curiously, the stability of the equilibrium positions changes with particle size and Reynolds number, a feature not previously discussed in the literature. For large particles, the diagonal equilibrium positions are stable, whereas those on the main axes are stable for small particles. Similarly, large Reynolds numbers render equilibrium positions on the diagonal axes stable. A possible explanation is that the diagonal equilibrium positions are in general positions further away from the channel walls. Both with increasing particle size and Reynolds number, the separation between particle and channel wall decreases. Hence, the hydrodynamic interactions increase and may destabilize the main axes. The particle size relative to the channel size is a fixed parameter, while the flow speed can be readily adjusted. Therefore, the dependence on Reynolds number allows to tune the stability of the equilibrium positions to separate particles by size.

Stable equilibrium positions on the diagonals have been observed for large deformable drops in lattice Boltzmann simulations [55]. Similarly, lattice Boltzmann simulations for hard spheres found stable diagonal equilibrium positions [53]. However, neither study discussed the dependence on size and Reynolds number. The studies [22, 54] did not observe diagonal equilibrium positions on the diagonals either in experiments or in finite-element simulations. We are not aware of the reason for this discrepancy. However, as we discuss in the next section, the stability of the diagonals is strongly dependent on the channel geometry. Even for small deviations away from \( w = h \), the diagonal
equilibrium positions become destabilized. In experiments, the strong pressures necessary for inertial microfluidics cause considerable deformations \[^{[159]}\]. We perform independent MPCD simulations with parameters \[^{[P2]}\] given in appendix \[^{E}\] to compare the equilibrium positions. We plot the profile of the lateral probability density of the particle for \(a/w = 0.5\), \(Re = 20\) in Fig. \[^{4.10}\]. In the probability density, stable equilibrium positions result in maxima and the unstable manifold of the saddle nodes results in areas with increased probability. The results agree with those of the LBM simulation. The main axes have saddle node stability, while the equilibrium positions on the diagonals are stable. Further, the distance \(d_{eq} \approx 0.45\) of the stable equilibrium positions from the channel center agrees with the value obtained by the LBM simulations.

### 4.2.2. Rectangular channel cross sections

The lift force profile changes drastically between different aspect ratios. For an aspect ratio of \(w/h = 1/2\) (Fig. \[^{4.9b}\]), the stable equilibrium positions lie on the short channel axis. The diagonal positions have vanished and the equilibrium positions on the long channel axis become saddle nodes. When starting close to the channel center, the particle first moves outside the \(y = 0\) plane before it approaches the stable equilibrium positions. A similar lift force profile for a smaller particle was reported in Ref. \[^{[13]}\]. For an even more asymmetric aspect ratio of \(w/h = 1/3\) (Fig. \[^{4.9c}\]), the lift force profile changes even further. The saddle node equilibrium positions on the long channel axes vanish and the channel center itself becomes a saddle node. Regardless of their initial position, particles always move into the \(y = 0\) plane. Hence, the motion in \(y = 0\) plane becomes stable. We discuss these drastic changes in the lift force profiles in the following paragraphs.

We consider, first, a particle with radius \(a = 0.4w\) and comment on smaller particles below. We plot the lift force for particles positioned on the \(y\) axis for different aspect ra-
The symmetry of the system prevents any lift force in the $x$ direction. However, all positions on the $y$ axes are unstable against perturbations in the $x$ direction and there are no stable equilibrium position on the $y$ axis. For aspect ratios $w/h > 0.46$, the lift force shows an unstable equilibrium position at the channel center and another equilibrium position located closer to the channel wall. The second equilibrium position is stable along the $y$ direction, but unstable along the $x$ direction. Therefore, it has saddle node stability. Increasing channel height, weakens the lift force close to the channel center. For intermediate aspect ratios $w/h \approx 0.46$, the channel center becomes stable against perturbation in the $y$ direction. In the full cross section, it is a saddle node, since it is still unstable along the $x$ direction. The change of stability of the channel center coincides with the change of the outer equilibrium position to a saddle node and the emergence of an additional unstable equilibrium position between the channel center and the outer equilibrium position. Further decreasing the aspect ratio $w/h$ drives the lift force to be negative for all $y$ values and the channel center remains the only equilibrium position on the $y$ axis.

The lift force for particles located on the $x$ axis (Fig. 4.11b) shows two equilibrium positions for all aspect ratios. The channel center is unstable against perturbation along the $x$ axis and the outer equilibrium position is always stable against perturbation in the $x$ direction. We discuss below the change of stability along the $y$ direction for both equilibrium positions with varying aspect ratio. With decreasing aspect ratio, the magnitude of the lift force decreases. For the smallest aspect ratios ($w/h \leq 0.33$), the lift force profile develops a constant shape. Then, the distance to the short channel faces is large and the flow in the channel center plane resembles a plane Poiseuille flow.

The equilibrium positions and their stability (Fig. 4.12a) characterize the bifurcation of the lift force profile. Although we only plot the equilibrium positions on the $y$ axis, the equilibrium positions on the $x$ axis for $w/h > 1$ correspond to the equilibrium positions on the $y$ axis for $w/h < 1$ and vice versa. First, we consider aspect ratios below unity, for which we show the lift forces in Fig. 4.11a. The outer equilibrium position shifts closer towards the channel wall as we decrease the aspect ratio. In the left inset of Fig. 4.12a, we illustrate the system for $w/h \approx 0.75$. For an aspect ratio $w/h \approx 0.48$, a subcritical pitchfork bifurcation occurs in which the channel center becomes a saddle node and an additional unstable equilibrium position appears. This bifurcation marks the point where the $y = 0$ plane becomes stable and the dynamics effectively two-dimensional. By further decreasing the aspect ratio, the newly created unstable equilibrium position moves towards the channel wall until it merges with the outer equilibrium position and both vanish in a saddle node bifurcation. For aspect ratios above unity, the equilibrium positions correspond to the force curves shown in Fig. 4.11b. Here, the position of the outer equilibrium position changes only little. At about $x/w > 1.33$, the outer equilibrium position becomes stable, while the diagonal equilibrium positions vanish. We illustrate the full cross section for this situation in the right inset.

For smaller particles, the bifurcation scenario changes. We plot the inertial lift force...
4.2. Rectangular channel cross sections

Figure 4.12.: (a) Equilibrium positions $y_{eq}$ on the $y$ axis as a function of aspect ratio $w/h$ for a particle with radius $a = 0.4w$. Here, we show the full stability along both $x$ and $y$ direction. The insets show typical equilibrium positions in a channel for $w < h$ (left) and $w > h$ (right). The plot corresponds to the lift forces shown in Fig. 4.11a. (b) The $y$ component of the lift force as a function of particle position on the $y$ axis for a smaller particle with radius $a = 0.2w$. The inset mirrors the main plot in (a). It shows the equilibrium positions $y_{eq}$ of the lift force in the main plot as a function of aspect ratio $w/h$. Both plots show data for channel Reynolds number $Re = 10$.

The lift force undergoes the subcritical pitchfork bifurcation for $w/h \approx 0.45$. However, it does not show the saddle node bifurcation for low aspect ratios. This difference is also visible in the qualitative difference between the lift force profiles for large particles (Fig. 4.9c) and small particles (Fig. 5.3a). Specifically, the lift force profile for smaller particles keeps a constant shape close to the channel wall for $w/h \leq 0.25$. For the channels with small aspect ratio the undisturbed flow field show significant shear gradients only close to the channel wall. However, only the small particle is able to explore these regions, where we expect a lift force according to the dynamic pressure model (Sect. 2.4.5). Furthermore, the outer equilibrium positions is stable for $w/h = 1$ and becomes unstable only for aspect ratios below $w/h < 0.9$. This change in stability coincides with the vanishing diagonal equilibrium positions.

The dynamic pressure model, introduced in Sect. 2.4.5, explains the features of the lift force profiles in term of the unperturbed flow profiles [20, 95]. The change in flow profile along the $y$ axis (Fig. 3.10b) mirrors the change in lift force (Fig. 4.11a). With increasing aspect ratio the flow profile develops a blunted shape close to the channel axis, with appreciable gradients visible only close to the channel wall. In particular, for aspect ratios $w/h \leq 0.5$, the flow profile changes drastically and the lift force profile undergoes the bifurcation to an effectively two-dimensional system. In contrast, on the short channel axis, the small change of the flow profile (Fig. 3.10a) mirrors the small
4. Channel geometry and inertial focusing

Figure 4.13.: The minimum height $h_{2D}$ required for a two-dimensional particle behavior as a function of Reynolds number for different particle sizes. The aspect ratio $w/h_{2D}$ corresponds to the pitchfork bifurcation in the main plot of Fig. 4.12a and the inset of Fig. 4.12b.

change in the lift forces (Fig. 4.11b).

Devices using optical methods often require a well defined focal plane such that particles always move in the focus of the optical instruments (for example [12]). Therefore, it is important to know the aspect ratio for which the system becomes effectively two-dimensional and particles move in the $y = 0$ plane. In the previous sections we found that the transition coincides with the change of stability of the channel center from unstable to saddle node. We plot the minimum channel height $h_{2D}$ required for this transition in Fig. 4.13. The required height decreases for increasing particle size. Furthermore, the required height is a monotonically decreasing function of Reynolds number for all particles but the smallest ($a = 0.2w$). For all investigated parameters, an aspect ratio below $w/h = 0.43$ is sufficient to render the system effectively two-dimensional. In experiments [12], the channel center plane was only for intermediate Reynolds numbers stable. In particular, for particle Reynolds numbers $Re_p = (a/w)^2Re < 5$, particles collected in the channel center plane consistent with our results. Increased flow rates however destabilize the channel center plane. Our results do not explain these findings. However, the experiment [12] used a dense suspension of particles with small inter-particle distances. Our simulations do not include the hydrodynamic interactions between particles. We therefore suspect that the missing hydrodynamic interactions explain the discrepancy.

4.3. Conclusions

In this chapter, we investigated how inertial focusing in microfluidic channels is influenced by particle size, Reynolds number, and the channel cross section. In channels with circular cross sections, the particles order on the Segré-Silberberg annulus, the radius of
4.3. Conclusions

which corresponds to the stable equilibrium position of the lift force. The magnitude of the lift force strongly increases with increasing particle size and Reynolds number. This change is well described by a scaling law in agreement with literature [22]. We demonstrated that the lift force profile can be connected to the radial probability distributions by a Langevin equation for the diffusion in the potential connected to the lift forces.

We continued to discuss inertial focusing in channels with square or rectangular cross sections. The reduced symmetry of the system lifts the degeneracy of the equilibrium position and particles collect at a set of discrete equilibrium positions. For square cross sections, particles order exclusively either on the main axes or on the diagonals. Beyond previous studies, we discussed how not only the placement but also the stability of the equilibrium positions changes with particle size and Reynolds number. This result has direct applications for particle separation. In rectangular cross sections, the lift force profiles undergo a sequence of characteristic bifurcations when the aspect ratio is varied. We investigated the bifurcation scenario in detail for particles of different sizes and discussed how the unperturbed flow profile explains the found features. In channels with low aspect ratios, not only the equilibrium positions, but the whole dynamics is restricted to the channel center plane. Here, we determined the minimum channel height necessary to observe this effect for different particle sizes and Reynolds numbers. This novel result simplifies devices design in inertial microfluidics, in particular, for control applications.
Control of inertial lift forces

In the previous chapter, we discussed how changing the channel geometry allows to control the lateral migration of colloidal particles in inertial microfluidics. However, many applications require further control over the system. Here, we investigate using external electric and magnetic fields that change the axial and angular velocity of particles to modify the inertial lift forces. We show how the external control influences the equilibrium positions and discuss possible applications to particle separation. Further, we demonstrate how axial control forces in combination with a hysteretic feedback scheme increase the particle throughput.

The results presented in this chapter have been published for axial control forces in [C] and for the control by rotational motion in [D].

At low Reynolds numbers, microfluidic devices often use external fields to control particle motion. Optical tweezers rely on strongly focused laser light to exert forces on colloidal particles [24, 28, 30] and can create complex potential landscapes, working as scanning optical tweezers [25–27] or holographic optical tweezers [28–30]. For example, Ref. [31] used optical lattices to sort particles by their size. Kim and Yoo used an electric field directed against the flow to slow down particles in a microfluidic channel with circular cross section [154]. For sufficiently high field strengths, the particles were focused onto the central axis of the channel.

External fields are not restricted to the control of translational motion, they can also modify rotational motion. Optical tweezers are able to rotate birefringent particles [28, 30]. Furthermore, rotating magnetic fields influence the rotation of superparamagnetic particles. A small anisotropy in the magnetic susceptibility of the particles defines an easy axis, that aligns to external magnetic fields [160]. When subjected to rotating magnetic fields, superparamagnetic particles assume their angular velocity [161]. Rotating particles in microfluidic devices self-organize in complex patterns [162, 163] and can further act as probes to test mechanical properties of DNA [164]. Both experiments [32, 33] and simulations [165, 166] studied rotating particles for micropumps.

Experiments in inertial microfluidics used external sheath flows as a control mechanism to sort particles by size [59] and test the mechanical properties of cells ("mechanical phenotyping") [14]. A recent experiment explored the combination of inertial focusing and external magnetic fields to isolate circulating tumor cells [34].

Depending on the specific control mechanism, its parameters are often changed over time by a predefined scheme. Here, we resort to the feedback control schemes. In contrast
5. Control of inertial lift forces

Figure 5.1.: Different control schemes. For both, the system state $x$ is described by a differential equation, which depends on the control force $u$. In open loop control (a), the control force $u(t)$ does not depend on the system state. In closed loop or feedback control (b), the system state $x(t)$ influences the control force $u(x(t))$.

To open loop control, feedback control takes the system state into account and adapts the control signal accordingly \[36\] (Fig. 5.1). A classic example of feedback control is the governor in steam engines \[36\], which adapts the fuel fed into steam engines such that they maintain a steady pace. The governor uses a mechanical feedback to decrease the fuel supply when the speed of the engine is above a target speed and conversely increases the fuel supply when the speed of the engine is below a target value. Feedback control schemes are often more robust to noise compared to open loop control schemes \[36\]. In microfluidics, feedback control was used with optical tweezers to increase the accuracy of force measurements in polymer solutions and molecular motors \[167–169\]. Further, lab on a chip devices used feedback control with optical tweezers and light microscopes to control the motion of particles \[170–172\].

In this chapter, we focus on genuinely inertial control methods. Specifically, we investigate axial control forces that change the particle velocity and external control torques that modify the particle rotation. These control methods do not modify the lateral particle position in the non-inertial regime (Sect. 2.4.3).

In the remainder of this chapter, we first demonstrate how axial control forces modify the particle motion in channels with rectangular cross section. Further, we show how a hysteretic feedback scheme increases the particle throughput in the system. Finally, we discuss how changing the rotational motion of the particle influences its lateral migration.

5.1. Axial control forces

Recently, Kim and Yoo demonstrated how applying an electric field focuses particles in a microfluidic channel with circular cross section onto the channel axis \[154\]. Without an electric field, the particles were uniformly distributed in the channel cross section, since the experiment was not performed in the regime of inertial focusing ($Re \approx 0.05$).
5.1. Axial control forces

Figure 5.2.: Schematic of the control methods explored in this chapter. The particle with radius \( a \) is placed in a channel with width \( 2w \). The particle is moving with axial velocity \( v_z \) parallel to the streamlines of the undisturbed flow and experiences the inertial lift force \( f_{\text{lift}} \) parallel to them. Further, the particle rotates with angular velocity \( \Omega \). In this system, we control inertial focusing by either applying the axial control force \( f_{\text{ctl}} \) (Sect. 5.1 and 5.2) or modifying the rotational motion (Sect. 5.3). In the latter case, we either apply the control torque \( T_{\text{ctl}} \) or prescribe a chosen angular velocity \( \Omega \).

When they applied an electric field directed against the flow, the particles slowed down and focused onto the central axis of axis. They explained the lateral migration by the Saffman lift force for particles lagging the flow \([74]\). Motivated by this experiment, we discuss a similar control scheme in inertial microfluidics. Here, the induced Saffman lift force has to compete with the inertial lift force and new effects arise. In particular, the control force changes the equilibrium position of the particle from the inertial focusing position to the channel center in a continuous manner.

In the following, we consider a channel with rectangular cross section (Fig. 4.8a). It has width \( 2w \), height \( 2h \), and an aspect ratio \( w/h = 0.33 \). We apply a pressure driven flow with maximum velocity \( u_{\text{max}} \) at the channel center, which defines the channel Reynolds number \( Re = 2wu_{\text{max}}/\nu \). Here, we choose \( Re = 10 \). Into the channel, we place a colloidal particle with radius \( a = 0.2w \). To control the particle we apply a control force \( f_{\text{ctl}} \) to it that is directed against the flow direction as shown in Fig. 5.2. We simulated the system with the lattice Boltzmann method and used the parameter set \([4]\) given in appendix E.

We plot the lift force profile profiles with and without control in Fig. 5.3. Without control (Fig. 5.3a), the particle is always focused into the \( y = 0 \) plane as discussed in Sect. 4.2.2. The stable equilibrium position of the particle is located halfway between channel center and channel wall at \( x_{\text{eq}} \approx 0.46w \). With a control force \( f_{\text{ctl}} = 2.5\rho u^2 \) (Fig. 5.3b), the particle is focused to the channel center regardless of its initial position. In contrast to the uncontrolled case, there exist no further equilibrium positions. Since the system is effectively two-dimensional with and without control, we focus on the lift forces along the short channel axis in the following.
5. Control of inertial lift forces

Figure 5.3.: Cross sectional lift force profiles in a channel with aspect ratio $w/h = 0.33$ for $Re = 10, a = 0.2w$ without control (a) and with an applied control force $f_{ctl} = 2.5\rho v^2$ (b). The gray lines show the trajectories of an unconstrained particle. The white squares indicate positions where we do not show the lift forces, as their magnitude exceeds $0.35\rho v^2$. We further indicate the equilibrium position and their stability.
5.1. Axial control forces

Figure 5.4.: (a) The lift force versus the particle position for different axial control forces $f_{\text{ctl}}$ with particle radius $a = 0.2w$ and channel Reynolds number $Re = 10$. (b) The positions of the stable equilibrium position $x_{\text{eq}}$ as function of applied control force $f_{\text{ctl}}$ for Reynolds number $Re = 33$ and varying particle sizes $a/w$. The inset shows the minimum control force $f_{0}\text{ctl}$ required to focus the particle onto the channel center ($x_{\text{eq}} = 0$) as a function of Reynolds number for different particle sizes.

We plot the lift force along the short channel axis as a function of particle position in Fig. 5.4a for different axial control forces. The axial control force changes the particle equilibrium position in a continuous manner. Slowing down the particle (positive control forces) decreases the lift force and moves the particle equilibrium position closer towards the channel center. Speeding up the particle (negative control forces) increases the lift force and moves the particles equilibrium position outwards closer towards the channel wall. As we discuss in detail below, the qualitative behavior is fully consistent with the dynamic pressure model (Sect. 2.4.5) and the Saffman lift force (2.53).

We plot the location of the equilibrium positions as a function of control force in Fig. 5.4b for different particle sizes. For all particles, the axial control force changes the equilibrium position in a similar manner. However, moving the equilibrium position for larger particles requires considerably larger control forces. We plot the minimum control force $f_{0}\text{ctl}$ required to focus the particle to the channel center in the inset. The minimum control force strongly increases with particle size and Reynolds number. When fitted to a power law, it scales like $f_{0}\text{ctl} \propto Re^{1.02}(a/w)^{2.60}$. The strong dependence on parameters suggest a simple separation scheme. For Reynolds number Re = 10 and control force $f_{\text{ctl}} = 2.5 \rho v^2$, a particle with radius $a = 0.2w$ is focused onto the channel center, while a particle with radius $a = 0.3w$ is only displaced by $\Delta x_{\text{eq}} \approx 0.1w$ (Fig. 5.4b).

We close this section by analyzing the control mechanism in detail for a particle size $a = 0.2w$ and channel Reynolds number Re = 10. We plot the change of velocity $\Delta v_z$ versus the applied control force for different lateral particle positions in Fig. 5.5a. The change of velocity follows the linear relationship $\Delta v_z = \xi^{-1} f_{\text{ctl}}$. Here, we introduced the effective
5. Control of inertial lift forces

Figure 5.5.: (a) The change of axial velocity $\Delta z = v_z - v_{z,0}$ as a function of applied control force $f_{ctl}$ for different particle positions $x/w$. For a fixed position the change of axial velocity is well described by $\Delta v = \xi_{\text{eff}}^{-1} f_{ctl}$. The inset plots the effective friction coefficient $\xi_{\text{eff}}$ as a function of particle position $x/w$. (b) Change in lift force $\Delta f_{\text{lift}}$ as a function of control force $f_{ctl}$ for different particle position $x/w$. The inset shows the transfer function (5.1). The red curve shows the Rubinow-Keller transfer function (5.2).

In both plots, the particle radius is $a = 0.2 w$ and the Reynolds number $\text{Re} = 10$.

We plot the effective friction coefficient as a function of particle position determined from a least-squares fit in the inset of Fig. 5.5a. The effective friction coefficient is at least six times higher than the Stokes friction coefficient (2.31) regardless of position. As the particle approaches the channel walls, the friction coefficient increases further. Fig. 5.5b shows the change of lift force $\Delta f_{\text{lift}}$ as a function of control force for different particle positions. The change of lift force $\Delta f_{\text{lift}}$ strongly depends on particle position. For small applied control forces, we restrict ourselves to the linear approximation

$$\Delta f_{\text{lift}} = \left. \frac{\partial}{\partial f_{ctl}} \Delta f_{\text{lift}}(x) \right|_{f_{ctl}=0} f_{ctl},$$

where we introduce the transfer function $\phi(x)$. We plot it in the inset of Fig. 5.5b. It grows linearly with distance from the channel center. Only close to the channel walls, it departs from the linear dependence. The focusing induced by the axial control force resembles the migration in shear flow investigated by Saffman [74]. He predicted a lift force (2.53) that has a square root dependence on the local shear rate. This prediction results in a transfer function $\phi(x) \propto x^{1/2}$ that is incompatible with our findings. Rubinow and Keller investigated the lift force acting on spinning sphere in a viscous fluid [45].
5.2. Axial feedback control

Figure 5.6.: Illustration of the feedback control scheme. The control becomes active when the particle leaves the target interval $[-b, b]$. Once the particle returns to the channel center, the control becomes inactive. (a) The applied control force as a function of particle position. When the control is inactive (blue), the particle does not experience any axial force. When the control is active (red), the particle experiences the constant axial control force $f_0$. (b) The axial velocity of the particle for the active and inactive control. Active control slows down the particle. (c) Example trajectory of the particle under the action of the feedback control scheme for $Re = 10, a = 0.2w, f_0 = 2.5\rho v^2$.

Their prediction results in a transfer function

$$\phi_{RB}(x) = -\frac{a^2\Omega_y(x)}{6\eta(1 + \frac{3}{8}(a/w)^2Re)},$$

where $\Omega_y(x)$ denotes the $y$ component of the angular velocity of the particle. We plot $\phi_{RB}$ as the red line in the inset and observe excellent agreement. The failure of the Saffman theory to describe the change in lift force is consistent with his assumption of weak shear flows [74]. In Ref. [74], Saffman notes that in strong shear flows the Rubinow-Keller theory [45] becomes relevant.

5.2. Axial feedback control

As discussed in the beginning of the chapter, feedback control is often used to improve the performance of external control. Here, we use axial control forces in a hysteretic feedback scheme and demonstrate that the feedback control increases the particle throughput.

In the following, we consider a particle with radius $a = 0.2w$ placed into the channel discussed in the previous section. We choose the Reynolds number $Re = 10$. The axial control force follows a hysteretic feedback scheme illustrated in Fig. 5.6. Whenever the particle is outside a target interval $[-b, b]$, we apply a constant control force $f_0$ until the particle reaches the channel center ($x = 0$). We then switch the control force off until the particle leaves the target interval again. In the following, we use control forces $f_0 \geq 2.5\rho v^2$ and, therefore, are able to focus the particle to the channel center.
Figure 5.7.: (a) The time averaged axial particle velocity $< v_z >$ as a function of target interval width $b$ for different control forces $f_0$. Without control, the particle moves with velocity $v_{eq}$ at its equilibrium position and $v_{max}$ at the channel center. (b) Distribution of active times $t_{on}$ for different target widths $b$. Here, the control force is $f_0 = 2.5 \rho v^2$. The symbols show the probabilities determined from simulations. The solid lines show the results expected from the mean first passage time of the Ornstein-Uhlenbeck process (5.4). In both plots, we choose Reynolds number $Re = 10$ and particle size $a = 0.2w$.

We model the particle motion using the Langevin equation (2.55)

\[
\frac{d}{dt} x = \xi^{-1} (f_{\text{lift}}(x, f_{\text{ctl}}) + \eta), \quad (5.3a)
\]

\[
\frac{d}{dt} z = v_z(x, f_{\text{ctl}}). \quad (5.3b)
\]

Here, both lift force and axial velocity are functions of the applied axial control force $f_{\text{ctl}}$. We choose the noise consistent with a channel width of $2w = 20\mu m$ and temperature of $T = 300K$. Under the influence of the control scheme, the particle oscillates inside the target interval (Fig. 5.6c). Only close to the channel center, where the lift forces are small, thermal fluctuations become important.

We plot the mean velocity of the particle averaged over time and independent realizations as a function of target width $b$ in Fig. 5.7a. If the target interval is chosen as $b = 0$, the particle is always outside the target interval and the control is always active. If the target interval includes the equilibrium position ($x_{eq} = 0.46w$), the particle is always inside the target interval and hence the control is always inactive. For intermediate target widths, the control switches from active to inactive and the particles oscillates as observed in Fig. 5.6c. To our surprise, the mean particle velocity increases compared to both constant control and no control. The increase is independent of the applied maximum control force and only weakly dependent on the target interval width. In short, the hysteretic feedback scheme increases the mean particle throughput by temporarily slowing down the particle.

Though the system is deterministic far away from the channel axis, thermal fluctua-
5.3. Control by rotational motion

As mentioned, inertial lift forces are weak and we linearize them as \( f_{\text{lift}}(x) = kx \). Then, the Langevin equation (5.3a) reduces to the Ornstein-Uhlenbeck process [96]. This equivalence allows us to use analytic approaches. For example, the time \( t_{\text{on}} \) the control is active is the mean time required for the particle to reach to the channel center from the target interval edge \( b \). Following Ricciardi and Sato, the active time \( t_{\text{on}} \) is distributed according to [173]

\[
P(\tilde{t}_{\text{on}}|\tilde{b}) = \frac{2\tilde{b}}{\sqrt{2\pi}}(e^{2\tilde{t}_{\text{on}}}-1)^{-3/2}e^{2\tilde{t}_{\text{on}}} \exp\left[-\frac{\tilde{b}^2}{2(e^{2\tilde{t}_{\text{on}}}-1)}\right],
\]

where we introduced \( \tilde{t}_{\text{on}} = t_{\text{on}}/\xi/k \) and \( \tilde{b} = b/\sqrt{k_B T/k} \). We plot the histogram of active times found the simulations in Fig. 5.7b and find good agreement with the analytic prediction.

5.3. Control by rotational motion

In this section, we investigate how to control a colloidal particle in inertial microfluidics via its rotational motion. The complex interplay between lift forces and rotational motion is an everyday phenomenon known by the name Magnus effect. A spinning particle moving through a fluid, such as a football through air, experiences a lift force resulting in a curved trajectory [81]. In microfluidic systems, the rotational motion of superparamagnetic beads can be controlled by rotating magnetic fields. A small anisotropy in the magnetic susceptibility of the particles results in an easy axis that aligns to external magnetic fields [160]. In rotating magnetic fields, the easy axis continues to be aligned and the particle follows the external field [101].

In the following, we consider a two-dimensional spherical particle with radius \( a \) in a planar channel with width \( 2w \) (Fig. 5.2). We apply a pressure driven Poiseuille flow with undisturbed flow profile \( u_z(x) \) (2.24) and flow vorticity \( \Omega_0(x) = [\nabla \times \hat{e}_z u_z]/2 \). The maximum flow velocity \( u_{\text{max}} \) both defines the Reynolds number \( \text{Re} = 2wu_{\text{max}}/\nu \) and the maximum vorticity at the channel wall \( \Omega_{\text{max}} = \nu \text{Re}/2w^2 \). To control the particle, we either apply a constant control torque \( T \) or control the angular velocity of the particle directly. The rotational motion of the particle is characterized by the rotational friction coefficient \( \xi_r = 4\pi \rho a^2 \) [94], as discussed in Sect. 2.4.2. We simulated the system with two-dimensional MPCD simulations using parameter set P3 given in appendix E.

5.3.1. Uncontrolled motion

As most of this work investigates three-dimensional systems, we review the basics of inertial focusing in two dimensions without external control in this section. We plot the probability distributions of the lateral particle position in Fig. 5.8a. The main plot shows...
5. Control of inertial lift forces

Figure 5.8.: (a) Lateral probability distribution $P(x)$ as a function of lateral position $x$ for $Re = 33$ and different particle sizes. The inset shows the lateral probability distribution for $a/w = 0.5$ and different Reynolds numbers. (b) The inertial lift force $f_{\text{lift}}$ as a function of lateral position $x$ for $Re = 33$ and two different particle sizes. The inset shows the angular velocity $\Omega$ of the particle as a function of lateral position for the same parameters.

The probability distribution for different particle sizes $a$ and a fixed Reynolds number $Re = 33$. The maximum of the probability distribution shifts closer towards the channel center with increasing particle size. Further, the width of the distribution strongly decreases for larger particles. In the inset, we show the lateral probability distribution for different Reynolds numbers and a fixed particle size $a/w = 0.5$. The probability distributions become narrower with increasing Reynolds number. The observed behavior is consistent with three-dimensional simulations discussed in Sect. 4.1.

We plot the inertial lift force experienced by the particle as a function of particle position in Fig. 5.8b for a Reynolds number $Re = 33$ and two different particle sizes $a = 0.3w$ and $a = 0.4w$. The inertial lift force points away from the channel center, which is an unstable equilibrium position. However, as the particle approaches the channel walls, strong wall lift forces push it back into the channel center. Both lift force contributions cancel at a stable equilibrium position halfway between channel center and channel walls. In contrast to three-dimensional simulations (Sect. 4.2), the difference magnitude of the inertial lift forces is less pronounced for different particle sizes. In the inset, we plot the angular velocity of the particle as a function of particle position. The angular velocity is close to linear and approximately follows Faxéns law (5.5). We further comment on this fact in Sect. 5.3.3.

5.3.2. Control by torque

The dynamic pressure model (Sect. 2.4.5) predicts that changes in the angular velocity of the particle also change the lift force. In this section, we investigate how a constant torque applied to the particle influences the lateral motion of the particle.

We plot the lateral probability distributions for a particle with radius $a = 0.4w$ and
5.3. Control by rotational motion

Reynolds number $Re = 33$ for varying positive torques applied to the particle in Fig. 5.9a. The applied torque breaks the symmetry of the system. Without it, the two peaks of the probability distribution have equal height. However, as the torque increases, the particle resides predominantly on the positive channel side. In particular, the height of the two peaks becomes strongly asymmetric with increasing torque. Finally, for the strongest torques, the probability distribution becomes unimodal.

To clarify this behavior, we plot the lift force profiles for different applied torques in Fig. 5.9b. The applied torque shifts the lift force profiles upwards and the changed lift force drives the particle closer towards the positive channel side. On the negative channel side, the unstable and stable equilibrium positions move closer towards each other. For sufficiently high torques, they merge and only the equilibrium position on the positive channel side remains. In the process, the equilibrium position on positive channel side does move little, as the induced lift force competes with the strong wall lift forces. At the same time, the torque applied onto the particle changes the angular velocity of the particle, as shown in the inset. Similar to the lift force, the angular velocity increases with increasing torque. The change in angular velocity is almost independent of the particle position and is well described by $\xi^{-1} T$ as we discuss in Sect. 5.3.3. In a similar system at Reynolds number $Re \approx 0 \[165\]$, changes in axial velocity $v_z$ of the particle have been observed. In our system, it does not change significantly (not shown), as the axial velocity is almost exclusively determined by the strong driving of the Poiseuille flow.

We investigate the behavior of the equilibrium positions in detail by plotting their position for different torques in Fig. 5.10. We determined the equilibrium positions from the distributions in Fig. 5.9a. Minima in the distribution correspond to unstable equilibrium positions and maxima to stable equilibrium positions. The equilibrium position

Figure 5.9.: (a) Lateral probability distribution $P(x)$ as a function of particle position $x$ for different applied torques $T$. (b) Inertial lift force $f_{\text{lift}}$ as a function of particle position $x$ for different applied torques $T$. The inset shows the angular velocity as a function of particle position. In all plots, we use a particle size $a/w = 0.4$ and Reynolds number $Re = 33$. 


5. **Control of inertial lift forces**

Figure 5.10.: The equilibrium position $x_{eq}$ as a function of applied torque $T$ for the system of Fig. 5.9a (Re = 33, $a/w = 0.4$). At critical torque $T_c \approx 3.4\rho\nu^2$, the system undergoes a saddle node bifurcation.

on the positive channel wall moves slightly outside. The unstable and stable equilibrium position on the negative channel side undergo a saddle node bifurcation. For small torques, they start to move closer towards each other. At sufficiently high torques, above $T_c \approx 3.4\rho\nu^2$, the two equilibrium positions annihilate each other and only the stable equilibrium position on the positive channel side remains.

For low Reynolds numbers, we do not expect any lateral migration. The argument of Bretherton discussed in Sect. 2.4.3 does still hold even with applied torques. Therefore, fluid inertia is necessarily the cause of the control mechanism. We check this statement by plotting the lateral probability distribution for different Reynolds numbers with a constant applied torque $T = 2.8\rho\nu^2$. As expected, inertial focusing becomes less prominent with decreasing Reynolds number.

Finally, we plot the inertial lift force for different sizes with and without applied torque in Fig. 5.11b. To our surprise, the applied torque changes the lift force profiles for both particle sizes almost equally. However, the change in angular velocity depends strongly on the particle size. In particular, the strong change of the angular velocity of the small particle is consistent with its lower rotational friction coefficient (2.39). We further comment on this fact in the next section.

### 5.3.3. Control by angular velocity

In experiments [161], super-paramagnetic beads follow rotating magnetic fields and assume their rotation velocity. In this section, we discuss the novel phenomena resulting from controlling the angular velocity directly instead of applying a constant control torque.

We plot the lateral probability distributions for different imposed angular velocities for Re = 33, $a = 0.4w$ in Fig. 5.12a. In contrast to the previous section, the distributions
5.3. Control by rotational motion

Figure 5.11.: (a) Lateral probability distribution $P(x)$ as a function of particle position $x$ for different Reynolds numbers, a constant applied torque $T = 2.8\rho \nu^2$, and particle radius $a/w = 0.4$. (b) The inertial lift force $f_{\text{lift}}$ with applied torque and without applied torque as a function of particle position $x$ for Reynolds number $Re = 33$ and two different particles sizes. The inset shows the angular velocity $\Omega$ as a function particle position $x$ for the same parameters.

Figure 5.12.: (a) Lateral probability distribution $P(x)$ as a function of particle position $x$ for different imposed angular velocities $\Omega$. (b) Inertial lift force $f_{\text{lift}}$ as a function of particle position $x$ for different imposed angular velocities $\Omega$. Here, $\Omega_{\text{eff}}$ is the angular velocity of a particle without control (Fig 5.8b, inset). In both plots, the particle radius is $a = 0.4$ and the Reynolds number is $Re = 33$. 


5. Control of inertial lift forces

![Graph](image)

Figure 5.13.: (a) Equilibrium position $x_{eq}$ as a function imposed angular velocity $\Omega$ for different combinations of particle radius $a$ and Reynolds number $Re$. (b) The deviation $\Delta T$ from the torque expected by Faxén’s law for different control strategies. For all curves, we choose Reynolds number $Re = 33$ and particle radius $a = 0.4w$. The inset shows the effective rotational friction coefficient $\xi_{r,eff}$ defined in the main text as a function of particle position $x$.

is unimodal for all angular velocities. When we prevent the particle from rotating ($\Omega = 0$), the distribution is symmetric and peaked in the channel center. With increasing angular velocity, the peak of the distribution shifts towards the positive channel side. Furthermore, the distribution becomes more narrow as the peak moves closer towards the channel wall.

The corresponding behavior is visible too in the lift force profiles plotted in Fig. 5.12b for different imposed angular velocities. For reference, we also show the lift force, when the particle is not controlled and it rotates with its free angular velocity $\Omega_{0,eff}(x)$. For a non-rotating particle ($\Omega = 0$), the lift force is always directed towards the channel center. This is in contrast to Ref. [22] where the particle could not be focused onto the channel axis. With increasing angular velocity, the stable equilibrium position moves closer to the channel wall. The overall magnitude of the lift force increases mirroring the reduced widths of the probability distributions (Fig. 5.12a). We plot the torque necessary to impose the angular velocity in the inset. When the particle is free to evolve, the torque is zero. However, when we impose a chosen angular velocity on the particle, its rotation has to compete with the viscous shear forces of the external Poiseuille flow. The torques required to impose the angular velocity are zero wherever the particle assumes the desired angular velocity on its own and increase linearly away from this position.

We determine the stable equilibrium position from the lateral probability distribution for different particle sizes and Reynolds numbers. We plot the equilibrium positions as a function of imposed angular velocity in Fig. 5.13a. For different particle sizes and Reynolds numbers, we are able to control the particle equilibrium position by changing
the angular velocity of the particle. However, the strong wall lift forces prevent us from moving the particle too close to the channel wall. Here, we scaled the angular velocity with the maximum vorticity $\Omega_{\text{max}} = \nu \text{Re}/2w^2$. Therefore, the angular velocities for $\text{Re} = 33$ are about 40\% higher than those for $\text{Re} = 13$.

Finally, we comment on the validity of Faxén’s law, that relates the torque a particle experiences to its angular velocity by

$$T = \xi_r (\Omega(x) - \Omega_0(x)),$$  \hspace{1cm} (5.5)

where we introduced the rotational friction coefficient $\xi_r = 4\pi \eta a^2$. To verify whether Faxén’s law does hold, we determine deviation from the expected torque $\Delta T = T - \xi_r (\Omega(x) - \Omega_0(x))$ and plot it in Fig.5.13b. Close to the channel center, the deviations are small and Faxén’s laws does indeed describe the relationship between the angular velocity of the particle and the torque it experiences. However, as the particle approaches the channel walls, the deviations become more pronounced. This behavior can be explained by the change in rotational friction coefficient. We determine the effective rotational friction coefficient by averaging the fraction $\xi_{r,\text{eff}} = T/(\Omega - \Omega_{0,\text{eff}})$ over all simulations shown in Fig.5.13b. We plot the result in the inset. For all positions, the effective rotational friction coefficient is larger than the friction coefficient expected by Faxén’s law. Furthermore, it increases drastically as the particle approaches the channel wall. This behavior mirrors the increase in translational friction coefficient we found for three-dimensional simulations (Fig.5.5a).

### 5.4. Conclusions

In this chapter, we investigated how to control the lateral particle migration in inertial microfluidics by changing the axial velocity of the particle with electric fields or by changing the angular velocity of the particle by rotating magnetic fields.

When the electric field is directed against the flow direction, the particles experience an axial control force as demonstrated experimentally in Ref. [154]. The control forces slow the particle down and decrease the lift force. For exemplary parameters, we discussed how the full lift force profiles change. As the lift forces drive particles into channel center plane with and without control, we concentrated in the remainder on the lift forces in this plane. The equilibrium positions of the particle change continuously with axial control force. Here, the strong dependence on particle size allows to separate particles. The relationship between induced lift force and axial control force is well described by the theory of [Rubinow and Keller][45]. Next, we combined the axial control forces with a hysteretic feedback law designed to keep the particle close to the channel center. To our surprise, the particle throughput in the system increases, even though we temporarily slow down the particle.
Finally, we investigated how rotating magnetic fields influence the inertial migration of paramagnetic beads. An applied torque changes the angular velocity and thereby also the lift force such that particles migrate towards the side with higher relative velocity. For strong torques, the system undergoes a saddle node bifurcation and only a single equilibrium position remains. When we controlled the angular velocity of the particle, the particle assumes only a single equilibrium position, the location of which changes with the angular velocity of the particle. The strong dependence of the lift force on the particle rotations allows to effectively separate magnetic from non-magnetic particles.
Optimal control of particle separation

In the previous chapter, we demonstrated how to apply feedback control in inertial microfluidics. We chose the control scheme in an ad-hoc fashion guided by physical intuition. Such an approach often results in suboptimal choices. The design of control schemes that are optimal with respect to a given control goal is addressed by optimal control theory. In this chapter, we apply optimal control theory to steer single particles to a target at the channel outlet and separate particles based on their size. We discuss how to formalize these problems and derive the optimal control force profiles. Finally, we demonstrate the approach on a number of systems inspired by experiments.

The results of this chapter have been published in [B].

Optimal control theory gathers diverse fields of mathematics all concerned with different systems under a common set of principles. Regardless of the application, they all state the control goal as the maximization of an objective functional. For the maximization, optimal control theory often uses concepts and methods from the calculus of variations. The field of optimal control started with optimizing the trajectories of missiles and rockets [37]. A typical question posed was, given finite amount of fuel, how can one maximize the distance traveled. Whereas the early applications of optimal control were concerned with deterministic systems, extension to stochastic systems are available. One application of stochastic optimal control theory is reinforcement learning, a field of artificial intelligence. In reinforcement learning, an agent tries to find the optimal strategy in an uncertain environment [174]. A successful application is TD-Gammon, a computer program learning to play backgammon [40]. However, most applications of stochastic optimal control can be found in finance [38]. For example, Merton’s portfolio problem, one of the rare solvable models, describes investment decisions in a volatile stock market [41]. In physics, optimal control theory has been applied to viscous flows [175] and, more recently, stochastic thermodynamics [176, 177].

We continue by introducing the channel geometry. Then, we discuss the optimal control formalism, for both particle steering and separation, and demonstrate its successful application to both problems.

6.1. System

In the following, we apply optimal control theory to inertial focusing in channels with rectangular cross section of width $2w$ and height $2h$. While we discuss devices with
6. Optimal control of particle separation

Figure 6.1.: Schematic of the optimal control problem in the \( y = 0 \) plane of the full system (Fig. 4.8). We try to steer a particle from its initial position \( x_i \) to the target interval \([x_t - b, x_t + b] \) at the channel outlet (green). The initial position is distributed according to \( P_0(x_i) \). We encode the target interval by the rewards function \( R(x) \), which we set \( R(x) = 1 \) inside the target interval and \( R(x) = 0 \) everywhere else. In axial direction, the particle moves with axial velocity \( v_z(x) \). In lateral direction, it experiences a combination of inertial lift force \( f_{\text{lift}}(x) \) and control force \( u(x,z) \).

finite length \( L \), we envision them as part of a larger microfluidic circuit. Concretely, we assume that particles entering through the channel inlet \((z = 0)\) are already focused to their stable equilibrium positions. Inside the channel, we aim to control the particle motion and position them in a target interval at the channel outlet \((z = L)\). We imagine the positioned particles to be then further manipulated or analyzed. Devices in inertial microfluidics often use similar design principles, where different parts with distinct functional properties constitute a larger circuits. Particles are first focused to controlled equilibrium positions. In a subsequent step, the well defined position of the particles allows to count cells [68], to test mechanical properties of cells with sheath flows [14], or to isolate circulating tumor cells with magnetic fields [34].

We restrict ourselves to a channel with aspect ratio \( w/h \approx 0.42 \). As we discussed in Sect. 4.2, the lift force drives colloidal particles for all lateral positions into the channel center plane \((y = 0)\). In particular, only two stable equilibrium positions on the short channel axis remain. Since we assume that the particles are already focused to their equilibrium position, when they enter the channel through its inlet, their movement continues in this plane. In the following, we use a stochastic description in terms of the Smoluchowski equation (2.62). The probability density \( P(x,z,t) \) to find a particle at lateral position \( x \) and axial position \( z \) at time \( t \) changes as

\[
\frac{\partial}{\partial t} P(x,z,t) = \mathcal{L} P(x,z,t),
\]

where the Smoluchowski operator \( \mathcal{L} \) includes all physical processes. Where appropriate, we specify the position by the vector \( \mathbf{x} = (x, z) \). Further, we denote the domain of the
channel in integrations by $\Omega = [-w, w] \times [0, L]$.

The Smoluchowski operator has contributions for the effects illustrated in Fig. 6.1. In lateral direction, the particle experiences a deterministic lateral force and a thermal noise force. The lateral force acting on the particle includes the inertial lift force $f_{\text{lift}}(x)$ and the control force $u(x, z)$. Physically, we think of optical tweezers as a possible implementation for the control force. We further comment on the implementation below. While the inertial lift force only depends on the lateral particle position, the control force depends both on lateral and axial position. In axial direction, the particle moves with the axial velocity $v_z(x)$. It is typically much higher than lateral velocities (Sect. 2.4.6). Therefore, we neglect any influence of control force and noise on the axial motion. The combination of all processes gives the complete Smoluchowski operator

$$\mathcal{L}[u] = -\frac{\partial}{\partial x} \left[ \xi^{-1} \left( f_{\text{lift}}(x) + u(x, z) \right) - D \frac{\partial}{\partial x} \right] - \frac{\partial}{\partial z} v_z(x),$$

where we made its dependence of the control force $u$ explicit. The operator agrees in form with (2.63), when we identify $f_{\text{ext}} = (f_{\text{lift}} + u)\hat{e}_x$. We assume the validity of the fluctuation-dissipation theorem (2.58), so $D = k_B T/\xi$.

To close the system, we have to give suitable boundary conditions for the channel inlet and the channel walls. We assume that the particles entering through the channel inlet are already focused. As demonstrated in Sect. 4.1.2.1 the initial position $x_i$ is then distributed according to

$$P_0(x_i) = \frac{1}{Z} \exp \left[ \frac{1}{k_B T} \int_0^{x_i} d x' f_{\text{lift}}(x') \right].$$

For typical parameters, this distribution is strongly peaked around the equilibrium positions $\pm x_{eq}$. The particle is confined to the channel and the lateral probability flux through the channel walls (2.67) has to vanish,

$$\left[ \xi^{-1} (f_{\text{lift}}(x) + u(x, z)) - D \frac{\partial}{\partial x} \right] P(x, z, t) = 0.$$  

We model the control force as a force profile $u(x, z)$, which we propose to implement by optical tweezers [28, 30]. They allow to generate optical potentials for complex tasks [25–30]. In particular, they have been used to generate optical lattices for particle separation [31]. Optical tweezers are able to exert forces up to hundreds of piconewtons [178, 179]. We explicitly model the limits of the forces that can be generated by optical tweezer by searching for the control force such, that $|u(x, z)| < u_{\text{max}}$. In the following, we choose $u_{\text{max}}$ no larger than 0.264 $\rho \nu^2$. Further, we assume that the control force is independent from the particle size, an assumption valid for wavelengths smaller than the particle size [180].
6. Optimal control of particle separation

6.2. Optimal control theory

Optimal control theory formalizes the control goal in an objective functional $J[u]$. It then searches for the optimal control force $u^*$ which maximizes the objective functional

$$u^*(x) = \arg \max_{u(x)} J[u].$$

(6.5)

In the next sections, we discuss how we choose the objective functional for particle steering and particle separation and how to perform the maximization.

6.2.1. Particle steering

In this section, we formulate the objective functional to steer a particle from its initial position into a given target interval $[x_i - b, x_i + b]$ at the channel outlet (Fig. 6.1). We cast this problem in the language of optimal control theory by introducing the rewards function $R(x)$, which is one if $x$ is inside the target interval, but zero everywhere else. We choose the probability that the particle reaches the target interval at the channel outlet as the objective functional. This probability is the integral of particle flux $j_z$ through the channel outlet weighted by the rewards function

$$J = \int_0^\infty dt \int_{-w}^{+w} dx \; j_z(x, z = L, t) R(x).$$

(6.6)

We further integrate over time as we are not interested in how long the particle takes to reach the goal, only that it reaches it at all.

As formulated, the optimal control problem is highly irregular, as we demonstrate with the following example. We try to steer a single particle to the target interval $[-b, b]$ at the channel outlet. The particle does not diffuse ($D = 0$), experiences no lift force ($f_{\text{lift}} = 0$), and has a constant axial velocity $v_z(x) = v_z$. The objective function has exactly two values: $J = 1$ if the lateral particle position at the channel outlet is inside the target interval and $J = 0$ if it is outside. Since we do not include diffusion, the particle moves deterministically and its position evolves according to

$$x = x_0 + \xi^{-1} ut,$$

(6.7)

$$z = z_0 + v_z t.$$

(6.8)

For this example, we determine the optimal control force profile by graphical considerations (Fig. 6.2). The target interval has two edges, the upper target edge located at $(b, L)$ and the lower target edge located at $(-b, L)$. From any point on the line $x_+(z) = b + \frac{u_{\text{max}}}{\xi v_z} (z - L)$ (red dashed line), the particle reaches the upper target edge if we control it with maximum control force $u_{\text{max}}$. Similarly, the particle reaches the lower
6.2. Optimal control theory

Figure 6.2.: Example control problem discussed in the main text. The optimal control force is only well defined on the dashed lines emanating from the target interval (green). For all other points the optimal control force is arbitrary.

target edge from any point on the line \( x_\pm(z) = -b - \frac{u_{\text{max}}}{\xi v}(z - L) \) (blue dashed line), if we control it with maximum negative control force \(-u_{\text{max}}\). For any point between the lines \( x_\pm(z) \), the control force is arbitrary as the particle hits either the target interval or one of the lines. Above \( x_+(z) \) or below \( x_-(z) \), the control force is arbitrary too as the particle never reaches the target interval regardless of the chosen control force. In summary, the optimal control force profile reads

\[
u^*(x, z) = \begin{cases} 
\mp u_{\text{max}} & \text{if } x = \pm (b + \frac{u_{\text{max}}}{\xi v}(z - L)), \\
\tilde{u}(x) & \text{otherwise},
\end{cases}
\] (6.9)

for an arbitrary function \( \tilde{u}(x) \). The control force profile is highly irregular, since for almost all positions its value is not unique and it does not necessarily vary continuously across space.

To obtain regular, well defined and smooth, control forces we add the following regularization terms to the objective function: To avoid excessively large control forces, we penalize nonzero control forces via \( \frac{1}{2} \int_\Omega d^2x |u(x)|^2 \). To ensure smooth control forces, we penalize gradients of the control force profile by \( \frac{1}{2} \int_\Omega d^2x \left[ \lambda_x^2 |\frac{\partial}{\partial x} u(x)|^2 + \lambda_z^2 |\frac{\partial}{\partial z} u(x)|^2 \right] \). The sum of both terms gives the regularization functional

\[
J_{\text{reg}} = -\frac{1}{2} \lambda_x^2 \int_\Omega d^2x |u(x)|^2 - \frac{1}{2} \int_\Omega d^2x \left( \lambda_x^2 |\frac{\partial}{\partial x} u(x)|^2 + \lambda_z^2 |\frac{\partial}{\partial z} u(x)|^2 \right) .
\] (6.10)

The total objective functional \( J_{\text{tot}} = J + J_{\text{reg}} \) is the sum of control goal and regularization. However, the regularization does no longer allow us to interpret the total objective functional as a probability, since it is no longer strictly positive.

We need to search the optimal control force under the constraint that the Smoluchowski equation (6.1) is satisfied. We do so by using the method of Lagrange multipliers as we discuss in Sect. C.1. The result is a set of partial differential equations which determine the optimal control force.
The objective functional becomes maximal if the control force satisfies
\[ u(x) - \frac{\lambda^2}{\lambda^2} \frac{\partial^2}{\partial x^2} u(x) - \frac{\lambda^2}{\lambda^2} \frac{\partial^2}{\partial z^2} u(x) = u_0(x), \] (6.11)
where we introduced the control force without gradient regularization
\[ u_0(x) = \frac{1}{\xi \lambda^2} W(x) \frac{\partial}{\partial x} V(x). \] (6.12)
Here, we defined the cumulated density \( W(x) = \int_0^\infty dt \ P(x, t) \) and the value function \( V(x) \).

The cumulated density satisfies the time-integrated Smoluchowski equation
\[ \mathcal{L}[u] W(x) = 0, \] (6.13)
with the boundary condition \( W(x, z = 0) = P_0(x) \) at the channel inlet and \( (\xi^{-1} f_{\text{lift}}(x) - D \frac{\partial}{\partial x} W(x) = 0 \) at the channel boundary. As the cumulated density fully defines the particle positions in the channel, the time-integrated Smoluchowski equation is also called the state equation in optimal control theory [181]. We express the cumulated density in terms of the transition probability as
\[ W(x) = \int_0^\infty dt \int_{\Omega} d^2x' P(x, x'|t) P_0(x'). \] (6.14)
Here, \( P(x, x'|t) \) gives the probability that we find the particle at position \( x \) after time \( t \) if it started at position \( x' \) (Sect. 2.4.6). In Sect. D.1 we use this formulation of the cumulated density to derive the numerical approximation of Eq. (6.13).

The value function satisfies the adjoint equation
\[ \mathcal{L}^+ V(x) = 0, \] (6.15)
with the boundary condition \( V(x, z = L) = R(x) \) at the channel outlet and the boundary condition \( \frac{\partial}{\partial z} V(x) = 0 \) at the channel walls. Here, the adjoint operator \( \mathcal{L}^+[u] \) take the form
\[ \mathcal{L}^+[u] = \xi^{-1} \left( f_{\text{lift}}(x) + u(x, z) \right) \frac{\partial}{\partial x} + D \frac{\partial^2}{\partial x^2} + v_z(x) \frac{\partial}{\partial z}. \] (6.16)

To gain further insight into the role of the value function \( V \), we express it in terms of the transition probability as
\[ V(x) = \int_0^\infty dt \int_{\Omega} d^2x' R(x') P(x', x|t). \] (6.17)
The value function $V(x)$ is the expected value of the rewards if the particle starts at position $x$. Therefore, it gives the probability for the particle to eventually reach the target interval at the channel outlet from initial position $x$. Just like the state equation is a time-integrated version of the Smoluchowski equation (2.62), the adjoint equation is a time-integrated Kolmogorov-Backward equation (2.70).

We interpret the optimal control force $u(x)$ as follows: the control force without gradient regularization (6.12) is the product of the cumulated density and the gradients of the value function. The cumulated density ensures that the control force at a given position increases when it becomes more probable that the particle visits this position. Furthermore, the control force is directed along the gradients of the value function $\partial V/\partial x$. Hence, it tries to move the particle into regions where the probability of it reaching the target interval increases. With the gradient regularization terms, the control force becomes smooth on length scales $\lambda_c/\lambda$ and $\lambda_z/\lambda$.

The optimal control force as the solution of Eq. (6.11) is in general outside the range of admissible control forces $[-u_{\text{max}}, u_{\text{max}}]$. Therefore, we first determine the control force without bounds and then project it into the allowed range by

$$u(x) \rightarrow \begin{cases} u(x) & \text{if } |u(x)| < u_{\text{max}}, \\ u_{\text{max}} & \text{if } u(x) > u_{\text{max}}, \\ -u_{\text{max}} & \text{if } u(x) < -u_{\text{max}}. \end{cases}$$

(6.18)

This procedure is only an approximation of the exact optimal control problem, but gives good results in practice.

Importantly, the equation for the control force (6.11), the state equation (6.15), and the adjoint equation (6.13) are a set of coupled partial differential equations and need to be solved self-consistently. We further comment on the resulting difficulties when discussing the numerical solution in Sect. 6.2.3.

6.2.2. Particle separation

In this section, we extend the formalism for particle steering to the problem of separating two types of particles with different sizes. We use the index $i$ to denote quantities relevant to the $i$-th particle type. For both particle types, we introduce separate reward functions $R_i(x)$, but try to find a single control force $u$ to steer the particles into their respective target intervals at the channel outlet. We choose the objective functional as the probability that both particles reach their respective target

$$J = J_1 J_2.$$  

(6.19)

When we choose the target intervals non-overlapping, the optimal control force separates the particles at the channel outlet. Therefore, we call $J$ the separation probability.
We add the regularization terms (6.10) and perform the maximization, as we discuss in Sect. C.2. The optimal control force is still determined by (6.11). However, the optimal control force without gradient regularization changes into

\[
    u_0(x) = \sum_i \frac{J}{J_i \xi_i \lambda^2} W_i(x) \frac{\partial}{\partial x} V_i(x). \tag{6.20}
\]

Here, the factor \(J/J_i\) gives the probability that all particles except particle \(i\) reach their target intervals. The remaining terms have the form of the single particle control force (6.12). The value function \(V_i\) satisfies the time-integrated Kolmogorov backward equation (6.13) and the cumulated density \(W_i\) satisfies the time-integrated Smoluchowski equation (6.13). In these equations, the lift forces and axial velocities depend on the particle type, while the control force is the same. While we restrict the discussion to two different particle types, the formulae are also valid for more particles. In setting up the formalism, we restricted ourselves to dilute suspensions and did not model hydrodynamic interactions between particles.

It is instructive to consider the special case of \(N\) identical particle types. Then, the optimal control (6.20) reduces to

\[
    u_0(x) = J^{N-1} \frac{N}{\xi \lambda^2} W(x) \frac{\partial}{\partial x} V(x), \tag{6.21}
\]

where we suppressed the indices for friction coefficient, value function, and cumulated density. This is the same control force as for the single particle problem (6.12) with an effective regularization constant

\[
    \lambda_{\text{eff}} = J^{\frac{1-N}{2}} \frac{1}{\sqrt{N}} \lambda. \tag{6.22}
\]

For typical steering problems, \(J \approx 1\) and the effective regularization constant \(\lambda_{\text{eff}}\) for separating \(N\) particles is reduced by a factor \(1/\sqrt{N}\). At the same time, the length scales of the gradient regularization \((\lambda_x/\lambda, \lambda_z/\lambda)\) stay the same since Eq. (6.11) is not modified.

6.2.3. Numerical solution

We are not able to solve Eqs. (6.11), (6.15), and (6.13) analytically and therefore resort to numerical means. Here we choose the Markov chain approximation method used in stochastic optimal control theory [182]. We discuss how to apply it to our problem in appendix D.2.

The Markov chain approximation method solves the partial differential equations independently. For example, we solve for the optimal control force in (6.11), while keeping the value function and the cumulated density fixed. To search for self-consistent solutions, we further use an iterative scheme. We denote the iteration of the self-consistency
6.2. Optimal control theory

In a single iteration, we first solve for $W^{(\alpha)}, V^{(\alpha)}$ and then continue to solve for $u^{(\alpha)}$. We observed that the control force strongly oscillates between iterations. Therefore, we use the damped update scheme for the control force

$$u^{(\alpha+1)} = (1 - \gamma^{(\alpha)}) u^{(\alpha)} + \gamma^{(\alpha)} \bar{u}(W^{(\alpha)}, V^{(\alpha)}),$$

(6.23)

where we introduced $\bar{u}(W^{(\alpha)}, V^{(\alpha)})$ as the solution of equation (6.11) with value function $V^{(\alpha)}$ and cumulated density $W^{(\alpha)}$. The update rate $\gamma^{(\alpha)}$ is in general small. Specifically, we choose it as $\gamma^{(\alpha)} = 0.1/(1 + \beta \times \alpha)$, with $\beta = 0.02$ for particle steering and $\beta = 0.05$ for particle separation. Such decaying update rates are a common choice in the context of stochastic optimization of neural networks [183]. After we obtain the optimal control forces, we verify their validity with Langevin simulations discussed in Sect. D.1.

We use multi-particle collision dynamics simulations with parameters $P_2$ given in appendix E to measure the inertial lift forces and axial velocities at discrete points. We determine the values of both quantities in between these points by using a least-squares fit. For the lift force, we use the ansatz

$$f_{\text{lift}}(x) = \phi_0 x + \phi_3 x^3 + \phi_w \left[ \frac{1}{x - (1 + \delta)(w - a)} + \frac{1}{x + (1 + \delta)(w - a)} \right],$$

(6.24)

where the last term models the wall part of the lift force. It strongly increases as the particle approaches the channel walls. The offset $\delta = 10^{-3}$ removes the singularity for points on the boundary. We model the axial velocity by the ansatz

$$v_z(x) = v_0 + v_2 x^2 + v_4 x^4.$$  

(6.25)

Here, the $x^4$ term models the deviation from the parabolic behavior as discussed for channels with circular cross sections in Sect. 4.1.2. Fig. 6.3 shows least squares fits for particles with sizes $a_1 = 0.3w$ and $a_2 = 0.4w$. 

Figure 6.3.: Fits for the inertial lift force $f_{\text{lift}}$ (a) and the axial velocity $v_z$ (b) as a function of particle position $x$. The rectangles show the data points estimated from MPCD simulations. The solid curves show the fits to the functions (6.24) and (6.25). Here, $v_0$ denotes the maximum velocity of the Poiseuille flow found at the channel center.
6. Optimal control of particle separation

6.2.4. Comparison with related optimal control problems

Before presenting the results, we discuss the connection to related optimal control problems in this section. The formalism we developed is closely related to stochastic optimal control theory \[35, 38\]. Specifically, we can derive the famed Hamilton-Jacobi-Bellman equation, when we change the regularization term to

\[
J_{\text{reg}} = -\frac{1}{2} \int_{\Omega} d^2x \ W(x) |u(x)|^2. \tag{6.26}
\]

Here, we did not use the gradient regularization and included the cumulated density in the regularization. Previously, the regularization penalized large control forces everywhere, now the regularization is only active if particles are close by. Choosing this regularization allows us to eliminate the cumulated density from the problem and the Hamilton-Jacobi-Bellman equation,

\[
\max_{u(x)} \left[ L_+ [u] V(x) + \frac{1}{2} |u(x)|^2 \right] = 0, \tag{6.27}
\]

fully describes the problem. As a result, the optimal control force,

\[
u(x) = \frac{1}{\xi \lambda} \frac{\partial}{\partial x} V(x), \tag{6.28}
\]

is independent of the density. In this formulation, gradients of the value function cause nonzero control force, even if the particle never experiences the control force. In our formulation, the control force is restricted to regions visited by the particle. We pay by having to consider set of coupled partial differential equations in contrast to a single one.

Another related optimal control problem is the control of general partial differential equations \[181\]. These problems commonly assume the form

\[
\max \int dx \ F[q, u], \tag{6.29}
\]

subject to \( Aq = u \), \( \tag{6.30} \)

with some differential operator \( A \) and reward functional \( F[q, u] \). Importantly, here the differential operator \( A \) is independent of the control \( u \) in contrast to our problem, where the Smoluchowski \( L[u] \) depends on the control. This seemingly insignificant difference does greatly complicate the numerical solution for our problem as we discuss in appendix D.2. In particular, guaranteeing positive densities renders our discretization scheme non-differentiable.
6.3. Optimal particle steering

We use the optimal control method described before to steer particles into a target interval at the channel outlet. Provided the control forces are strong enough, we can steer the particles to any position at the channel outlet. Here, we consider particles with size $a/w = 0.4$ at a channel Reynolds number of $Re = 10$. We choose the channel length $L = 200w$ and the maximum control force $u_{\text{max}} = 0.264\rho v^2$. The regularization constants are $\lambda^2 = 10^{-3}$, $\lambda_x^2 = 10^{-7}$, and $\lambda_z^2 = 10^{-4}$.

In Fig. 6.4a, we plot the optimal control force profile to steer the particles into the target interval $[0.05w, 0.15w]$. We also plot 100 example trajectories obtained by Langevin simulations as the black lines. Since the Péclet number is high (Sect. 2.4.6), the stochastic fluctuations connected to thermal noise are small and the different trajectories collapse. At the channel inlet, the particles start at the equilibrium positions $x_{\text{eq}} \approx \pm 0.33$ and then move towards the channel outlet. The control force profile succeeds to guide the particles into the chosen target interval at the channel outlet.

The optimal control without smoothing (6.12) is proportional to the product of cumulated density and gradients of the value function. Hence, the control force profile follows the gradients of the value function shown in Fig. 6.4b. The value function $V(x, z)$ gives the probability that the particles reach the target interval, if they start at position $(x, z)$. Therefore, the region with $V(x, z) = 1$ extends from the target interval at the channel outlet and follows the trajectories. At the channel inlet, we find $V = 1$ for all lateral positions and the particles reach the target interval with certainty.

The control force is concentrated narrowly around the trajectories and varies smoothly in space. Changing the regularization parameters $\lambda, \lambda_x, \lambda_z$ modifies these features of the control force profile. We plot the control force profile for different values of the regularization parameter in Fig. 6.5 for $x_t = 0.1w, b = 0.15w$. With increasing $\lambda$, the

Figure 6.4.: Optimal control force $u(x, z)$ (a) and value function $V(x, z)$ (b) for steering particles into target interval (green) at the channel outlet with particle size $a = 0.4w$, Reynolds number $Re = 10$, and maximum control force $u_{\text{max}} = 0.264\rho v^2$. The black lines show independent Langevin simulations (white lines in (b)).
6. Optimal control of particle separation

Figure 6.5.: Influence of the regularization parameter $\lambda$. The control force steers the particles into the target interval $[-0.05w, 0.25w]$. All other parameters are the same as in Fig. 6.4a. With increasing regularization parameter, the control force profile becomes more confined to the trajectories.

Figure 6.6.: (a) The cumulated density $W(x_f)$ as a function of final position $x_f$ at the channel outlet for different target widths $b$ and fixed target position $x_t = 0.2w$. (b) Position $x_p$ of the peaks of the cumulated density at the channel outlet as function of target position $x_t$ for different target widths $b$. In both, the dashed black lines indicate the equilibrium position without control and the solid black line the target position.

control force profile becomes more confined and the particles remain on the equilibrium positions for longer times before the control force steers them into the target interval.

We further analyze the behavior of the particles by plotting the cumulated density at the channel outlet in Fig. 6.6a. The width of the distributions is only determined by the system temperature and is close to the line width. The particles enter the system through the channel inlet at their two equilibrium positions. For most target widths, these two positions are also reproduced at the channel outlet. Only for the smallest target interval do the peaks coalesce. We further observe how for the largest target width the outer peak aligns with the equilibrium position shown in dashed.

We plot the peak positions at the channel outlet in Fig. 6.6b as a function of target positions for different target widths. For the smallest target width $b = 0.02w$, the...
6.4. Optimal particle separation by size

The concepts used in steering particles directly apply to the problem of separating differently sized particles. In this section, we consider particles with sizes $a_s = 0.3w$ and $a_l = 0.4w$. For clarity, we use the indices $s, l$ to denote the small and large particles respectively. As in the previous section, the channel Reynolds number is $Re = 10$ and we use a maximum control force $u_{\text{max}} = 0.264\rho u^2$, if not otherwise stated. The regularization constants are $\lambda_2 = 10^{-3}$, $\lambda_x^2 = 10^{-7}$, and $\lambda_z^2 = 10^{-4}$. In the following, we neglect hydrodynamic interactions between particles. Again, we assume that the particles are already focused to their respective equilibrium positions ($x_{\text{eq},s} = \pm 0.33w$, $x_{\text{eq},l} = \pm 0.38w$), when they enter the system at the channel inlet.

First, we position the target intervals such that they contain the equilibrium positions of the particles. We try to steer the small particles to the target position $x_{t,s} = +0.3w$ and the large particles to the target position $x_{t,l} = -0.3w$, where both targets have a width $2b = 0.2w$. We plot the optimal control force profile and particle trajectories obtained by Langevin simulations for this setup in Fig. 6.7a. We are able to steer both types of particles into their respective target intervals. For both particle types, there

![Figure 6.7: Control force profile $u(x, z)$ to separate particles based on their size for wide targets which include the equilibrium position (a) and narrow targets shifted away from the equilibrium positions (b). The dashed and solid lines indicate the particle trajectory determined from independent Langevin simulations. The green bars show the target positions for the two particles.](image)
6. Optimal control of particle separation

Figure 6.8.: Value function $V(x, z)$ for the separation problem of Fig. 6.7a for the small (a) and large (b) particle. The green bars indicate the respective target intervals. The solid lines show trajectories obtained from Langevin simulations.

are particles which need to cross the channel side, and particles that do not. First, we concentrate on latter. The equilibrium positions of the small particles are closer to the channel wall than the equilibrium position of the large particles. Therefore, the small particles starting already on the correct channel side do not require any control and move directly towards their target. However, the large particles on the negative channel side have to swap places with the small particles. The control force pulls particles of both types to a single spot, where the difference between the lift force for different particle types separates them (Fig. 6.3a). Here, the optimization shapes the control force profile such, that it separates the particles close to the lateral position with maximum difference between the lift force. Finally, those particles remain, that need to change the channel side. The control force pulls these particles for both sizes together and separates them, again at the position where the difference in lift force is maximal. In sum, the control mechanism exploits the different lift forces the particles experience and steers the particles into their respective target intervals with certainty.

Fig. 6.7b shows a more complex example, which we discuss below. However, we explain the origin of the control force profile first. Similarly to the single particle problem, the control force for particle separation \((6.20)\) is the product of the cumulated density and the gradients of the value function. We plot the value function for the small particles in Fig. 6.8a and for the large particle in Fig. 6.8b. Starting from the target interval the region, where the value function is unity, widens for both particle types as we approach the channel inlet. Due to the small temperature the value function has a sharp edge. For the small particle, the trajectories closely follow this edge, whereas for the large particles, the edge of the value function is further away. As before the control force profile follows the gradients of the value function and the trajectories. Since we separate multiple types of particles, the effective regularization constant \((6.22)\) is lowered and results in nonzero control force even for regions with low particle density.

We also treat a more challenging separation problem where the target intervals are
6.4. Optimal particle separation by size

Figure 6.9.: Separation of particles in a bifurcating channel. (a) Schematic of the proposed device. At the channel inlet \((z = 0)\), particles enter the channel at their equilibrium positions. At the bifurcating channel outlet \((z = L)\), particles leave the system through the different channel arms. (b) Optimal control force profile \(u(x, z)\) to separate particles at the channel outlet. The lines show the trajectories. The green bars indicate the targets.

much small and they do not overlap with the equilibrium positions. Here, we choose the target width \(b = 0.02\) and the target positions \(x_{l,s} = 0.45w\) and \(x_{l,l} = -0.4w\). We plot the resulting control force profile in Fig. 6.7b. The separation process is similar to the setup chosen before (Fig. 6.7a). However, after the control force separates the particles, it has to further overcome the strong wall lift forces. Therefore, the control force profile is more pronounced compared to the previous system.

As we discussed in the introduction to this chapter, we imagine the control region to be part of a larger microfluidic circuit. In experiments, [Mach and Di Carlo] have demonstrated how to use a bifurcating channel outlet for particle separation [15]. Their experiment relied on the large size differences between bacteria and red blood cells. Here, we demonstrate how external control forces increase the sensitivity and reduce the required difference in particle size. Specifically, we consider the setup illustrated in Fig. 6.9a. We position the targets such that large particles exit through the side arms, while small particles exit through the center outlet. We plot the control force profile and the particle trajectories in Fig. 6.9b. Similar to the previous setups, the control force profile pulls the particles together and separates them at the position where the lift force difference is maximal. Here, the required channel lengths are much shorter compared to the previous setup. We discuss the necessary channel length in detail below. In the experiments of [Mach and Di Carlo], the bacteria and red blood cells had a size difference of approximately 900% [15]. With external control forces, we are able to separate particles with a more modest difference of only 33%. Importantly, we are also able to separate particles, that are already focused, which is not possible without external control.

For experimental realizations, the robustness against noise is an important question.
6. Optimal control of particle separation

Figure 6.10.: (a) The cumulated densities $W(x)$ for 100 different realizations of the noise of the control force for two different noise strengths $\sigma$. The shaded areas show the targets for the two particle types. The channel has a length $L = 300w$. The black solid line shows the equilibrium positions of the small particle type, the dashed black line for the large particle type. (b) The separation probability $J$ as a function of noise strength of the control force $\sigma$ over different realizations. In both plots, the setup is that of Fig. 6.7a.

To address this issue, we introduce the control force with noise

$$u_{\text{noise}}(x, z) = u(x, z) + \eta(x, z). \quad (6.31)$$

Here, the spatial noise $\eta$ has variance $\langle \eta(x, z)\eta(x', z') \rangle = \sigma^2 \delta(x - x')\delta(z - z')$ and zero mean. We use the setup of Fig. 6.7a as the basis for the following discussion, but choose the maximum control force $u_{\text{max}} = 0.226 \rho v^2$. First, we determine the control force profile $u$ without noise and then perform independent Langevin simulations with the added noise (6.31). For each simulation we averaged over 100 different realizations of the noise of the control force and 250 different realizations of the thermal noise. We plot the distributions at the channel outlet for two different noise strengths in Fig. 6.10a. The noise broadens the distributions, but the majority of the particles still reach the target interval. Here, the noise affects the small particles more strongly than the large particles.

To analyze the robustness in detail, we plot the separation probability (6.19) as a function of noise strength for different channel lengths in Fig. 6.10b. For $L \geq 180w$, the separation probability is close to unity for noise strengths $\sigma < u_{\text{max}}$. When $\sigma > u_{\text{max}}$, the separation probability decreases continuously. Here, the influence of spatial noise becomes more pronounced for decreasing channel length. Below a minimum channel length $L < 160w$, the separation probability suddenly drops even for $\sigma = 0$. For $L = 150w$, we are not able to separate the particles. However, we are still able to steer the small particles into their target intervals and reach $J = 0.5$. The robustness of the control force against spatial noise is remarkable, since we did not include this type of noise in our optimization.
6.5. Conclusions

In this chapter, we discussed how we can design control laws in inertial microfluidics with optimal control theory. Specifically, we determined optimal control force profiles for steering particles to desired target positions at the channel outlet and separating particles by size. For these problems, we formulated the objective functional and maximized it numerically.

We are able to steer particles to almost arbitrary positions at the channel outlet. The profiles of optimal control force are concentrated narrowly around the trajectories of the particles, greatly simplifying an experimental realization.

We extended the formalism to separate different particle types by size. Here, the different particle types experienced the same control force, but different inertial lift forces depending on their size. The profile of optimal control force separates the particles with help of the inertial lift forces, by steering them to positions where the difference in inertial lift force is maximal. The separation was successful for different systems inspired by experiments, provided sufficient channel length. Here, the external control greatly increases the sensitivity of the separation mechanism. Further, we are able to separate already focused particles, which is not possible in straight channels without external control. Finally, we found that the control schemes are extremely robust against imperfections in their realization. Even with variation on the order of the maximum control force, we are able to separate the particles. This resilience is surprising in so far as we did not explicitly optimize for robustness.
Conclusions

Motivated by the seminal experiments of Segré and Silberberg in 1961 [7], theory and experiment explored inertial migration since the early sixties. For years, the consensus was that fluid inertia is irrelevant in microfluidic devices [3]. Only recently, experimental and numerical studies started to explore how inertial effects influence microfluidic systems, when flow speeds are increased [10, 11]. Colloidal particles in flow experience inertial lift forces, which induce a self-organized order between the particles. A single particle assumes stable equilibrium positions in the channel cross section. In particle suspensions, particles trains along the channel axis and ultimately microfluidic crystals form [12, 19]. Over the last years, different microfluidic devices using inertial lift forces have been designed for biomedical applications. They perform functions ranging from counting particles [12], analysis of mechanical cell properties [14], to particle separation by size [15, 16].

Using external control to improve the performance of microfluidic devices has a long history [154, 184–186]. Electric and magnetic fields permit to control translational [28, 30, 185, 186] and rotational motion [28, 30, 160, 161] of particles in microfluidic flows. Notably, strongly focused laser beams known as optical tweezers [24, 28, 30] allow to create complex potential landscapes for particle motion [25–30], which can be used to separate particles by size [31]. Recent experiments started to explore external control for inertial microfluidics. External flows can probe the mechanical properties of cells [14] and magnetic fields can be used to isolate circulating tumor cells [34].

In this thesis, we explored how external control methods improve the performance of inertial microfluidic devices. We shortly review the main results in the following.

We investigated in chapter 4 how the channel geometry determines the features of inertial lift forces. We concentrated on straight channels with circular and rectangular cross sections. For circular cross sections, particles order on a Segré-Silberberg annulus consistent with the symmetry of the system. The annulus formation can be understood in terms of inertial lift forces. In particular, the stable equilibrium positions of the lift force profiles coincide with the annulus radius. We investigated in detail how the inertial lift force profiles depend on particle size and Reynolds number and found that the profiles are described in good approximation by scaling laws consistent with literature [22]. The lift forces can be related to the radial particle distributions by a Langevin equation for the diffusion inside the potential connected to the lift forces. Channels with square or rectangular cross section are characterized by discrete rotational symmetries in contrast to the continuous symmetry of circular cross sections. Therefore, the degenerate equilibrium positions in circular cross sections is replaced by a set of discrete equilibrium
7. Conclusions

positions. In square cross sections, the placement and the stability of the equilibrium positions depends on both particle size and Reynolds number. This novel result suggests a simple separation scheme by particle size. For increasing channel height only two stable equilibrium positions on the short channel axis remain. Furthermore, for sufficiently large aspect ratio the complete dynamics becomes two-dimensional. This result simplifies the design of devices using external control.

In chapter 5, we explored how electric and magnetic fields influence inertial migration and control particle motion. Specifically, we investigated electric fields directed along the channel axis and rotating magnetic fields perpendicular to the channel axis. The axial electric fields change the axial velocity of the particle. Increasing this control force slows down the particles, the lift forces decreases, and the equilibrium position of the particle moves continuously closer towards the channel center. We discussed the minimum control force required to fully control the particle as a function of Reynolds number and particle size, as this knowledge is crucial to design devices. The control mechanism resembles Saffman’s discussion of particles in shear flow [74] and is well described by the Rubinow-Keller theory [45]. In combination with a hysteretic feedback scheme the axial control force keeps the particle close to the channel center. To our surprise, the average particle speed increases even when the control force temporarily slows down the particles. Thereby, we were able to increase the particle throughput independent of the magnitude of the control force.

Next, we considered how rotating magnetic fields control inertial focusing in two dimensions. Rotating magnetic field exert torques on superparamagnetic beads and change their angular velocity [160, 161]. Here, the torques exerted on colloidal particles modify the lift force profile and drive the particle towards the channel side with higher relative surface velocity. For sufficiently strong torques only a single equilibrium position remains. When we controlled the angular velocity, the particles assumed a single equilibrium position, the location of which depends on the angular velocity. Importantly, both control methods, by axial forces and by torques, are genuine inertial and are of no avail at low Reynolds numbers.

Finally, we investigated how optimal control theory allows to design control force profiles for inertial microfluidics in chapter 6. Here, we considered two specific problems: First, we steered particles to a given target at the channel outlet. Second, we used optimal control theory to design control force profiles to separate particles based on their size. For both problems, the optimal control force profile is determined by the maximization of an objective functional, which we perform numerically. The control force profiles steer single particles with certainty to an almost arbitrary position at the channel outlet. The required control force profiles are strongly concentrated around the particle trajectories in the channel simplifying the experimental realization. For a mixture of two particle types of different size, the control force profiles separate them by size. Here, both particle types experience the same control force, but different lift forces due to the difference in size. The control force profile is designed such that the particles experience the maximum
difference in lift force. We demonstrated successful particle separation in systems inspired by experiments. The added control increases the sensitivity to particle size compared to previous designs and separates particles with similar sizes. The separation mechanism is extremely robust against stochastic variations in the control force profile.

In the context of this thesis, some questions have been left unanswered and we outline directions for future research in the following paragraphs.

Experiments and numerical simulations observe complex collective dynamics in inertial microfluidics. In particular, the dynamic assembly of particle trains and two-dimensional particle lattices was reported [12, 19]. Particle pairs show complex oscillatory motion at low and high Reynolds numbers [19, 187]. Therefore, we expect collective oscillations of particles in self-assembled microfluidic crystals similar to phononic excitations. The control of these complex structures has not yet been explored and may offer novel insights into self-organized matter.

Applied to biomedical systems, inertial microfluidics treats the inertial migration of biological cells. These cells are typically neither spherical nor rigid. Consequently, future works should consider more complex particle models either rigid non-spherical particles or flexible particles which deform in response to local shear forces. In particular, the collective behavior of soft objects and the possible existence of soft inertial crystals promise avenues for future research.

While we focused on the specific problem of particle separation, optimal control can be extended to other control goals. A possible control target is optimizing the particle throughput as we did in chapter [5]. Furthermore, extending optimal control theory to time-delayed or hysteretic systems could result in new control strategies. Finally, we propose to use optimal control theory to design channel geometries for particle separation.

In experiments cylindrical pillars were placed in microfluidic channels to modify fluid streamlines and thereby the lateral migration of colloidal particles [18]. The lateral displacement of a colloidal particle after a sequence of pillars can be described by the composition of transfer matrices which depend on the pillar positions. In this formulation, optimal control theory is applicable and determines the optimal placement of these pillars.
# Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>(x, y)</td>
<td>lateral coordinates</td>
</tr>
<tr>
<td>(z)</td>
<td>axial coordinate</td>
</tr>
<tr>
<td>(r)</td>
<td>radial coordinate</td>
</tr>
<tr>
<td>(d)</td>
<td>number of dimensions</td>
</tr>
<tr>
<td>(a)</td>
<td>vector (a = (a_x, a_y, a_z))</td>
</tr>
<tr>
<td>(a_x/a_i, (a)_i)</td>
<td>the (x)-component/ the (i)-th component of a vector</td>
</tr>
<tr>
<td>(</td>
<td>a</td>
</tr>
<tr>
<td>(A_{ij}, (A)_{ij})</td>
<td>the ((i, j))-th component of a tensor</td>
</tr>
<tr>
<td>(\hat{n})</td>
<td>normal of a surface</td>
</tr>
<tr>
<td>(\hat{e}_x, \hat{e}_y, \hat{e}_z, \hat{e}_r)</td>
<td>unit vectors in (x, y, z, r) direction</td>
</tr>
<tr>
<td>(a \cdot b)</td>
<td>dot product between two vectors (a \cdot b = \sum_i a_ib_i)</td>
</tr>
<tr>
<td>(a \cdot A)</td>
<td>tensor vector contraction ((a \cdot A)<em>i = \sum_j a_j A</em>{ji})</td>
</tr>
<tr>
<td>(A : B)</td>
<td>tensor contraction: (A : B = \sum_{ij} A_{ij}B_{ji})</td>
</tr>
<tr>
<td>(a \otimes b)</td>
<td>Kronecker product ((a \otimes b)_{ij} = a_ib_j)</td>
</tr>
<tr>
<td>(\delta_{ij})</td>
<td>Kronecker delta, (\delta_{ij} = 1) if (i = j), else (\delta_{ij} = 0).</td>
</tr>
<tr>
<td>(\nabla \cdot f)</td>
<td>divergence of a vector field (\nabla \cdot f = \frac{\partial}{\partial x} f_x + \frac{\partial}{\partial y} f_y + \frac{\partial}{\partial z} f_z)</td>
</tr>
<tr>
<td>(\nabla \cdot A)</td>
<td>divergence of a tensor field ((\nabla \cdot A)<em>i = \sum_j \frac{\partial}{\partial x_j} A</em>{ji})</td>
</tr>
<tr>
<td>(\nabla f)</td>
<td>gradient of a function (\nabla f = \left( \frac{\partial}{\partial x} f_x, \frac{\partial}{\partial y} f_y, \frac{\partial}{\partial z} f_z \right))</td>
</tr>
<tr>
<td>(\nabla \times f)</td>
<td>rotation of a vector field (\nabla \times f = \left( \frac{\partial}{\partial y} f_z - \frac{\partial}{\partial z} f_y, \frac{\partial}{\partial z} f_x - \frac{\partial}{\partial x} f_z, \frac{\partial}{\partial x} f_y - \frac{\partial}{\partial y} f_x \right))</td>
</tr>
<tr>
<td>(\nabla^2)</td>
<td>Laplace operator (\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})</td>
</tr>
<tr>
<td>(w/h)</td>
<td>half channel width / half channel height</td>
</tr>
<tr>
<td>(R)</td>
<td>channel radius</td>
</tr>
<tr>
<td>(u)</td>
<td>fluid velocity</td>
</tr>
<tr>
<td>(M)</td>
<td>colloid mass</td>
</tr>
<tr>
<td>(I)</td>
<td>colloid moment of inertia</td>
</tr>
<tr>
<td>(\xi/\xi_r)</td>
<td>translational friction coefficient / rotational friction coefficient</td>
</tr>
<tr>
<td>(x/x_\perp)</td>
<td>colloid position (x = (x, y, z)) / lateral colloid position (x_\perp = (x, y))</td>
</tr>
<tr>
<td>(v)</td>
<td>colloid velocity</td>
</tr>
<tr>
<td>(\Omega)</td>
<td>colloid angular velocity</td>
</tr>
<tr>
<td>(f)</td>
<td>force on colloid</td>
</tr>
<tr>
<td>(T)</td>
<td>torque on colloid</td>
</tr>
<tr>
<td>(P(x, t))</td>
<td>colloid probability density</td>
</tr>
</tbody>
</table>
## A. Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P(x)$</td>
<td>steady-state colloid probability density</td>
</tr>
<tr>
<td>$P(x, x'</td>
<td>t)$</td>
</tr>
<tr>
<td>$\mathcal{L}$</td>
<td>Smoluchowski operator</td>
</tr>
<tr>
<td>$\rho/\eta/\nu$</td>
<td>fluid density / dynamic shear viscosity / kinematic viscosity $\nu = \eta/\rho$.</td>
</tr>
<tr>
<td>$\eta/\eta$</td>
<td>noise</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>variance</td>
</tr>
<tr>
<td>$b$</td>
<td>full width at half maximum, target interval width</td>
</tr>
<tr>
<td>$r_{\max}, x_{\max}$</td>
<td>maximum of a probability density</td>
</tr>
<tr>
<td>$r_{eq}, x_{eq}, y_{eq}$</td>
<td>equilibrium position</td>
</tr>
</tbody>
</table>

In chapter 6 we introduce the following specific notation:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J$</td>
<td>objective function</td>
</tr>
<tr>
<td>$W(x)$</td>
<td>cumulated density, $W(x) = \int_0^\infty dt \ P(x, t)$</td>
</tr>
<tr>
<td>$V(x)$</td>
<td>value function</td>
</tr>
<tr>
<td>$R(x)$</td>
<td>rewards function</td>
</tr>
<tr>
<td>$u(x)$</td>
<td>control force</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>area of integration</td>
</tr>
<tr>
<td>$\lambda, \lambda_x, \lambda_z$</td>
<td>regularization parameters</td>
</tr>
</tbody>
</table>
Kernel density estimates

For stochastic processes, we only observe a time series of individual samples. This time series represents one specific realization of this process and repeating the experiment or simulation gives another time series. While they are certainly instructive themselves, often the system is better characterized by probability densities. Although we cannot determine these densities directly, we can estimate them from the observed samples. Here, we use the method of kernel density estimates (KDEs), which we shortly explain in this section. For a more detailed review, we refer to Ref. [188].

To explain the advantages and properties of KDEs, we contrast them with histograms, another common method used to estimate probability densities. Histograms work by subdividing the system into non-overlapping regions, called bins. For each bin, they count the number of samples inside and thereby estimate the probability density inside the bin. A popular choice in one dimension is to subdivide space into regular intervals with width $\Delta x$. Then, the histogram estimates the density $P_{\text{hist}}(x)$ at the bin center $x$ as

$$P_{\text{hist}}(x) = \frac{1}{N \Delta x} \sum_{i=0}^{N} \Theta(x_i - x + \frac{1}{2} \Delta x) \Theta(x + \frac{1}{2} \Delta x - x_i), \quad (B.1)$$

where $\Theta(x)$ is the Heaviside step function and the $x_i$ are the observed samples. Since the samples are stochastic quantities, also the density estimate is a stochastic quantity. Its reliability is commonly expressed by the variance, which gives the deviation around the expected value. The histogram estimator in its current form has a number of disadvantages, most importantly, its high variance and its discontinuous nature [188].

An alternative are kernel density estimates, which use the kernel function $K(x)$ to provide a smooth estimate of the local density. Specifically, they estimate the density as

$$P_{\text{kde}}(x) = \frac{1}{Nh} \sum_{i=1}^{N} K\left(\frac{x - x_i}{h}\right), \quad (B.2)$$

where the bandwidth $h$ gives the scale over which the density is smooth.

A typical choice of kernel function is the Gaussian kernel

$$K(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}x^2\right]. \quad (B.3)$$
B. Kernel density estimates

Figure B.1.: Comparison of histogram and KDE used to estimate the radial probability density $P(r)$. For both methods, we choose the same characteristic width ($h = 0.02R$, $\Delta x = 0.02R$). The gray lines at the bottom show about 0.05% of all radius samples used in the plot.

The kernel density estimate has two major advantages over the histogram estimator. First, it has lower variance [188]. Second, it has the same continuity properties as the employed kernel. For a Gaussian kernel, the KDE and all its derivatives are continuous. In this thesis, we typically use the method proposed by Sheather and Jones to determine the bandwidth [189].

For cylindrical coordinate systems, the transformation from Cartesian to cylindrical coordinates introduces the local area element $2\pi r$ into the probability density. Jones proposed a KDE scheme to correct for the area element [190], in which each sample is weighted proportional to the inverse of its radial distance. Then, the estimate of the probability density reads

$$P_{\text{KDE}}(r) = \frac{1}{Nh} \sum_i w_i K\left(\frac{r - r_i}{h}\right),$$  \hspace{1cm} (B.4)

were we introduced the weights

$$w_i = W/r_i.$$  \hspace{1cm} (B.5)

The normalization factor $W$ ensures that all weights sum to one.

As an example, we compare a histogram and the corresponding KDE in Fig. B.1. While both methods agree in the general behavior, the histogram shows more fluctuations compared to the KDE. Furthermore, the discontinuous nature of the histogram manifests itself as jumps, which make numerical differentiation infeasible.
C.1. Optimal particle steering

In this section, we discuss how to derive the optimal control force $u$ for the problem of particle steering introduced in Sect. 6.2.1. In the maximization of the objective functional (6.6), we have to ensure that the density satisfies the Smoluchowski equation (6.1) and the boundary conditions (6.3), (6.4). We include these constraints by using the method of Lagrange multipliers [181].

As we are not interested in the time-evolution of the system, we integrate out the time variable. Then, the objective functional (6.6) simplifies to

$$J = \int_{-w}^{+w} dx \ W(x, z = L)v_2(x)R(x),$$ \hspace{1cm} (C.1)

where we introduced the cumulated density

$$W(x) = \int_{0}^{\infty} dt \ P(x, t).$$ \hspace{1cm} (C.2)

To derive the partial differential equation describing the cumulated density, we integrate the Smoluchowski equation (6.1) and the boundary conditions over time. For the Smoluchowski equation, we obtain a time-integrated Smoluchowski equation

$${\mathcal L}W = [P(x, t)]_{t=0}^{t=\infty} = 0,$$ \hspace{1cm} (C.3)

where the density term vanishes as there are no particles in the channel initially and all particles leave the channel eventually.

The boundary conditions at the channel walls (6.4) become

$$\left( \xi^{-1}[f_{\text{lift}}(x) + u(x)] - D \frac{\partial}{\partial x} \right) W(x, z) = 0 \quad \text{for} \ x = \pm w.$$ \hspace{1cm} (C.4)

The boundary condition at the channel inlet (6.3) becomes

$$W(x, z) = P_0(x) \quad \text{for} \ z = 0.$$ \hspace{1cm} (C.5)
C. Optimal control with Lagrange multipliers

We include all constraints by functional Lagrange multipliers and further include the regularization terms (6.10). Thereby, we construct the total objective functional

\[ J_{\text{tot}}[u] = \int_{-w}^{+w} dx \, W(x, z = L)v_z(x)R(x) - \frac{1}{2} \lambda_x^2 \int_{\Omega} d\Omega \, |u(x)|^2 \]

\[ - \frac{1}{2} \int_{\Omega} d\Omega \left[ \lambda_x^2 \left( \frac{\partial}{\partial x} u(x) \right)^2 + \lambda_z^2 \left( \frac{\partial}{\partial z} u(x) \right)^2 \right] \]

\[ + \int d\Omega \, V(x) \left[ - \frac{\partial}{\partial x} [\xi^{-1}[f_{\text{lift}}(x) + u(x)] - D \frac{\partial}{\partial x}] - \frac{\partial}{\partial z} v_z(x) \right] W(x) \]  \hspace{1cm} (C.6)

\[ + \sum_{x = \pm w} \int_0^L dz \, \phi_x(z) \left[ \xi^{-1}[f_{\text{lift}}(x) + u(x, z)] - D \frac{\partial}{\partial x} \right] W(x, z) \]

\[ + \int_{-w}^{+w} dx \, \chi(x) [W(x, 0) - P_0(x)] . \]

Here, the value function \( V(x) \) acts as the Lagrange multiplier for the time integrated Smoluchowski equation. We also introduce the function \( \phi_{\pm w}(z) \) for the boundary conditions on the channel walls and the function \( \chi(x) \) for the boundary condition at the channel inlet. To obtain the optimal control under the constraints, we have search \( u \) such, that the variations of \( J_{\text{tot}}[u] \) with respect to \( W, u, V, \phi_{\pm w}, \chi \) vanish independently.

By construction, a vanishing variation with respect to the Lagrange multipliers yields the constraints and only the variation with respect to the cumulated density \( W \) and the control force \( u \) remain. Since the objective functional contains spatial derivatives boundary terms require special care, similar to the Euler-Lagrange equations in classical mechanics [91]. We resolve this problem by using integration by parts and demanding that the surface terms vanish. This procedure yields partial differential equations and boundary conditions for the Lagrange multipliers.

By varying the cumulated density, we arrive at

\[ J[W + \delta W] - J[W] = \int d\Omega \, \delta W \left[ D \frac{\partial^2}{\partial x^2} + \xi^{-1}[f_{\text{lift}} + u(\partial_x + v_z \partial_z)] V \right] \]

\[ + \int_{-w}^{+w} dx \, \delta W v_z(V - R) \bigg|_{x=L} + \int_{-w}^{+w} dx \, \delta W (\chi(x) - v_z V) \bigg|_{x=0} \]

\[ + \int_0^L dz \, \delta W \left[ \phi_x(z) - V \right] \xi^{-1}[f_{\text{lift}} + u] - D \frac{\partial}{\partial z} V \bigg|_{x=\pm w} \]

\[ - \int_0^L dz \left( \frac{\partial}{\partial x} \delta W \right) D(\phi_x(z) - V) \bigg|_{x=\pm w} + O(\delta W^2) . \]  \hspace{1cm} (C.7)

Demanding that the derivate of the variation \( \delta W \) does not enter the first order variation
of $J$ gives the condition
\[ \phi_x(z) = V(x, z) \quad \text{for } x = \pm w. \quad (C.8) \]

The remaining terms give the partial differential equation for the value function
\[ \left[ D \frac{\partial^2}{\partial x^2} + \xi^{-1}(f_{\text{lift}} + u) \frac{\partial}{\partial x} + v_z \frac{\partial}{\partial z} \right] V = 0, \quad (C.9) \]
with the boundary conditions
\[ \frac{\partial}{\partial x} V(x, z) = 0 \quad \text{for } x = \pm w, \quad (C.10) \]
\[ V(x, z) = R(x) \quad \text{for } z = L. \quad (C.11) \]

We also find that the Lagrange multiplier for the boundary condition at the channel inlet has to satisfy
\[ \chi(x) = v_z(x) V(x, z) \quad \text{for } z = 0. \quad (C.12) \]

The variation of the objective functional with respect to $u$ reads
\[ J[u + \delta u] - J[u] = \int dx \delta u \left[ \xi^{-1}W(x) \frac{\partial}{\partial x} V(x) - \lambda u(x) + \lambda^2_x \frac{\partial^2}{\partial x^2} u(x) + \lambda^2_z \frac{\partial^2}{\partial z^2} u(x) \right] 
\]
\[ + \int_0^L dz \delta u \left[ \lambda_x \frac{\partial}{\partial x} u + \xi^{-1} (\phi_x(z) - V(x, z)) \right]_{x=\pm w} 
\]
\[ + \int_{-w}^{+w} dx \delta u \left[ \lambda_z \frac{\partial}{\partial z} u \right]_{z=0,L} + O(\delta u^2). \quad (C.13) \]

Demanding that the variation of $J$ vanishes for all $\delta u$, yields the following partial differential equation for $u$
\[ \lambda^2_x u(x) - \lambda^2_x \frac{\partial^2}{\partial x^2} u(x) - \lambda^2_z \frac{\partial^2}{\partial z^2} u(x) = \xi^{-1}W(x) \frac{\partial}{\partial x} V(x), \quad (C.14) \]
with the boundary conditions
\[ \frac{\partial}{\partial x} u = 0 \quad \text{for } x = \pm w, \quad (C.15) \]
\[ \frac{\partial}{\partial z} u = 0 \quad \text{for } z = 0, L. \quad (C.16) \]

We discretize the resulting equations by using Markov-chain approximation methods introduced in Sect. D.2.
C. Optimal control with Lagrange multipliers

C.2. Optimal particle separation

For optimal particle separation, we try to steer different particle types to different target intervals at the channel outlet (Sect. 6.2.2). We index all quantities by \( i \) to denote the particle type. The probability that particles of type \( i \) reach their targets reads

\[
J_i = \int_{-w}^{+w} dx \ W_i(x, z = L)v_{z,i}(x)R_i(x). \tag{C.17}
\]

To include the Smoluchowski equation and the boundary conditions, we use independent Lagrange multipliers for each particle type. In the following, we use the symbol \( \tilde{V}_i \) for the Lagrange multipliers of the Smoluchowski equation, as they are related, but not equal to the value function. We comment on this fact below.

The total objective function reads

\[
J_{\text{tot}} = \prod_i J_i + \sum_i \int_\Omega dx^2 \tilde{V}_i \mathcal{L}_i W_i + \sum_i \int_{-w}^{+w} dx \chi_i (W_i - P_{0,i}) + \sum_i \sum_{x=\pm w} \int_0^L dz \phi_{x,i} \left[ \xi_i^{-1}(f_{\text{fin}},i + u) - D_i \frac{\partial}{\partial x} \right] W_i \tag{C.18}
\]

\[- \frac{1}{2} \int_\Omega dx^2 \left[ \lambda^2 |u|^2 + \lambda_x^2 \frac{\partial}{\partial x} |u|^2 + \lambda_z^2 \frac{\partial}{\partial z} |u|^2 \right].\]

Since the necessary steps are identical to the ones presented in the previous section, we state only the results and do not present their derivation. When varying the objective functional with respect to \( W_i \), we arrive at the partial differential equation for \( \tilde{V}_i \)

\[
\mathcal{L}_i^+ \tilde{V}_i = 0, \tag{C.19}
\]

with the boundary conditions

\[
\tilde{V}_i(x, z) = \frac{J}{J_i} R_i(x) \quad \text{for } z = L, \tag{C.20}
\]

\[
\frac{\partial}{\partial x} \tilde{V}_i(x, z) = 0 \quad \text{for } x = \pm w. \tag{C.21}
\]

Here, the factor \( J/J_i = \prod_{k \neq i} J_k \) is the probability that particles of all types but the \( i \)-th reach their respective target intervals.

The variation with respect to \( u \) yields

\[
\lambda^2 u(x) - \lambda_x^2 \frac{\partial^2}{\partial x^2} u(x) - \lambda_z^2 \frac{\partial^2}{\partial z^2} u(x) = \sum_i \frac{1}{\xi_i} W_i(x) \frac{\partial}{\partial x} \tilde{V}_i(x), \tag{C.22}
\]
with the boundary conditions
\[
\frac{\partial}{\partial x} u = 0 \quad \text{for } x = \pm w, \quad (C.23)
\]
\[
\frac{\partial}{\partial z} u = 0 \quad \text{for } z = 0, L. \quad (C.24)
\]

We introduce the value function with the same interpretation as before by defining it as \( V_i = J_i \tilde{V}_i / J \). Finally, we arrive at the adjoint equation
\[
\mathcal{L}_i^+ V_i = 0, \quad (C.25)
\]
with boundary conditions
\[
V_i(x, z) = R_i(x) \quad \text{for } z = L, \quad (C.26)
\]
\[
\frac{\partial}{\partial x} V_i(x, z) = 0 \quad \text{for } x = \pm w. \quad (C.27)
\]

Then, the partial differential equation for the control force changes into
\[
\lambda^2 u(x) - \lambda_x^2 \frac{\partial^2}{\partial x^2} u(x) - \lambda_z^2 \frac{\partial^2}{\partial z^2} u(x) = \sum_i \frac{J_i}{J \xi_i} W_i(x) \frac{\partial}{\partial x} V_i(x), \quad (C.28)
\]
with the boundary conditions (C.23) and (C.24).
### Numerical methods for stochastic systems

#### D.1. Euler method for the Langevin equation

Throughout this thesis, we use the overdamped Langevin equation (2.55) to describe the motion of particles under the influence of thermal noise. To model it numerically, we discretize it using the Euler scheme for stochastic processes [191]

\[
x(t + \Delta t) = x(t) + \frac{\Delta t}{\xi} f_{\text{lift}}(x(t)) + \Delta W(t).
\]  

Here, the increment \(\Delta W\) describes the noise. To reproduce the correct diffusive behavior, it has to satisfy \(\Delta W(t) = 2\Delta t k_B T / \xi g(t)\), where the components \(g_i(t)\) are independent Gaussian variables with zero mean and unit variance.

#### D.2. Markov chain approximation methods

In this section, we explain how we solve the partial differential equations for the optimal control problem in chapter 6 numerically. First, we describe how solve the adjoint equation (6.15) and state equation (6.13). Then, we describe how to solve the optimality condition (6.11) for the control force.

##### D.2.1. Adjoint equation and state equation

The Smoluchowski equation (2.62) describes the evolution of probability densities in time. In this section, we discuss its numerical solution by the Markov Chain Approximation Method (MCAM) [182]. The MCAM describes a continuous random process by a jump process on a lattice. It offers great flexibility in constructing the approximating lattice process and is, therefore, highly beneficial for optimal control problems. In these problems, the control force is constantly adapted and the coefficients of the Smoluchowski equation change. The MCAM allows to construct the jump process such that densities are guaranteed to stay positive even under changing control force.

Our aim is to describe the density in the area \(\Omega = [-w, w] \times [0, L]\), introduced in Sect. 6.1. We discretize the area by an equidistant lattice with spacing \(\Delta x\) in \(x\) direction and lattice spacing \(\Delta z\) in \(z\) direction. On this lattice, we introduce the jump probability
$P_{ij}(u)$ to jump from lattice position $x_j$ to lattice position $x_i$ in a single time step $\Delta t$. Here, the probability depends on the current control force $u$. For simplicity, we only consider next nearest neighbor jumps and define the set $NN(j)$ of next nearest neighbors for lattice position $x_j$. We construct the jump probability such, that the first two local moments of the displacement $\Delta x_{ij} = x_i - x_j$ approximately coincide for the discrete and continuous system (Sect. 6.1). The drift, or mean displacement, in time $\Delta t$ has to satisfy

$$\sum_{i \in NN(j)} P_{ij}(u) \Delta x_{ij} = [(f_{\text{lift}}(x) + u(x,z))\hat{e}_x + v_z(x)\hat{e}_z] \Delta t.$$  \hspace{1cm} (D.2)

Further, the diffusion, or mean squared displacement, in time $\Delta t$ has to satisfy

$$\sum_{i \in NN(j)} P_{ij}(u) \Delta x_{ij} \otimes \Delta x_{ij} = 2D\hat{e}_x \otimes \hat{e}_x \Delta t + O(\Delta t^{3/2}).$$  \hspace{1cm} (D.3)

Whereas we reproduce the local drift exactly, we can do so only approximately for the local mean squared displacement.

To satisfy these conditions, we choose the jump probability as

$$P_{ij}(u) = \begin{cases} 
\xi^{-1} ([f_{\text{lift}}(x_j)]^+ + [u(x_j)]^+) \frac{\Delta t}{\Delta x} + \frac{D\Delta t}{(\Delta x)^2} & \text{if } \Delta x_{ij} = +\Delta x \hat{e}_x, \\
\xi^{-1} ([f_{\text{lift}}(x_j)]^- + [u(x_j)]^-) \frac{\Delta t}{\Delta x} + \frac{D\Delta t}{(\Delta x)^2} & \text{if } \Delta x_{ij} = -\Delta x \hat{e}_x, \\
v_z(x_j) \frac{\Delta t}{\Delta z} & \text{if } \Delta x_{ij} = +\Delta z \hat{e}_z, \\
0 & \text{if } \Delta x_{ij} = -\Delta z \hat{e}_z, \\
\xi^{-1}(u_{\text{max}} - |u(x_j)|) \frac{\Delta t}{\Delta x} & \text{if } x_i = x_j.
\end{cases}$$  \hspace{1cm} (D.4)

Here, we defined $[u]^\pm = \max(\pm u, 0)$ and similarly $[f_{\text{lift}}]^\pm$. This choice of jump probabilities ensures that they are always positive and, thereby, the particle density assumes only positive values. However, the terms involving $[u]^\pm$ render the jump probabilities non-differentiable in $u$. Finally, the jump probabilities have to sum to one, $P_{jj} + \sum_{i \in NN(j)} P_{ij} = 1$. We choose the time step $\Delta t$ such that this relation holds. As the drift depends on the grid position, the time step depends too on the lattice position. It is defined by

$$\Delta t_{\text{j}}^{-1} = \frac{1}{\xi \Delta x} ([f_{\text{lift}}(x_j)] + u_{\text{max}}) + v_z(x_j) \frac{1}{\Delta z} + D \frac{1}{(\Delta x)^2}.$$  \hspace{1cm} (D.5)

By construction, the local control force $u(x_j)$ does not enter the time step, since the probability to stay at a lattice positions $P_{jj}$ cancels any contribution. The local time step does not allow to define a globally consistent time. However, as we are only interested in steady-state solutions, this fact does not pose a problem. On the contrary, the local
time step is always the maximum time step possible and the system approaches steady state as fast as possible.

To close the system, we include the boundary conditions by modifying the transition probabilities on the boundaries. For the channel inlet \((z = 0)\) and channel outlet \((z = L)\), we set the probability to jump in positive \(z\) direction to unity. Therefore, all other probabilities are zero. On the channel walls, we set the probability to jump through the wall to zero and add its contribution to the probability to stay at the current position.

The matrix \(P_{ij}(u)\) gives the probability of a jump after a single step, for \(n\) steps the probability of jumping from \(x_j\) to \(x_i\) is given by the matrix exponential

\[
[P^n(u)]_{ij} = \sum_{k_1} \cdots \sum_{k_n} P_{i_{k_1}k_1} P_{k_1k_2} \cdots P_{k_{n-1}k_n} P_{k_nj}.
\]

The matrix \(P^n(u)\) is analogous to the transition probability defined in Sect. 2.4.6. However, we measure time in the number of jumps performed not in the actual time passed.

We expressed the cumulated density \(W\) as the integral (6.14). A straightforward discretization on the lattice is the sum

\[
W_i = \sum_{n=0}^{\infty} \sum_j \Delta t_i [P^n(u)]_{ij} P_{0,j},
\]

where \(P_{0,j}\) is the initial density at lattice position \(x_j\). We rewrite this equation as follows

\[
W_i = \sum_{n=1}^{\infty} \sum_j \Delta t_i [P^n(u)]_{ij} P_{0,j} + \Delta t_i P_{0,i}
\]

\[
= \sum_k P_{ik}(u) \sum_{n=0}^{\infty} \sum_j \Delta t_k [P^n(u)]_{kj} P_{0,j} + \Delta t_i P_{0,i}
\]

\[
= \sum_k P_{ik}(u) W_k + \Delta t_i P_{0,i}.
\]

This form suggests, that \(W_i\) is the steady state of the dynamic equation

\[
W_i^{(n+1)} = \sum_j P_{ij}(u) W_j^{(n)} + \Delta t_i P_{0,i}.
\]

The properties of the jump matrix ensure that the fix point \(W\) exists, and further, that it is the unique solution \([182]\). Therefore, the cumulated density \(W = W^{(n)}\) satisfies Eq. (D.7), for \(n \to \infty\).

Analogous to the cumulated density, we discretize the integral definition of the value function (6.17) by the sum

\[
V_i = \sum_{n=0}^{\infty} \sum_j \Delta t_j R_j [P^n(u)]_{ji},
\]
where $R_j$ is value of the rewards function at lattice position $x_j$. By similar arguments as before, we interpret the value function as the steady state of

$$V_i^{(n+1)} = \sum_j P_{ji}(u)V_j^{(n)} + \Delta t_i R_i.$$  \hfill (D.13)

Again, the steady state does always exist and is unique [182].

**D.2.2. Optimal control equation**

In this section, we discretize the partial differential equation that gives the optimal control force (6.11),

$$u(x) - \frac{\lambda_x^2}{\lambda_x^2} \frac{\partial^2}{\partial x^2} u(x) - \frac{\lambda_z^2}{\lambda_z^2} \frac{\partial^2}{\partial z^2} u(x) = u_0(x),$$  \hfill (D.14)

with $u_0$ being dependent on the cumulated density $W$ and value function $V$, both approximated in the last section.

We use the MCAM to solve this equation too, after we interpret its solution $u(x)$ as the steady state of the diffusion equation

$$\frac{\partial}{\partial t} u(x,t) = \frac{\lambda_x^2}{\lambda_x^2} \frac{\partial^2}{\partial x^2} u(x,t) + \frac{\lambda_z^2}{\lambda_z^2} \frac{\partial^2}{\partial z^2} u(x,t) - u(x,t) + u_0(x),$$  \hfill (D.15)

with the source term $u_0(x)$ and the loss term $u(x,t)$. The optimal control force is given by the steady state $u(x) = \lim_{t \to \infty} u(x,t)$. Here, the time variable $t$ has no physical meaning and is only introduced to interpret the optimality condition (D.14) as a diffusion equation. For the diffusion part of this equation, we introduce the probability to jump from lattice position $x_j$ to $x_i$ as

$$\Gamma_{ij} = \begin{cases} 
\frac{\lambda_x^2 \Delta t_u}{\lambda_x^2 (\Delta x)^2} & \text{if } \Delta x_{ij} = \pm \Delta_x \hat{e}_x, \\
\frac{\lambda_z^2 \Delta t_u}{\lambda_z^2 (\Delta z)^2} & \text{if } \Delta x_{ij} = \pm \Delta_z \hat{e}_z, \\
0 & \text{if } x_i = x_j.
\end{cases}$$  \hfill (D.16)

In the continuous equation, the loss term removes the particle with rate 1 from the lattice. For the discrete process, the particle is removed in each time-step with probability $\Delta t_u$. The probabilities of jumping to another lattice position and removal of the particle from the lattice have to sum to one

$$\Delta t_u + \sum_{i \in NN(j)} \Gamma_{ij} = 1.$$  \hfill (D.17)

This relationship fixes the time step $\Delta t_u$. In contrast to the previous section, the time step does not depend on the lattice position.
Then, the complete lattice process for the discretized control force reads

\[ u_{i}^{(n+1)} = \sum_{j} \Gamma_{ij} u_{j}^{(n)} + \Delta t_u u_0. \] (D.18)

In the limit \( n \to \infty \), \( u^{(n)} \) gives the optimal control force.

We have to discretize the source term \( u_0 \) in Eq. (D.18) with special care. Since the value function may develop discontinuities, we have to use one sided differences in the approximation of Eq. (6.12). Depending on the chosen direction, we obtain two possible discretizations of the source term

\[ u_0^{\pm}(x) = 1/\lambda^2 \sum_{i} J_i \xi_i W_i(x) \frac{\pm[V_i(x+\Delta x, z) - V_i(x, z)]}{\Delta x}. \] (D.19)

We choose the control force resulting in the larger increase of the objective functional, which is the control force with the larger absolute value \( |u_0^+| \) or \( |u_0^-| \).
In this chapter, we present the simulation parameters used throughout the thesis. For multi-particle collision dynamics (MPCD), we discuss how choose the parameters in Sect. 3.2.5. For the lattice Boltzmann method (LBM), we discuss it in Sect. 3.3.5.

[P1] MPCD for channels with circular cross section

We use the number of particles per cell \( n = 10 \) and Knudsen number \( \text{Kn} = 0.004 \) for all Reynolds numbers. We implement these parameters by using particle mass \( m = 1 \), temperature \( k_B T = 1 \), and collision time step \( \Delta t_c = 0.1 \). The channel has radius \( R = 25 \) and length \( L = 250 \). Along the axial direction, we apply periodic boundary conditions. Here, we vary the number of cells per radius to satisfy the Mach bounds for different Reynolds numbers as discussed in Sect. 3.2.5. In particular, we use \( N_R = 25 \) for \( \text{Re} = 40 \) and \( N_R = 20 \) for \( \text{Re} < 40 \). We implement these parameters by choosing the cell size \( l_c = 1.0 \) for \( \text{Re} = 40 \) and \( l_c = 1.25 \) for \( \text{Re} < 40 \).

[P2] MPCD for channels with rectangular cross sections

We choose the cell size \( l_c = 1 \), \( n = 20 \) particles per cell with mass \( m = 1 \), temperature \( T = 1 \), and collision time \( \Delta t_c = 0.1 \). The channel has width of \( 2w = 25 \), height \( 2h = 60 \), and length \( L = 125 \). We apply periodic boundary conditions along the axial directions. These parameters result in \( N_w = 12.5 \) cells per half width and a Knudsen number \( \text{Kn} \approx 0.008 \).

[P3] MPCD for two-dimensional, planar channels

For the two-dimensional simulations, we choose temperature \( T = 1 \), collision time \( \Delta t_c = 0.1 \), and \( n = 10 \) particles per cell with mass \( m = 1 \). The channel has width \( 2w = 36 \) and length \( L = 100 \) with periodic boundary conditions in \( z \) direction. Further, we use \( N_w = 18 \) cells per half width and obtain a Knudsen number \( \text{Kn} \approx 0.008 \).

[P4] LBM for channels with rectangular cross sections

For the LBM simulations, we discretize the total channel width including walls by \( N_x = 101 \) lattice points in \( x \) direction. In \( y \) direction, we choose \( N_y \) lattice points such that we reproduce the correct aspect ratio \( (w/h \approx N_x/N_y) \). To minimize the influence of
E. Parameters

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<th>Re</th>
<th>Ma</th>
<th>$\tau$</th>
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</tr>
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</table>

Table E.1.: The Mach number Ma and relaxation time $\tau$ used in the lattice Boltzmann simulations.

the periodic images of the colloidal particle, we use $N_z$ lattice points in the periodic $z$ direction such that the length of the channel satisfies $N_z/N_x \approx L/2w = 10a/w$, with the colloid radius $a$. To increase the accuracy of the immersed boundary method, we use the Mach number Ma and relaxation time $\tau$ for a given Reynolds number Re given in table E.1.
List of publications


Bibliography


Bibliography


Bibliography


Bibliography


Zusammenfassung


Zuletzt untersuchen wir die Anwendungen der Theorie der optimalen Kontrolle, um damit Profile von Kontrollkräften in optimaler Weise zu gestalten. Wir entwickeln den notwendigen Formalismus und beschreiben die numerische Methode um Profile optimaler Kontrolle zu bestimmen. Wir zeigen, dass die Kontrollprofile in der Lage sind Teilchen zu gewünschten Positionen am Kanalende zu steuern. Darüber hinaus demonstrieren wir die Trennung verschiedener Teilchen anhand ihrer Größe. Dabei erhöht die zusätzliche Kontrolle die Effizienz verglichen mit passiven Systemen und ist extrem robust gegenüber Störungen.
Abstract

The young field of inertial microfluidics investigates fluid inertia to enhance the performance of microfluidic devices. The scope of inertial microfluidics expanded rapidly to cover a diverse set of applications, after the first devices were proposed in the early 2000s. Recently, devices have been demonstrated for counting, cells, testing the mechanical properties of cells, and separating particles by size. Devices in inertial microfluidics rely on a self-organized order between particles induced by inertial lift forces.

In this thesis, we investigate how inertial microfluidics benefits from the application of external control. Here, we place a special emphasis on feedback control and optimal control theory. In contrast to open-loop control, feedback control does not use a fixed control law, but adapts it to the current system state. Therefore, feedback control is typically less sensitive to noise. Optimal control theory offers a mathematical way to design (feedback) control laws that are optimal with respect to a given performance measure.

First, we use mesoscopic simulations methods, specifically multi-particle collision dynamics and the lattice Boltzmann method, to investigate inertial focusing. In particular, we concentrate on how the channel geometry influences the inertial lift force profiles. In channels with circular cross sections, particles collect on the Segré-Silberberg annulus. In channels with rectangular cross sections, the reduced symmetry restricts the particles to a discrete set of equilibrium positions. Particle size and flow speed strongly influence the position and stability of the equilibrium positions. The system becomes effectively two-dimensional if the height of the channel is large compared to its width.

We further investigate the control of the inertial lift forces profiles using external electromagnetic fields. First, we slow particles down by an external electric field directed against the flow velocity. The field reduces the inertial lift forces and moves the equilibrium positions closer to the channel center. Thereby, we are able to control the particle motion. In combination with an hysteretic feedback law, axial control forces increase the particle throughput. Second, magnetic fields exert additional torques on the particles and change their angular velocity. As a result, they too change the inertial lift force profiles. When we control the angular velocity of the particles, we are able to focus them onto a single equilibrium position controlled by the chosen angular velocity.

Finally, we investigate optimal control theory for designing optimal control force profiles for particle steering and separation. We develop the necessary formalism and describe the numerical solution technique to determine the optimal control force. We show that the designed control force profiles are able to steer single particles into a target interval at the channel outlet. Furthermore, we demonstrate how to separate particles by size. Here, the external control force strongly increases the sensitivity compared to similar passive devices. Importantly, the optimal control force profiles are very robust against imperfections.
Acknowledgments

The shape and form of this thesis is influenced by many people and its successful completion would not have been possible without them. First, I would like to acknowledge the continuing support by Prof. Dr. Holger Stark. His supervision and guidance played a vital role in shaping this work. I am equally grateful to Prof. Dr. Roland Netz, who kindly examined this work, and Prof. Dr. Martin Oestreich, who served as head of the committee in the defense. I am happy to have received funding by the Deutsche Forschungsgemeinschaft. The framework program SFB910 provided an extremely welcoming atmosphere and allowed me to meet and learn from many inspiring people. While working on this project, I was lucky enough to work with great colleagues. I am indebted to the working group as a whole for discussions, support, and inspiration. In particular, I want to extend my thanks to Dr. Katrin Wolff and Dr. Andreas Zöttl. Their knowledge and advice has shaped many facets of this work. Special thanks belong to my friends who offered countless hours of advice and helped shape this thesis in so many aspects. I am most grateful to my family, my mother and my two sisters. Their love and support accompanied me every step of this journey and made its completion possible.