Multi-scale simulations with complex automata: In-stent restenosis and suspension flow

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Citation for published version (APA):
Chapter 4

Suspension Flow

In this chapter a multi-scale system will be described in which we apply a coupling scheme which is different to those used in the ISR model in the previous chapter. Focusing on simulations of macroscopic flow behavior of non-Brownian monodisperse hard-sphere suspensions we will investigate the application of the Heterogeneous Multi-scale Method (HMM) [7] to this type of systems.

The original aim of the work on suspension modeling has been to provide a submodel for detailed simulations of blood flow on the scale of the blood cells in a layer along the boundary to the SMC domain which would then have been coupled to the coarser bulk flow. However, instead of appropriate coupling of two models in a multi-domain approach (as for example in [89]) we consider the flow domain to be a single domain where a macro-scale model for the non-Newtonian hydrodynamics is coupled everywhere to a micro-model for the suspension’s micro-dynamics (see Chapter 2 and the classification of multi-scale problems in Fig. 2.5). Each of the model’s spatio-temporal domains $A_{m,M}(\Delta x_{m,M}, \Delta t_{m,M}, L_{m,M}, T_{m,M})$ is chosen such that typical temporal, $\tau_{m,M}$, and spatial scales, $\xi_{m,M}$, of the phenomena can be resolved on the micro scale (denoted by subscript m), or macro scale (denoted by subscript M), respectively.

The remainder of this chapter will be as follows. In Sec. 4.1 an overview of the rheology of hard-sphere suspensions is given in the aspects that are important to our simulation approach. In Sec. 4.2 the idea of how suspension flow can be simulated using the HMM approach will be presented. Subsections discuss the scales and their separation in this type of systems (Sec. 4.2.4) and consequences of the choice of simulation methods. Also, the proposed multi-scale model will be discussed with the help of the scale separation map and sub-execution loops, helpful tools offered by the CxA formalism. The subsequent section will discuss the modeling of the fully resolved micro-scale of the suspension with the Lattice-Boltzmann method (LBM). In that two major improvements regarding this method are proposed. First, Lees-Edwards boundary conditions (LEbc) are presented which remove the side-effects that walls have in a commonly used Couette type of shear flow on the microstructure. Second, a correction to the momentum exchange algorithm (MEA) commonly used in LBM suspension methods is proposed that restores Galileian invariance of the particle dynamics. Section 4.5 is dedicated to the phenomenon of shear-induced diffusion in non-Brownian suspensions including a description of diffusivity measurements on the micro-scale as well as the appropriate modeling of...
advection-diffusion with a flow-aligned anisotropic diffusivity tensor on the macro-scale. Section 4.6.2 discusses the possibility of using a database coupled in between micro and macro-models which significantly reduces the number of micro simulations to be launched. In the last two sections simulation results for macroscopical flow through a straight channel are presented and discussed in a comparison to other models and experiments addressing the same flow problem.

4.1 Rheology of Hard-Sphere Suspensions

The dynamics of dense liquid-particle suspensions is of great importance for many physical, biological and industrial processes. Suspension behavior is rich in rheological aspects triggered by various properties such as particle-fluid volume density, particle shape, size distribution and properties of the suspending fluid [90, 91, 92, 93]. Depending on the situation, the apparent viscosity $\nu_{\text{app}}$, the crucial property describing a (complex) fluid at the macroscopic scale in general, is a function of almost all the parameters characterizing these properties. The effect of the volume ratio $\phi$ is best described by the Krieger-Dougherty relation

$$\nu_{\text{app}} = \nu_t \left( 1 - \frac{\phi}{\phi_{\text{max}}} \right)^{-[\eta] \phi_{\text{max}}}$$

(4.1)

which describes the divergence of $\nu_{\text{app}}$ when $\phi$ gets closer to the maximum density $\phi_{\text{max}}$ at which the suspension jams. For a system of disks in 2D $\phi_{\text{max}} = \pi/4 \approx 0.785$ which is the density of the densest square lattice packing and which lower than the maximum packing density of $\approx 0.95$ for hexagonal packing of monodisperse particles. The square lattice packing gives the maximum packing density at which layers of particles still can move in a sheared flow. When particles get stuck in formations that percolate the whole system no further movement is possible. This leads to a divergence of the apparent viscosity scaling like a power law $\nu_{\text{app}} \sim (\phi - \phi_{\text{max}})^{-\alpha}$ with a critical exponent $\alpha \approx 2$ in 2D. In case of non-spherical particles this effect sets in at even lower $\phi$ whereas suspensions with a non-Dirac distribution of particle sizes have higher $\phi_{\text{max}}$ [94]. The factor $[\eta]$ in (4.1) is the intrinsic viscosity which depends on shape and additional interactions between the particles. For spherical non-colloid particles $[\eta] = 2.5$. In the limit of small $\phi$ (4.1) reproduces the linear increase $\nu_{\text{app}} = \nu_t (1 + 2.5\phi)$ as derived by Einstein [95, 96] under the assumption that particles do not interact hydrodynamically and Brownian motion can be neglected.

Central role in this work plays the influence of the shear rate $\dot{\gamma}$ on $\nu_{\text{app}}$. Different types of viscosity behavior can be observed in an unit-less parameter space described by the Reynolds number $\text{Re}_p = 4\dot{\gamma} R^2 / \nu_t$, expressing the ratio of inertial forces to viscous forces, and the Peclet number $\text{Pe}_p = 4\dot{\gamma} R^2 / D$, the ratio of advection time scale to that of diffusion (where $\dot{\gamma} R$ denotes a typical velocity, $R$ the particle radius, $\nu_t$ the kinematic viscosity of the fluid, and $D$ the Stokes-Einstein diffusivity of a single particle).

In general, from low to high $\text{Pe}_p$ a hard-sphere suspension shows the following behavior [97] (see Fig. 4.1): for small $\text{Pe}_p < 1$ thermal fluctuations govern the system dynamics and lead to an increased viscosity due to the increased effective volume of the particles. In this regime $\nu_{\text{app}}(\text{Pe}_p)$ shows a high plateau. Increasing the shear rate $\dot{\gamma}$ to mediate $1 < \text{Pe}_p < 50$ causes the viscosity to exhibit
shear-thinning due to the decreasing influence of Brownian motion, followed by a Newtonian plateau where particle dynamics is governed by Stokesian drag forces and particles are believed to form layers that are easily sheared \([98, 94]\). Increasing \(\dot{\gamma}\) further causes the suspension to thicken as consequence of a breaking of the layers in a order-disorder transition (ODT) \([98, 99]\) where particles now collide with smaller impact parameters and therefore higher momentum exchange. Going to even higher \(Pe_p\) on the microstructural level this is accompanied by ever closer approaches of particles and the formation of non-compact elongated (hydro-)clusters whose sizes in case of dense suspensions eventually diverges in the process of jamming \([100, 101, 102, 103]\).

The question about the origin of shear-thickening is still not answered consistently. Considerable experimental effort has been applied through the study of mono-disperse steric stabilized particles and charged latices. However, these are contradictory in some aspects. Theoretical approaches are limited by the need to include both many-body non-equilibrium distribution functions and hydrodynamic interactions.

Both processes might contribute to the increase in \(\nu_{app}\), the breaking of particle layers that might have formed as a consequence of leveled Brownian and hydrodynamical forces and the formation of clusters at higher shear rates as a consequence of particle inertia and the dissipative nature of the hydrodynamical interaction between particles. The two components of the viscosity, Brownian thermodynamical (elastic-like) and hydrodynamic (viscous-like), respectively, differ substantially between clustering theory and the order-disorder transition theory. The thermodynamical component decays as \(Pe_p^{-1}\) \([105]\) (constant elastic stress) whereas the hydrodynamical component is clearly associated to the onset and course of shear-thickening. Based on our simulations of sheared non-Brownian suspensions presented in the next sections and the last chapter of this thesis we see a clear correlation between shear-thickening and the formation of particle clusters. Brownian forces, however, were not considered and, related to that or not, we could not observe layering at small or medium \(Pe_p\). Also the dimensionality might play a role here as the additional degrees of freedom in three dimensions will have impact
on the dynamics in the shear plane compared to the pure two dimensional system where particle movement is much more restricted. It might be that particles in a 3 dimensional suspension at small shear rates use the additional dimension to arrange in two dimensional layers.

For small perturbations from equilibrium Brady suggested a master curve for Brownian hard-sphere suspensions at any volume fraction can be produced by plotting reduced viscosity against $Pe_s = R^2 \gamma / D_s$ [106], the Peclet number calculated using the short-time self-diffusivity, $D_s$. The short-time self-diffusivity quantifies the instantaneous mobility of a particle in the suspension. Its value is reduced below that for a single particle in the solvent because hydrodynamic interactions with adjacent particles in the suspension slow particle motions. Therefore, only at infinite dilution is the short-time self-diffusivity equal to the Stokes-Einstein diffusivity $D$. As we do not consider Brownian fluctuations in this work, and are more interested in the regime far from equilibrium, the scaling can not be extended.

Depending on the volume fraction $\phi$ two distinct shear thickening regimes have been observed. A critical value $\phi_c$ exist below which only continuous shear-thickening occurs, characterized by a smooth increase with $\dot{\gamma}$. For $\phi > \phi_c$ a sudden increase in $\nu_{app}(\dot{\gamma})$ can be observed. In the literature values for $\phi_c$ vary with suspension type and particle size distribution between $0.52 \leq \phi_c \leq 0.575$ [107, 108, 109]. Any colloidal interaction can drastically effect $\phi_c$ and weaken or amplify the effect of discontinuous viscosity increase. In the present work we simulated two-dimensional suspensions at $\phi$ which apparently in all cases was below the critical $\phi_c^{(2D)}$. This was probably due to the fact that the flow did not reach high enough $\dot{\gamma}$ for $\phi > \phi_c^{(2D)}$ in the diffusion coupled simulations presented to see a crossover to discontinuous shear-thickening. Another reason for not seeing discontinuity in $\nu_{app}$ might be because Brownian motion was neglected. For volume fractions that clearly showed discontinuous shear-thickening the increase of $\nu_{app}$ was accompanied by an increase of the viscous-like viscosity component and a slow decay of the stress after shear cessation [105] giving rise to the assumption that when particles are densely packed Brownian motion again might play an important role.

In search for the origins of clustering inertia of the particles can be identified as playing a central role as we observe Stokes number scaling of the shear-thickening curves, i.e. $\nu_{app} = f((\rho_s/\rho_f)\dot{\gamma})$, shown in Fig. 5.5. The influence of particle inertia on microstructure and shear-thickening will be subject of Sec. 5.

Another question remaining open is whether ideal non-colloidal hard-sphere suspensions jam at very high shear rates at all. Some experiments on real suspensions give rise to the assumption that the shear-thickening regime again is followed by a shear-thinning region [90, 108]. Against that can be argued that while experimenting with real suspensions the influence of the experimental setup and additional forces between the particles can not be absolutely excluded in most cases [110, 111, 112, 109]. Also, in our simulations we see a continued increase of $\nu_{app}$ up to the highest shear rates allowed by the methods we used [113] in contrast to comparable simulations which resemble more the experimental setup of real viscometers [114, 115, 116].

Simulation approaches to address suspension rheology range from, in decreasing order of abstraction, (i) modeling the suspension as non-Newtonian fluid, (ii) continuum models of two-phase flows and (iii) fully resolved particulate suspen-
sions where the fluid dynamics is governed by the Navier-Stokes equations and the motion of the solid particles is governed by Newton’s laws. In many practical problems, the more detailed level of description turns out to be necessary and Brownian motion has to be incorporated [117] for small particle sizes at small Reynolds numbers.

4.2 HMM Modeling of Suspension Flow

4.2.1 Description of the Problem

The emergent rheology on the macro-scale is dictated by the details of fluid-particle, and particle-particle interactions on the micro-scale. In systems where the typical spatial scale on the particle level is much smaller than that of macroscopic properties the scales can be split using a heterogeneous multi-scale method (HMM) approach [7]. In a simple test case for this multi-scale approach we consider the pressure driven flow of a 2-dimensional suspension of hard-discs in a straight channel with a wall-to-wall distance $L_y = 5 \cdot 10^{-3} \text{m}$ and a no-slip condition at the boundaries. In $x$-dimension the channel is infinitely long implemented by means of periodic boundary conditions. As the actual computational domain we consider only a length of $L_x = \Delta x_M$ of the channel where $\Delta x_M$ is the spatial resolution of the macro model we will use. With that we impose a symmetry on the system so that the macroscopic fluid velocity has a zero $y$-component under the assumption of non-compressible flow. With this we rule out any effects related to non-laminar flow. We will discuss the possible extension to this class of flow problems in an outlook at the end of this chapter. As any mapping of additional effects between the scales might be another source of scale splitting error in the current work we enforced laminar flow to minimize the complexity already present in the coupling of the models described here.

**Momentum Transport: Viscosity** Complex fluids, in which constituents on the micro-scale interact in various ways leading to a shear-dependent microstructure, mostly show strong non-Newtonian behavior. That is, in local shear stresses

$$\tau(x_M) = \frac{\nu_{\text{app}}(x_M)}{\rho(x_M)} \frac{\partial \mathbf{u}}{\partial x} \bigg|_{x=x_M} = \frac{\nu_{\text{app}}(x_M)}{\rho(x_M)} \dot{\gamma}(x_M)$$ \hspace{1cm} (4.2)

the local apparent viscosity $\nu_{\text{app}}$ of the suspension strongly depends on the local shear rate $\dot{\gamma}(x_M)$. Furthermore $\nu_{\text{app}}$ is a function of the local volume fraction of the solid phase so that we have

$$\nu_{\text{app}}(x_M, t) = F_{\nu_{\text{app}}}^{\nu_1, \rho_f, \rho_s}(\dot{\gamma}(x_M, t), \phi(x_M, t)).$$ \hspace{1cm} (4.3)

Additionally, $\nu_{\text{app}}$ strongly depends on parameters like the kinematic fluid viscosity $\nu_1$, the fluid mass density $\rho_f$, and the solid phase mass density $\rho_s$. Although there is tremendous progress in understanding the rheology of hard-sphere suspensions, so far scaling and other more complete relations could only be derived under conditions where the hydrodynamic interaction between suspended particles was simplified. Most of them are only valid in the limits of small $\dot{\gamma}$ and $\phi$. A full functional form for the whole variable space of interest does not exist and the higher $\dot{\gamma}$ and $\phi$ the
more open are the discussions on how $\nu_{\text{app}}$ behaves in this regime. In Sec. 4.1 we discuss the rheology of hard-sphere suspensions regarding these aspects in relevant detail. In case of suspensions that deviate from the ideal monodisperse hard-spheres even less consensus on the form of $\nu_{\text{app}}(\dot{\gamma}, \phi)$ exists. If we want, and this is the further aim of this work, to develop a tool to study the rheology of various types of suspensions involving numerous parameters $\{P\}$ characterizing properties such as shape and size distributions, additional inter-particle forces and maybe even dynamic processes like the shear-stress activation of inter-cellular forces in blood, we simply have to conclude that full knowledge about the function $\nu_{\text{app}} = \mathcal{F}^{\{P\}}_{\nu_{\text{app}}} (\dot{\gamma}, \phi)$ does not exist and the constitutive equation as (4.2) cannot be given in complete form (see e.g. [97] for a review on the rheology of dense suspensions).

Particle Transport: Diffusivity In the presence of variations in the solid volume fraction $\phi(x_M)$, e.g. particle concentration, a net flux of particles will try to relax the concentration gradient according to Fick’s law of diffusion

$$J = -D \frac{\partial \phi(x)}{\partial x} \bigg|_{x=x_M} \quad (4.4)$$

However, the diffusivity tensor $D$ is, similar to the momentum transport coefficient $\nu_{\text{app}}$, dependent on the shear rate $\dot{\gamma}$ and the volume fraction $\phi$. In the limit of vanishing Brownian fluctuations in the momentum exchange with the fluid, the case we consider in this work, there is no force that could drive the diffusive motion of the particles through the suspension. With the resulting zero diffusivity a concentration gradient would not be enough to cause a flux of particles. However, when the suspension is sheared particles will collide with each other and, like random walkers, will be progressively displaced from their origin. This results in a dynamics that is found to be diffusive [118]. This so-called shear-induced diffusivity is a strong function of the shear rate and the volume fraction, e.g.

$$D(x_M, t) = \mathcal{F}^{\{P\}}_D (\dot{\gamma}, \phi)(\dot{\gamma}(x_M, t), \phi(x_M, t)) \quad (4.5)$$

where $\{P\}$ is again the set of parameters that characterizes the exact type of suspension. Here, the situation is similar to that of $\mathcal{F}^{\{P\}}_{\nu_{\text{app}}} (\dot{\gamma}, \phi)$; we know its behavior only in some limits and then mostly only for the case of monodisperse hard-spheres [119] (see also Sec. 4.5 for a brief discussion on that). However, because a non-trivial feedback loop exists between shear rate $\rightarrow$ diffusivity $\rightarrow$ volume fraction $\rightarrow$ viscosity $\rightarrow$ shear rate, we cannot just neglect diffusive effects. We rather expect non-trivial particle distributions dynamics $\phi(x_M, t)$.

4.2.2 The Heterogeneous Multi-scale Method

The Heterogeneous Multi-scale Method [7] is a general methodology grouping approaches to the efficient numerical computation of multi-scale and multi-physics problems (see Sec. 2 for a classification of multi-scale problems). The fact that the involved submodels might be of very different nature gave rise to the characterization of being “heterogeneous”. They all have in common that the macro-scale model, whose observables and dynamics we are interested in, lacks completeness
in one or more aspects. That could be in case of the non-existence of constitutive
equations or if the macro-scale is not valid due to localized singularities,
e.g. boundaries. To provide the missing information, micro-models are employed
which typically are descriptions of the underlying process on a much smaller scale.
HMM is thus a strategy for designing multi-scale algorithms that are driven by
data. A very typical and descriptive example for a HMM coupling could be a
molecular dynamics (MD) model with which the state space of a gas system of
specifically interacting atoms is sampled for a given subset of the local state vari-
ables of a macroscopical flow field. The subset is used as boundary conditions to
the MD micro-model which in turn completes the set of state variables acting as a
replacement (or other form) of a constitutive equation that might not be available
but is needed on the level of the Navier-Stokes description of the fluid. Although
the micro-scale model contains all the information, its level of detail makes it too
costly to be applied to the whole macroscopic domain. Based on the multi-scale
system we investigated in the current work we will also see that this argument can
even be extended. Due to the possible limited validity range of the methods used in
a micro-model, the concept of independent micro realizations that communicate in
a compressed way (exploiting the symmetries of the physical system) via a macro-
scale makes simulations spanning the complete range of scales feasible in the first
place.

Several other or related existing multi-scale methods fall in the HMM category
such as ab initio molecular dynamics [120], quasi-continuum methods [121] and
projective methods for multi-scale systems [122]. The approach is different to the
more traditional multi-scale methods such as multi-grid, fast multipole method,
adaptive mesh refinement, or wavelet representation that make explicit use of multi-
scale decomposition of functions and signals, and thus, in contrast to HMM, resolve
the details of the solutions of the micro-scale model as general purpose micro-scale
solvers.

A trade-off can always be found between completeness of the information gained,
accuracy of the solution, computational efficiency and straightforwardness of the
implementation. Using a HMM strategy we have to cut back in the following two
main aspects. First, we won’t gain information on the micro-scale level everywhere
but only on parts of the physical domain. For the rest of the macro-scale domain we
have to be satisfied with the solutions of the macro-scale solver and/or interpolated
solutions of the micro-scale model. Also, due to the coupling of different types of
models, an estimation of the error we make on the macro-scale is not always simple.
Second, we must explore possible special features of the micro-scale problem, such
as scale separation and self-similarity. The HMM strategy only gives us a starting
point, applications of HMM to specific problems can be a highly non-trivial task.
A great understanding of the multi-physics system on all involved scales is needed,
formulation issues have to be resolved and technical tools have to be developed
along the way.

4.2.3 Submodels and Coupling

With the ideas of HMM in mind we will now construct an abstract computa-
tional model for flow of a non-Brownian monodisperse suspension of hard spheres
through a macroscopic channel. As elaborated in Sec. 4.2.4 the scales of the micro-
and macrodynamics are separated and lead to a classical micro-macro coupling. In Sec. 2.2.2 we have identified this type of scale separation as interaction region 3.1 in scale separation map in Fig. 2.3. This corresponds to the case that the full spatio-temporal extend of MiS is smaller than a single spatio-temporal step of MaF, i.e. $T_m \times L_m < \Delta t_M \times \Delta x_M$. We also learned that when we face the problem of incomplete constitutive equations we need to obtain the missing information by means of explicit simulations of the microdynamics. As another property, we see that all the submodels are defined on the same single domain (sD). Using the classification of multi-scale systems we have motivated in chapter 2 the present multi-scale system falls into the group of hierarchical coupling problems (see Fig. 2.5). The HMM approach will be an applicable guideline to construct an appropriate multi-scale model.

Besides the macro-model for the fluid dynamics MaF, a model MaS is introduced on the macro-scale in order to handle the evolution of the local volume fraction $\phi(x_M)$ consisting of advection with the velocity field $u(x_M)$ and diffusion induced by a local shear rate which is a function of the velocity gradient field, e.g. $\dot{\gamma}(u(x))$.

In Fig. 4.2 an HMM suspension is depicted in a way as to show the coupling between the macro-scale level consisting of a non-Newtonian fluid model and an advection-diffusion model, and a fully resolved suspension model on a micro-scale level. At every point on the macro-scale lattice and time step the macro-models need information on collision parameters which can not be provided due to the lack of constitutive equations. Instead, a “micro pocket” is opened up, running a fully resolved simulation of suspended particles in a shear flow. The initial and boundary conditions of the micro-simulation are determined from the local macroscopic shear rate $\dot{\gamma}(x_M, t_M)$ and volume ratio $\phi(x_M, t_M)$, i.e. the microscopic shear rate and the number of particles in the micro domain given by

\[
\begin{align*}
\dot{\gamma}_m &= s^{-1}_\gamma \dot{\gamma}(x_M, t_M) \\
N_p &= N_p(\phi(x_M, t_M)).
\end{align*}
\] (4.6) (4.7)

We will discuss this mapping in some more detail in the section on the preparation of the initial conditions of the micro simulations.

From the simulation run of the micro-model the apparent viscosity $\nu_{\text{app}}(\dot{\gamma}_m, N_p)$ and anisotropic diffusivity tensor $D_m$ are determined. They are converted into the macro-scale unit system according to

\[
\begin{align*}
\nu_M(x_M, t_M) &= s_\nu \cdot \nu_{\text{app}}(\dot{\gamma}_m, \phi) \\
D_M &= s_D \cdot D_m
\end{align*}
\] (4.8) (4.9)

and then passed as collision parameters to the macro-scale model. Also, $u(x_M, t_M)$ is passed from MaF to MaS within the macro-scale spatio-temporal domain, therefore without conversion. In this formulation we introduced a scale factor $s_Q$ which is a scalar constant translating a quantity $Q$ between the units of the micro and macro model. It is defined as

\[
s_Q = \frac{Q_M}{Q_m}
\] (4.10)

where $Q_m$ and $Q_M$ are the numerical representations of the quantity $Q$ in the unit base formed by $\Delta x_m, \Delta t_m$ and $\Delta x_M, \Delta t_M$, respectively. The scale factor $s_Q$ therefore can be expressed in terms of $\Delta x_{m,m}, \Delta t_{m,M},$ and $s_x$ and $s_t$. In Table 4.4
Figure 4.2: HMM type of coupling for the multi-scale simulation of the flow of a suspension. On the macro-scale a non-Newtonian fluid dynamics model (MaF) computes the evolution of the suspensions pressure and velocity fields. Besides that, an advection-diffusion model treats the evolution of the particle concentration field, i.e. the local volume ratio, on the same macroscopical scale. As no constitutive equations are present to compute the collision parameters $\nu$ and $D$ needed at every spatio-temporal point $(x_M, t_M)$, a “micro pocket” is opened where a fully resolved suspension simulation is run. The initial and boundary conditions, i.e. shear rate $\dot{\gamma}_m$ and $N_p$, of the micro simulation are determined from the local macroscopic $\dot{\gamma}_M(x_M, t_M)$ and volume fraction $\phi(x_M, t_M)$ (a). From the simulation run apparent viscosity $\nu_{app}$ and diffusivity tensor $D$ are determined and passed to the macro-scale (b). Also the local macroscopic velocity is passed from MaF to MaS.
this is done for the quantities describing the suspension system together with the actual numerical values for the scales given in Table 4.3.

As useful tools to construct an algorithmic description of a complex multi-science multi-scale system, the CxA formalism offers the concepts of the scale separation map (SSM), a generic sub-execution loop (SEL) and coupling templates. The SSM will prove its usability in the next subsection where we discuss the scales that have to be resolved and their coupling. The coupling will be specified at hand of coupled SEL’s in the subsection thereafter.

4.2.4 Scales of the Problem and their Separation

The scales to be resolved are not only dictated by the processes in the system that should be modeled. In all cases of multi-scale modeling the limitations of the chosen models and methods itself have to be taken into account carefully because their application might be limited to a certain range of $\Delta x$ or $\Delta t$, or the ratio $\Delta x/\Delta t$. Typically, outside the validity range of a model its results become meaningless, either because the assumptions it is based on are not true anymore, or a numerical method involved becomes unstable.

On the spatial scale, the two central properties that define the upper and lower limits of the scales to be resolved are the size of the particles and the dimension of the domain. The particle diameter in the experiments we will compare the results of the simulations to is in the $\mu$m range [123, 124]. We have chosen a particle radius $R_p = 3.15\mu$m. To resolve the fluid in sufficient detail with LBM a resolution of $1\mu$m is appropriate [125], we thus define $\Delta x_m = 1\mu$m. Clusters of particles that form at higher $St \sim \dot{\gamma}$ are spatial structures giving rise to a correlation length $\xi_m$ (see Chapter 5). They are believed to be the origin of changes in mesoscopic properties such as the diffusivity $D_{xy}$ of particles or the apparent viscosity $\nu_{app}$ (see discussions in Sec. 4.1 and Chapter 5). Choosing a mass-density ratio of $M = \rho_s/\rho_f$ = 10.0, for $\phi_0 = 0.40$ we find a typical cluster size of $N \approx 10$ for the highest shear rates feasible with LBM (see Chapter 5). With an observed fractal dimension of $D = 1.15$ and a typical orientation angle of $\approx 45^\circ$ we can estimate a typical size of the clusters in the direction of the velocity gradient to $2^{-1/2}N^{1/1.15} \cdot 2R_p \approx 36\Delta x_m$. To lower the probability that clusters percolate the system we set the spatial extend of the micro system to $L_m = 72\Delta x_m > \xi_m$. Under the Mach number limitation of the LB method, i.e. $u < 0.8c_s \approx 0.46$, and practicable fluid viscosity $\nu_t = 0.1$ this allows us to reach a maximum Reynolds number of $Re_p = 4R_p^2\dot{\gamma}/\nu_t \approx 2.535$. This is approximately an order of magnitude higher than the Reynolds number at which shear thickening sets on. These settings can thus be used to sample the state space of the suspensions in a sufficient $\dot{\gamma}$-range to find interesting behavior.

On the macro-scale, the width of the channel is $L_M = 50$mm and we have chosen a spatial resolution $\Delta x_M = 1.25$mm which should be fine enough to resolve the properties of the macroscopic flow which will be laminar due to very low flow Reynolds numbers and due to the symmetry enforced by setting $L_{M,x} = \Delta x_M$. For the spatial scale factor,

$$s_x = \frac{\Delta x_M}{\Delta x_m},$$  \hspace{1cm} (4.11)

we get $s_x = 1.25 \cdot 10^3$. 

The advection-diffusion model $\text{MaS}$ relies on the velocity field $u(x_M,t_M)$ provided by $\text{MaF}$ and its spatio-temporal resolution. It will also output information on the local volume fraction $\phi(x_M,t_M)$ in the same spatio-temporal resolution. Consequently, it is reasonable to write $A_{\text{MaS}} = A_{\text{MaF}} = A(x_M,L_M,t_M,T_M)$ although the dynamics of $\phi(x_M,t_M)$ will be solved using a Lagrangian point particle representation (LPAD) for $\phi(x_M,t_M)$ whose actual spatial resolution and timestep are smaller.

In contrast to the freedom in setting $\Delta x$ according to the scales of the physical system, the temporal scale is dictated by the range of fluid viscosities $\nu_f$ we can simulate with LBM. Using a LBGK relaxation collision, due to the limited stability of the LBM the relaxation parameter is limited to $0.5 < \tau < 2$. We have chosen $\frac{1}{100} < \nu_f < \frac{2}{5}$ as a “save” range in units of the macro-system, $\Delta x_M^2 \Delta t_M^{-1}$. Expecting the apparent viscosity of the micro-system to be in the range of $1 \cdot \nu_f < \nu_{\text{app}} < 50 \cdot \nu_f$, we chose a viscosity scale factor,

$$s_\nu = \frac{\Delta \nu_M}{\Delta \nu_m} = \frac{\Delta x_M^2 \Delta t_M^{-1}}{\Delta x_m^2 \Delta t_m^{-1}},$$

of $s_\nu = 1 \cdot 10^1$ to map viscosities from the micro-scale to the macro-scale by $\nu_M = s_\nu^{-1} \nu_m$. This results in a time scale factor,

$$s_t = \frac{\Delta t_M}{\Delta t_m} = s_\nu^{-1} s_x^2,$$

of $s_t = 1.5625 \cdot 10^4$.

The typical time scale on the micro level $\tau_m$ is given by the shear rate set. From autocorrelation measurements of the apparent viscosity we find that the correlation time scales linearly with $\dot{\gamma}$ and can be estimated as 1 in normalized strain units. A maximum shear rate $\dot{\gamma}_{\text{max}} = M a_{\text{max}} c_s L_m^{-1}$ results from the Mach number constraint and the system size $L_m = 72$ used. For a range of shear rates $10^{-8} \Delta t_m^{-1} < \dot{\gamma}_m < 6.42 \cdot 10^{-3}$ we estimate

$$10^8 > \tau_m > 1.56 \cdot 10^2.$$

Averages of mesoscopic properties will be taken over a normalized strain of 100. Assuming equivalence of averages in space and time we don’t extend $T_m$ for the considerations here. We still can assume that averaging out fluctuations at this instance does not influence the macro-dynamics. To picture the average case at later stages of the channel flow simulations we consider a typical micro simulation time $T_m = 100 \cdot (10^{-4})^{-1} = 10^6$ for the estimation of the computational benefit using the HMM approach for such simulations.

The maximum time scale of the system $T_M$ depends on what feature of the system we want to investigate. In this work we focus on the macroscopic equilibrium of a suspension flowing through a channel. The relaxation dynamics of the fluid is relatively fast and the dynamic equilibrium is reached after a few $10^3 \Delta x_M$. Base on that, we assume $T_M = 1 \cdot 10^4 \Delta t_M$. In contrast, the diffusive motion of suspended particles is much slower and particle concentration profiles develop on a larger time-scale only. The fluid adapts rather quickly to the change in the distribution of particles. This type of scale separation will be discussed in section Sec. 4.8.1 where we motivate a legitimate rescaling of $D_M$ to accelerate the diffusive dynamics.
without violating the scale separation. As long as the separation is intact, this will change only the time scale the system reaches the macroscopic equilibrium. The equilibrium itself will not be biased. For the maximum simulated time we thus still consider $1 \cdot 10^4 \Delta t_M$.

In Table 4.3 all dimensions are summarized. In Table 4.4 the scale factors are listed defining the conversion of quantities from one level to the other.

The scale-separation map in Fig. 4.5 shows the micro and the macro-models placed according to the scales we have discussed. On the lower left (small spatial and temporal scale region) we find the fully resolved suspension model $\text{MiS}$ which itself consists of a LBM solver and the Newtonian dynamics solver for Lagrangian particles (see Sec. 4.4). The dynamics of the particles in the micro-model are described on a relatively fine spatial scale. Also, their dynamics is resolved on a finer temporal scale than the fluid to increase the numerical stability of the integration scheme (see Sec. 4.4.1). To reflect the dynamically adapted time-step the particle box was symbolically extended to lower temporal and spatial scales. However, because interaction between fluid and solid phase is realized via a grid representation of the particles we will assume the spatio-temporal domain of $\text{MiS}$ to be $A_{\text{MiS}} = A(\Delta x_m, L_m, \Delta t_m, T_m)$.

Looking at the relations expressing the scale separation, $L_m < \Delta x_M$ and $T_m < \Delta t_M$, we find the typical micro-macro coupling, identified as interaction region 3 in the classification of CxA in chapter 2.

Based on the points on the scale map defining lower-left and upper-right corners of the models on both scales we can make a theoretical estimation of the reduction of the computational cost due the application of the scale separation. Assuming that the time needed for the computation of one iteration of each of the models is the same (the extra effort due to the particles in the resolved suspension model and that due to the advection-diffusion solver on the macro scale is indeed comparable).
Figure 4.5: Scale separation map for the suspension system showing the spatio-temporal scale domains of the micro and macro models and thereby illustrating the scale separation between them. On the macro-scale both models, MaS and MaF, respectively, are defined on the same scales. The shaded extension of MiS towards smaller spatial scales results from the fact that suspended particles in MiS are described in a Lagrangian framework. The extension towards smaller temporal scales is due to the application of a scale splitting of the fluid and particle dynamics in MiS allowing the particle dynamics to be resolved on much finer temporal scales (see Sec. 4.4.1). The extension towards larger temporal scales (indicated by dashed gray lines) illustrates the temporal extension of the simulation to obtain a better statistics over the measurements of viscosities and diffusivities.

we can estimate the computational effort of the HMM simulation as

\[ C_{\text{HMM}} = c_m \left( \frac{L_m}{\Delta x_m} \right)^{D_m} \left( \frac{T_m}{\Delta t_m} \right)^{D_m} + c_M \left( \frac{L_M}{\Delta x_M} \right)^{D_M} \left( \frac{T_M}{\Delta t_M} \right)^{D_M}. \] (4.15)

Here the dimensions of the models are \( D_m = 2 \) and \( D_M = 1 \). The effort of simulating the whole problem using the fully resolved suspension model, thus at \( \Delta x_m, \Delta t_m \), would be

\[ C_{\text{full}} = c_m \frac{L_M}{\Delta x_M} \frac{L_m}{\Delta x_m} \frac{T_m}{\Delta t_m}. \] (4.16)

Here we assume the otherwise quasi-1D system has a second dimension of \( L_m \) necessary to resolve the typical length scale of the micro-dynamics.

To obtain a measure of the gain through scale splitting with the HMM approach we calculate the ratio

\[ \frac{C_{\text{full}}}{C_{\text{HMM}}} \approx 1.1 \cdot 10^7. \] (4.17)

This means, using the HMM approach we can reduce the computational effort by seven orders of magnitude. If we would use \( L_{M,x} = \Delta x_M \) here, the speedup is \( 1.9 \cdot 10^8 \) and in the case of a full 2-dimensional macroscopical flow, i.e. \( D_M = 2 \) and \( L_{M,x} = L_{M,y} \), using the same scales we can estimate the speedup to

\[ \frac{C_{\text{full}}}{C_{\text{HMM}}} \approx 5.8 \cdot 10^9. \] (4.18)
The reduction of the computational effort is not the only advantage of the HMM approach in this case. Applying the Lattice-Boltzmann method, due to the Mach number limit of lattice velocities a simulation of the whole system of size $L_M = 50000\Delta x_m$ at a resolution $\Delta x_m$ would limit the shear rate drastically to very small values. It would not be possible to study the effect of shear-thickening on the concentration and velocity profiles. Comparable to the situation with parallelization under usage of the Lees-Edwards boundary conditions in Sec. 4.4.2, splitting the whole domain into domains that can be Galilei-transformed and therefore can reach arbitrary absolute velocities (in the reference frame of the macroscopic domain). The problem of limited validity range is inherent to practically every method, not only numerical, so splitting and re-coupling scales of the considered problem can also be considered a problem solving strategy.

4.2.5 More on Coupling

In Fig. 4.6 the sub-execution loops for the single-scale models are shown together with their coupling. Although the models for the particle dynamics on the microscale, respectively the dynamics of their continuous representation on the macroscale, are not of CA type we still can express their computational structure in the sub-execution loops conventionalized in the CxA formalism.

The MaF model being based on the LB method clearly fits into the CA description. In Fig. 4.6 we find a collision step as well as a propagation step that directly correspond to those of the LBM. In the collision step, however, information on the local relaxation parameter $\tau(x_M, t_M)$ is missing. Inside the iteration
loop, and, since $\tau$ is also a function of $x_M$, inside the loop over all nodes of the domain, observables $u(x_M, t_M)$ and $\dot{\gamma}(x_M, t_M)$ are computed from the state variable vector $f_i(x_M, t_M - \Delta t_M)$. Those are passed to $\text{MaS}$ and $\text{MiS}$, respectively, and the execution is halted until $\tau = f(\nu_{app})$ was made available by $\text{MiS}$.

The execution of the coupled system as depicted in Fig. 4.6 is different to a CxA as introduced in chapter 2 due to not using MUSCLE to couple the submodels\(^1\). Realizing the coupling with MUSCLE would mean all submodels are brought to life by a centralized initialization routine called plumber who also spawns the conduits who would contain the mapping functionality. The plumber would wire the submodels with the conduits and terminate leaving a fully decentralized system behind. Instead, the coupling to the micro-model was realized the “classical” way via a function call, which also has the effect that a send primitive is blocking instead of a non-blocking send provided by MUSCLE. This later fact has no consequence on the execution because the graphs in Fig. 4.6 and Fig. 4.7 are cyclic. The fact that the coupling via the collision operators of $\text{MaF}$ and $\text{MaS}$ was realized by implementing $\text{MiS}$ as a subroutine of the combined $\text{MaF+MaS}$ kernel, however, results in a master-slave coupling where the combined $\text{MaF+MaS}$, once launched by the user, will trigger the execution and termination of $\text{MiS}$.

The macro-model $\text{MaS}$ for the advection and diffusion of the field of local volume fraction $\phi(x_M, t_M)$ is based on a Lagrangian model for a finite number of massless point particles that are advected with a velocity interpolated from $u(x_M, t_M)$ (passed by $\text{MaF}$) and a random step according to the interpolated value from the diffusivity field $D(x_M, t_M)$ (passed by $\text{MiS}$) in real coordinate space. It could therefore be viewed as an agent based model with the tracer particles as agents whose dynamics are functions of external fields comparable to the situation in the CxA model for in-stent restenosis discussed in chapter 3 where the dynamics of the Lagrangian agents representing smooth muscle cells is influenced by the external fields of drug concentration and wall shear stress which were both provided by Eulerian models. In the ISR model mappers had the function to translate between lattice-based data and agent-based data. In the present situation of the coupling of $\text{MaS}$ to the other models data for velocity and diffusivity is based on the same macroscopic lattice $x_M$. It has to be mapped to each of the Lagrangian tracer particles. Vice versa, particle based data (their positions) have to be mapped back to the volume fraction lattice field $\phi(x_M)$. We could therefore think of the Lagrangian particle advection-diffusion model (LPAD) be separated from the data mapping and include the mapping functionality into “smart conduits” for each of the couplings $u$ from $\text{MaF}$, $D$ from $\text{MiS}$, and $\phi$ to $\text{MiS}$. Same is true for the models of the fluid and solid phase in $\text{MiS}$, respectively. When treating them as separate submodels, the functionality of mapping the positions of the suspended particles to the lattice of the fluid solver, the mapping of exchanged momentum per boundary node to forces and torque on single particles, the mapping from lattice-based shear stress in the fluid and internal stress per particle to a single value of $\nu_{app}$, as well as creating the initial velocity field from $\dot{\gamma}(x_M)$ and the initial particle distribution from $\phi(x_M)$ could be defined as functionalities of appropriate mappers.

\(^1\)MUSCLE does not allow to spawn several instances of the same submodel agent, a functionality which necessary to run several micro-model realizations in a farming approach to parallelization. Later, we found that with the use of the database described in Sec. 4.6.2 a farming approach would not be of much advantage. However, at that time the implementation of the coupling was already too advanced to rebuild it using MUSCLE.
Figure 4.7: The complete coupling scheme shows also mappings of data structures internal to the submodels MaF, MaS and MiS. There are multiple ways to define submodels and their coupling based on which data mapping functionality is covered by them. In one extreme case, MaF, MaS and MiS can be viewed as agents that communicate via data structures defined on the lattice of the macro domain, i.e. \( \nu_{app}(x_M), D(x_M), u(x_M) \) and \( \phi(x_M) \). All internal mapping is hidden in this definition. The other extreme case is to consider the submodels of MaS and MiS as submodels. Then the mapping between lattice-based data and off-lattice data (Lagrangian particle models as “solid” in MiS and MaS) would be seen as functionality of mapper agents similar to the coupling schemes for the ISR CxA’s presented in chapter Sec. 3. Throughout this chapter we will use the first definition.

The complete coupling scheme in Fig. 4.7 shows both ways to define submodels and their coupling including the data conversions which either could be seen as part of the submodels or as external “mappers”.

There is a third way to understand the coupling of MaF, MaS, and MiS, though not clear from Fig. 4.7. The submodel MiS is coupled to the collision operators of both macro-scale models, MaF and MaS, completing the information on the constitutive relations there. In principle, viscosity and diffusivity measurements could be split in two micro-models at the same (micro-)scales and sharing the same domain. This would result in a coupling scheme where the dynamics of fluid phase and that of the solid phase would have their own cycles between micro- and macro-model constituting a kind of dual micro-macro coupling.

As we did not make use of any multi-scale simulation framework, such as MUSCLE, we are free to chose one of both views (ignoring the third as this is not applicable), or a compromise of them, to base the construction and implementation of the multi-scale model and its coupling on. Throughout the remainder of this chapter we keep viewing MaS as a black box, i.e. “some” solver for the advection-diffusion of the lattice field \( \phi(x_M, t_M) \), as the choice for a solver might change in the future. This is also true for MiS where the internal implementation of the solver for the flow of suspended particles could be changed in favor of a Stokesian dynamics solver, for example.
4.3 Macroscopic Non-Newtonian Flow (MaF)

To solve the flow of the suspension on the macro-scale the Lattice-Boltzmann method is applied. The first section will briefly introduce LBM in a general manner in order to base also the extension to suspended particles on it that is addressed in Sec. 4.4 which introduces the micro-model. The last paragraph will discuss the coupling to the other models.

4.3.1 Lattice-Boltzmann Method

The Lattice-Boltzmann method [41, 126] method is an alternative approach to hydrodynamics offering a very efficient way to solve the discretized Boltzmann equation on regular lattices. It has in common with its predecessor, the Lattice-Gas Automaton (LGA) [127], that particles kinetics are abstracted to a collision and streaming step but instead of single particles particle distributions collide at and propagate between the nodes of the lattice. This step from a microscopic to a mesoscopic representation comes with the advantage of eliminating the noise using all possible particle states. (See [128] for a derivation of LBM from LGA).

Despite being based on a description for dilute gases viscous flow behavior emerges automatically from this scheme (in the limit of small mean free path of the particles) so that with a properly chosen equilibrium function the Navier-Stokes equations are reproduced to second order of approximation, even for large viscosities. Due to its local nature implementation of complex boundaries and parallelization is comparatively straightforward.

When Richard Feynman was asked to explain why people spend a lot of time and money on building large parallel computers for the computation of particles that hop from one lattice node to the other (LGA) he put it this way\(^2\):

\[
\text{We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, the flow of sand is very similar to the flow of water or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids.}
\]

The same argument is true for Lattice-Boltzmann methods as direct successor of LGA. With this Feynman illustrates fundamental universality we find in physics which gives some freedom in constructing algorithms which produce similar behavior on a higher scale which we want to study.

There are several choices for the collision operator. The most simple is derived from the insight that the collision operator in the Boltzmann equation brings the particle velocity distribution closer to the equilibrium distribution [129]. This leads to the single-relaxation time collision scheme, named LBGK after Bhatnagar, Gross and Krook. More sophisticated collision operators exist, most notably the multi-relaxation-time collision (MRT) [130, 131]. The MRT lattice Boltzmann equation overcomes some obvious defects of the LBGK model, such as fixed Prandtl

\(^2\)http://www.longnow.org/essays/richard-feynman-connection-machine/
number ($\text{Pr} = 1$ for the BGK model) and fixed ratio between the kinematic and bulk viscosities. It can be shown that by applying the MRT scheme the numerical stability of LBM simulations can be significantly increased in comparison with LBGK [131, 132]. However, choosing the numerous relaxation parameters, many of which correspond to the damping of modes that have no physical meaning, is not straightforward; a reason why they sometimes are called “magic parameters”. Another notable approach to increase the stability of LBM calculations is the entropic LBM collision operator [133] which is characterized by an equilibrium function of exponential form which satisfies the first four moments of the Maxwellian and a relaxation parameter which is dynamically adjusted to satisfy a lattice version of the H-theorem. The later fact guarantees stability, but provokes criticism based on the fact that with the relaxation parameter the viscosity changes locally. Simulations of time-dependent problems therefore should be considered carefully. It also should be noted that efforts were undertaken to improve the stability of the LBGK scheme which allow simulations of unsteady flow at above $\text{Re} = 10^4$ [134].

In this work a two-relaxation-times (TRT) relaxation scheme [135] was used, which offers a good balance between quality of the results, computational cost and implementation effort. It achieves a slight improvement in comparison to the lattice-BGK scheme in terms of damping unphysical high-frequency modes, leading to more stable simulations at higher $\text{Re}_{\text{p}}$.

At each time iteration $t$ and at every node $r$ of the lattice, $f_i = f_i(r, t)$ are the particle densities traveling in directions $e_i$, where $\{i = 1, \ldots, b\}$ denotes the discrete velocity space. During the collision step, these distributions are relaxed towards an equilibrium distribution $f_{eq}^i$. Unlike LBGK the TRT model uses two different relaxation times and a collision operator

$$C_f = \frac{1}{\tau} (f_{eq}^i(f) - f_i)^+ + \frac{1}{\tau_-} (f_{eq}^i(f) - f_i)^- + g_i.$$  

(4.19)

where $F_i^+$ and $F_i^-$ denote the even and the odd part, respectively, of a function on the discrete velocity space:

$$F_i^+ = \frac{F_i + F_i'}{2}, \quad F_i^- = \frac{F_i - F_i'}{2}$$  

(4.20)

where $i'$ is such that $e_i' = -e_i$. Then, defining a propagation operator $P$, the propagation step reads

$$P f_i(r, t) = f_i(r + e_i, t + 1).$$  

(4.21)

In this notation the LB equation becomes

$$P f_i(r, t) = C f_i(r, t).$$  

(4.22)

The relaxation parameter $\tau$ is related to the kinematic viscosity by $\nu = c_s^2 (\tau - 1/2)(\Delta x^2 / \Delta t)$ [129, 135] where $c_s$ is the speed of sound. The second relaxation parameter $\tau_-$ is set to 1, a choice in favor of stability. Simulating flows of dense suspensions at relative high Reynolds numbers, setting $\tau_-=1$ effectively damps checkerboard effects and numerical pressure waves, therefore improving the robustness. With the choice for $\tau_-$, also the position of the numerical boundaries [136] can be controlled. The equilibrium function is a function of the local velocity distribution
through the density $\rho(f)$, and the velocity $u(f)$, in accordance to the kinetic theory of gases computed as the 0th and 1st moments of $f$

$$
\rho(r, t) = \sum_i f_i(r, t) \quad (4.23)
$$

$$
\rho(r, t)u(r, t) = \sum_i e_i f_i(r, t). \quad (4.24)
$$

For simplicity of notation, in what follows, we will identify $f_i^{eq}(f) = f_i^{eq}(\rho(f), u(f))$.

Besides density and velocity, the momentum tensor can be computed as

$$
\Pi_{\alpha\beta}(r, t) = \sum_i e_{i\alpha} e_{i\beta} f_i(r, t). \quad (4.25)
$$

Conservation of mass, momentum and kinetic energy are constraints to any equilibrium function $f_i^{eq}(r, t)$ (and the Navier-Stokes equations for weakly compressible fluids are obtained [137]). Isotropy requires a multi-speed model which involves at least nine lattice velocities $e_i$ in 2D [129]. A suitable choice for $f_i^{eq}$ for this model is

$$
f_i^{eq} = w_i \rho \left(1 + \frac{1}{c_s^2} e_i \cdot u + \frac{1}{2c_s^4} (e_i \cdot u)^2 - \frac{1}{2c_s^2} u^2\right) \quad (4.26)
$$

with the lattice velocities

$$
e_1 = (1, 0), \quad e_2 = (0, 1), \quad e_3 = (-1, 0), \quad e_4 = (0, -1),
$$

$$
e_5 = (1, 1), \quad e_6 = (-1, 1), \quad e_7 = (-1, -1), \quad e_8 = (1, -1)
$$

and $e_0 = (0, 0)$ for the rest particle distribution. The parameters $w_i$ and $c_s$ depend on the particular realization of LBM scheme. For the D2Q9 model with $f_i^{eq}$ given in (4.26) the speed of sound is defined as $c_s = 1/\sqrt{3}$ and the direction dependent weights $w_i$ read

<table>
<thead>
<tr>
<th>$w_i$</th>
<th>$i = 0$</th>
<th>$i = 1..4$</th>
<th>$i = 5..8$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1/3</td>
<td>1/18</td>
<td>1/36</td>
</tr>
</tbody>
</table>

so that (4.26) agrees with an expansion of the Maxwell-Boltzmann distribution in small Mach numbers $u/c_s$ to the order of $u^2$.

The term $g_i$ in (4.19) is an extra momentum added to $f_i$ in every time step, therefore acting as a volume force $G$ that can be used to drive the flow according to the application of the simulation.

$$
g_i = \Delta x^2 w_i c_s^2 e_i G \quad (4.27)
$$

with the properties

$$
\sum_i g_i = 0, \quad \sum_i e_i g_i = \Delta x^2 G. \quad (4.28)
$$

It can be related to a pressure driven flow by

$$
G = \frac{\Delta p}{L \rho} \quad (4.29)
$$
where $\Delta p$ is the difference between the pressure at the inlet and the outlet of a pipe of length $L$, for instance.

The LBM scheme can be written as

$$P f_i(r, t) = C f_i(r, t) \quad (4.30)$$

using propagation and collision operators defined in (4.21) and (4.19).

It can be shown that in the asymptotic limit, the stress tensor,

$$S_{\alpha\beta}(r, t) = (\Pi_{\alpha\beta}(r, t) - C(r, t)) (\Delta x/\Delta t)^2 \quad (4.31)$$

and pressure, $p = (\rho - \rho_0) c_s^2 (\Delta x/\Delta t)^2$, can be obtained locally. Here, $\rho_0$ denotes a constant reference density which is typically set to 1 in simulations. In practice, $\Pi_{\alpha\beta}$ has to be calculated as mean over pre-collision and post-collision densities $f_i$ and $C f_i$. $C(r, t) = \rho(r, t) u(r, t) u(r, t)$ is the local convection tensor.

We remark that in problem relevant units time step $\Delta t$ and space step $\Delta x$ satisfy

$$\frac{\Delta t}{\Delta x^2} = \text{const.} \quad (4.32)$$

a relationship called diffusive scaling in the literature being a prerequisite to recover the incompressible Navier-Stokes equations in the limit $\Delta x \to 0$ [138].

### 4.3.2 Coupling

As a CA-type of method there is a propagation of properties at one lattice node to the adjacent nodes and a collision at each node. It therefore can be directly translated into the sub-model execution loops as has been done in Fig. 4.7. In case of LBM, observables are obtained from the local state variables $f_i$, the phase-space one-particle distribution function, on which the propagation and collision rules of the CA are defined.

The local shear rate $\dot{\gamma}(x_M, t_M)$ can be determined from the local shear stress tensor and $u(x_M, t_M)$. However, a more direct approach was applied reading

$$\dot{\gamma}(u) = \sqrt{\frac{1}{2} (\partial_\beta u_\alpha + \partial_\alpha u_\beta)(\partial_\alpha u_\beta + \partial_\beta u_\alpha)}. \quad (4.33)$$

When passing the shear rate to MiS it is translated to the micro-scale by

$$\dot{\gamma}_m = s^{-1}\dot{\gamma}(x_M, t_M). \quad (4.34)$$

After MiS finished the simulation run for $\dot{\gamma}_m$ and $\phi(x_M, t_M)$ from MaS the apparent viscosity $\nu(x_M, t_M)$ is received from MiS. The relaxation parameter is then obtained through the relation $	au(x_M, t_M) = (3\nu(x_M, t_M) + 1)/2$.

The local velocity $u(x_M, t_M)$ needed as input for MaS is obtained using (4.24) and does not have to be scaled since MaF and MaS share the same spatio-temporal domain.
4.4 Fully Resolved Suspension Flow (MiS)

In order to introduce the micro-model MiS for the simulation of fully resolved suspensions this section will first describe how Lagrangian particles can be coupled to a Lattice-Boltzmann fluid and how the time-scales of the two subsystems can be decoupled to increase the numerical stability of the whole scheme. Thereafter Lees-Edwards boundary conditions will be introduced for LBM suspensions which allow to simulate shear flow in a quasi-infinite system, thus not resembling Couette-type of viscometers but a simulation box that presents a realized small part of a (virtual) bigger system and which is in this sense very similar to the HMM idea of a micro-model. In the subsequent subsection a correction to the momentum exchange algorithm as a part of the coupling of the LBM fluid to the suspended particles is proposed to recover Galileian invariance of the particle dynamics. When validating simulations are presented the method to measure the apparent viscosity is addressed. At the end the preparation of the initial condition is discussed. How shear-induced diffusivity can be measured in MiS will be described later in a subsection of section Sec. 4.5.2.

4.4.1 Direct Simulation of Suspended Particles

When modeling particles living in continuous space but suspended in a lattice-Boltzmann fluid, interaction between fluid and solid has to be realized via the intermediate representation of the particle on the lattice. Except for techniques similar to immersed boundary conditions [139], this is done by appropriate boundary conditions applied in the propagation step. In two dimensions, a spherical, that is disk-like, particle is represented by solidification of all nodes \( x \) for which \( |x - x_p| < R_p \) where \( x_p \) is the location of the particle’s center and \( R_p \) its radius. Mapping a particle to the lattice therefore is like cutting cookies out of a flat dough. It leaves broken links at which we have to apply appropriate boundary conditions. In some of the methods the fluid on the nodes inside the particle shell is kept alive as either physical or virtual fluid. The (dis-)advantages of this approach will be addressed in the next sections.

To implement no-slip conditions at the surface of the particles, in this work the bounce-back at the links method (bbl) was applied, assuming the boundary to be always located at the midpoint of boundary links, i.e. of the lattice links that are cut by the solid-fluid interface. More sophisticated and accurate methods [140, 141, 142] (see also [143] for a review) exist and, in principle, can be combined with the ideas of the following sections. However, for clearness we stick here to the bbl description where in the standard formulation a distribution \( f_i(x) \) is reflected if the associated link \( e_i \) intersects a particle surface. In case of bbl at moving solid surfaces, an additional term accounts for the change due to the velocity of the surface at the intersection point, and the propagation step is now given by

\[
P f_i(r, t_+) = \begin{cases} R_{u_b} f_{i'}(r, t_+) & \text{if } i' \text{ is BL,} \\ f_i(r + e_i', t_+) & \text{else,} \end{cases}
\]

using a reflection operator

\[
R_{u_b} f_i = f_i + 2 w_i c_s^{-2} u_b \cdot e_i
\]
where $u_b$ is the velocity of the midpoint of the boundary link and $i'$ denotes the opposite direction to $i$. If the fluid node is not virtual, an amount of momentum

$$\delta p_i = 2e_{i'}[Cf_i(r, t + 1) - \rho w_i(c_s^{-2}u_b \cdot e_i + TCJ)]$$

(4.37)

is transferred to the particle. $TCJ$ is a correction term. With $TCJ = 0$ the Momentum Exchange Algorithm (MEA) as first published by Ladd [144, 125] is reproduced. As we will see later in this section, MEA causes strong deviations from Galilean invariance in some situations and an accordingly set $TCJ$ can successfully correct for these effects.

Regarding hydrodynamical properties of suspended particles, it has been shown that the use of the bounce-back rule for boundaries not orientated along the lattice results in an effective hydrodynamic boundary slightly displaced from the physical boundary. In the case of spherical particles with a radius $a$ this leads to a hydrodynamic radius $a_{hd} = a + \Delta$, where the deviation $\Delta$ depends on the fluid viscosity [144, 145]. An a priori correction of $a_{hd}$ can achieve more accurate dynamics of the solid particles.

**Fluid-particles forces**

We begin focusing on two approaches to deal with the interaction between fluid flow and solid suspensions, the method proposed by Ladd [144, 125], and the ALD method [146, 147] (Fig. 4.8). Both techniques employ the Momentum Exchange Algorithm [144] to deal with hydrodynamical forces exerted on the particles. According to its original formulation, the MEA is used to approximate the momentum given to the particle by the surrounding fluid.

The transferred momentum $\delta p_i$ gives rise to a force and a torque acting at the boundary point $r_b = r + \frac{1}{2}e_{i'}$ according to

$$F(r_b, t + 1/2) = \delta p_i / \Delta t$$

(4.38)

$$T(r_b, t + 1/2) = [r_b - R] \times F(r_b, t + 1/2),$$

(4.39)

where $R$ is the center of mass of the particle. The total force and torque on a particle are then obtained by a summation over the contribution from all boundary links $i_b$.

In its original version [144] also the nodes inside the solid particles are treated as fluid, which contribute to the hydrodynamical forces as well. In other words, the summations (4.38) contain both fluid-solid and solid-fluid links. A particle is therefore composed of a rigid shell and the inner fluid in this description.

However, for solid phase densities $\rho_s \leq \rho_f$ the explicit update of particle positions has been found to become unstable [125] and improvements on the update have been proposed [148, 145]. The applicability was later extended [145] to smaller ratios $\rho_s/\rho_f$ by omitting the action of the inner fluid on the shell.

In the ALD method, the inner fluid is only virtual, but is still used to bypass an explicit treatment of the nodes which become fluid when the particle moves. In this description, the fluid momentum of a new fluid node has to be taken from the particles momentum, while, when the particle 'absorbs' a fluid site its momentum is given to the particle. Formally, the momentum exchange

$$p_{t \rightarrow s} = \rho(n, j)[u(n, j) - U_p]$$

(4.40)
Figure 4.8: LBM approaches for suspended particles. **Left.** Ladd method: Particles are represented by a solid shell. Inner points, belonging to the physical solid domain, are treated as normal fluid nodes. **Center.** ALD method: The inner fluid has no physical meaning, but it is still used to initialize new fluid nodes. Solid nodes of different particles are turned into fluid nodes if they are in contact. Bridge-links are created via which lubrication force elements are applied. **Right.** In the present work we use an improved method applying a corrected momentum exchange (4.60) in combination with a refill method (4.61). The latter removes the need for an explicit simulation of inner fluid.

leads then to another contribution $F_{f \rightarrow s}$ to force and torque on the particle.

When particles come closer than the lattice spacing $\Delta x$ the fluid between the particle can not be resolved if no grid refinement is applied in ever increasing depth. To overcome this lubrication breakdown problem, an explicit model for the lubrication forces based on (asymptotic) lubrication theory \[145\] has to be included. In most suspension models a single particle-particle force term is used. With the ALD method link-wise lubrication correction \[147\] were introduced which provide a better resolution of lubrication forces between arbitrary shaped particles or walls. In the present work we applied the lubrication correction as proposed in \[149, 114\]. It was derived from a first order approximation of the stress tensor based on the stream function for the flow in the gap between two particles that approach each other on their centerline. As a function of the gap $d_{12} = |r_2 - r_1|$ and speed of approach $u_{12} = -\partial_t (r_2 - r_1)$ it reads

$$F_{\text{lub}}(d_{12}, u_{12}) = \left( \frac{d_{12}}{R} \right)^{-\frac{3}{2}} \nu \rho u_{12} \left( F_0 + \frac{d_{12}}{R} F_1 \right)$$

where $F_0$ and $F_1$ are numerical constant given in the references. The lubrication force is only applied for gaps $d_{12} < h_0 = 0.8\Delta x$ as for gaps larger $h_0$ the lubrication force is resolved by the LBM fluid. The actually applied lubrication force has to be reduced by the lubrication force at $h_0$, i.e.

$$F_{\text{lub,eff}}(d_{12}, u_{12}) = \begin{cases} F_{\text{lub}}(d_{12}, u_{12}) - F_{\text{lub}}(h_0, u_{12}) & \text{if } d_{12} \leq h_0 \\ 0 & \text{else} \end{cases}$$

Unlike in \[149, 114\] where only the squeeze mode of the lubrication interac-
tion (4.41) was introduced, we also applied the according rotation mode which also leads to a contribution to the torque on the particles.

Combining hydrodynamical forces $F_{\text{hd}}$, possible $F_{f \rightarrow s}$, lubrication forces $F_{\text{lub}}$ and according torques, positions and velocities of the particles are updated by an integration of the equations of motion for rigid bodies. Usually this is done based on a time stepping $\Delta t$ equal to that of the LBM, and higher order schemes as 4th order Runge-Kutta integration methods can be applied.

**Time-Splitting of the Dynamics of Fluid and Particles** Ever increasing the shear rate the numerical simulation of the fluid and the particles suspended therein eventually leads to numerical instabilities even before reaching the rule of thumb limit for the lattice velocity $Ma(u) < 0.8$. This is not only due to the sensitivity of the LBM iteration to high pressure and velocity gradients, also the interaction with the moving boundaries give raise to unphysical oscillations that build up and lead to a breakdown when the relaxation step leads to over-relaxation and therefore to stripe and checkerboard effects. The fast change of boundary velocities at higher shear rates and primarily the frequent covering and release/refill of fluid nodes are sources for these misfeatures. Also, when two particles approach each other, small pressure waves induced by covering and refill of fluid nodes interact with the particle dynamics and their slightly delayed response might lead to building up oscillations in this coupled system. Of course, the accuracy of the whole scheme suffers already before these effects are visible. All these phenomena are high-frequency effects, spatial as well as temporal, i.e. clear discretization effects as consequences of $\Delta x$ and $\Delta t$.

However, the most sensible subsystem to an integration with a finite time step we found solving the dynamics of two approaching particles for small distances and high relative velocities, even in case of a resting center of mass of those two particles, therefore under exclusion of effects caused by singular events like covering/refill of fluid nodes. It is thus purely related to the integration of the lubrication correction (4.41).

In a model system we neglect the coupling to the LBM fluid and only consider the following ODE

$$\ddot{r} = -a \frac{\dot{r}}{r} - b$$

which has the same functional form as (4.41). With $r$ we denote the distance between the two particles, $a$ is a constant defining the strength of the coupling between the acceleration $\ddot{r}$ and the ratio of velocity $\dot{r}$ and $r$. The constant $b$ is an acceleration pushing the particles towards each other mimicking the interactions with other particles and the fluid in a shear flow. It is clear that in the limit $r \rightarrow 0$ the acceleration diverges. With any $b < 0$, the velocity $\dot{r} < 0$ and the gap inevitably $r \rightarrow 0$. With it the gradient $\partial_r \ddot{r}$ (constant $\dot{r}$ assumed here) also diverges leading to the breakdown of any numerical integration method with finite time step $\Delta t$.

In Fig. 4.9(a) the numerical solutions for $r(t)$ are shown for several values for $b$, all for the initial condition $r(t) = 1$, $\dot{r} = 0$, $\ddot{r} = 0$. The coupling constant $a$ was adapted so that always $a/b = \text{const}$ leading to the same $r(t)$ behavior but at higher $\ddot{r}(t)$. We see that the larger $b$ the earlier the numerical integration breaks down characterized by high frequency oscillations around a constant $r_{\text{break}}(b)$. In Fig. 4.9(b) the trajectories $\dot{r}(r)$ are shown. The coupling constant $a$ was adapted so that al-
Figure 4.9: (a) The time course of the gap \( r \) in the system (4.43) for different \( a > 0 \) and \( b > 0 \) with constant \( a/b \). The larger \( b \) the earlier the integration breaks down. Initial conditions were \( r(t = 0) = 1 \) and \( \dot{r}(t = 0) = 0 \). (b) The trajectories in the \((\dot{r}, r)\) space show that the breakdown correlates with the convergence with \( \dot{r}(r) \rightarrow \text{const} \cdot r \).

As expected, comparing integration schemes we found improved stability for a 4th order Runge-Kutta scheme over the Velocity-Verlet integration and the 1st order Euler method. However, even the Runge-Kutta scheme improved stability only by one order of magnitude in the minimum distance \( r_{\text{break}} \) reached. We therefore decided to treat the particle dynamics on a timescale \( \Delta t_p \) much finer than the time step \( \Delta t \) of the LBM fluid the particles are coupled to. This approach has been described earlier [150] but an explicit dependence of the splitting factor \( \Delta t_p/\Delta t_{\text{LBM}} \) on the shear rate or mass-density ratio has not been given. Incorporating the Krieger-Dougherty relation (4.1), the approximate scaling of \( \nu \sim St^{1/2} \) we find in shear-thickening (see Sec. 5), and the viscosity-stress relation we define the particle-dynamics time step according to

\[
\Delta t_p = c \cdot \frac{\nu_{KD}(\phi)}{\nu_t} \mathcal{S}(\rho_p/\rho_t, \nu_t, \dot{\gamma})^{3/2} \Delta t_{\text{LBM}}.
\tag{4.44}
\]

If this formula gives values below \( \Delta t_{\text{LBM}} \), \( \Delta t_p = \Delta t_{\text{LBM}} \), of course. For the prefactor a value \( c = 1.5 \) was found to be a good choice, leading to a first increase at approximately \( Re_p \approx 0.3 \) and approximately \( \Delta t_{\text{LBM}}/\Delta t_p \approx 1000 \) for the highest Reynolds numbers for which data is presented in Fig. 4.14.

Ideally, one would like to decrease the time step \( \Delta t_p \) only for those particles for which \( \dot{r}/r \) is large. However, due to multi-particle interactions this is not straightforward and we keep this idea for future works.

The application of the time-splitting of fluid and particle dynamics together with the improvements described before in this section allowed us to simulate sheared suspensions of hard-spheres at Reynolds numbers up to 10 before instabilities occurred again. In Fig. 4.14 we plotted data of the apparent viscosity only...
Table 4.1: Comparisons of the approaches of Ladd [144, 125], ALD [146, 147] and CMES combined with an accurate refill (section 4.4.3), concerning the main algorithmic issues for LB suspension flows. In the case of Ladd method, the algorithm from [144, 125] has been combined with the later proposed lubrication correction [145]. Some features are formally independent from each other, which leads to numerous combinations. For simplicity, we restricted this work to the original formulations.

<table>
<thead>
<tr>
<th>feature</th>
<th>Ladd</th>
<th>ALD</th>
<th>present work</th>
</tr>
</thead>
<tbody>
<tr>
<td>inner fluid</td>
<td>active</td>
<td>virtual</td>
<td>no</td>
</tr>
<tr>
<td>refill (un-)cover</td>
<td>inner fluid nodes</td>
<td>inner fluid nodes</td>
<td>equil + noneq. refill [151]</td>
</tr>
<tr>
<td>lubrication</td>
<td>linear theory, 2-part. term [145]</td>
<td>linear theory, link-wise forces</td>
<td>linear theory, 2-part. term [149]</td>
</tr>
<tr>
<td>force computation</td>
<td>MEA</td>
<td>MEA</td>
<td>Corrected MEA [152]</td>
</tr>
</tbody>
</table>

up to \( \text{Re}_p = 4 \) because of finite size effect for larger \( \text{Re}_p \) (particle clusters that percolate the system).

The additional computational costs due to the smaller time step \( \Delta t_p \) are admittedly not negligible. However, for a constant strain over one simulation of 100 the total time steps needed increase with inverse shear rate. By chance costs for the computation of the fluid and that of the particles added up to an almost constant total runtime, regardless of the shear rate.

To summarize the methods, in Tab. 4.1 the main features of the approaches are compared. Note that some features are independent from others (e.g. refilling new fluid nodes and lubrication corrections) and this produces several combinations. For simplicity, we focused on setups reflecting the original ideas.

### 4.4.2 Lees-Edwards Boundary Conditions

When simulating sheared suspensions, Lees-Edwards boundary conditions allow more realistic computational setups as they remove the need of a domain bounded by shearing walls (like in Couette-type flow) which bias typical flow structures. Lees-Edwards boundary conditions therefore allow to investigate pure bulk properties in a quasi-infinite system. Besides that, they improve the computational efficiency of the simulations as the whole domain can be used to calculate averages.

We propose an implementation of Lees-Edwards boundary conditions for Lattice-Boltzmann simulations of particulate suspensions, combined with an accurate treatment of fluid-particle interaction. The algorithm is validated using a simple single-particle benchmark and further applied to a fully resolved suspension flow. Shear-thickening behavior, that is prolonged to higher shear rates as compared to Couette flow results, could be observed.

Lees-Edwards boundary conditions (LEbc) [153] are routinely used in MD simulations to maintain a constant shear over a periodically continued simulation box. They allow to realize a sheared system without the need of explicit shearing solid

---

Periodic boundary conditions are applied in the directions perpendicular to a shear velocity gradient while in the direction of the velocity gradient it is assumed that a copy of the system is moving with a velocity \( \mathbf{u}_{\text{LE}} = (u_{\text{LE}}, 0) \) with respect to the original system and a velocity \( \mathbf{u}'_{\text{LE}} = (-u_{\text{LE}}, 0) \) on the opposite side. This induces a shear rate \( \dot{\gamma} = u_{\text{LE}}/L_y \) over the system height \( L_y \).

The need to develop LEbc for suspension simulations arises from the fact that the application of the common planar Couette viscometer scheme, where two moving parallel planar walls shear the fluid in between, gives results that are unavoidably affected by the presence of the walls. Interested in pure bulk properties we can only use a limited system fraction for measurements. Wall effects are the formation of a depletion zone near the wall and the resultant wall slip, both clearly observable in real suspensions \([154, 155, 111]\) as well as in numerical simulations \([156, 149]\). Suspended particles are limited in their mobility near the wall leading to different particle structure and lower solid-fluid density near the wall resulting in a lower apparent viscosity in that region. Also, the wall slip decreases the shear rate over the bulk leading to a different situation than intended.

The use of viscometer theme in LBM simulations has even greater impact. Here fluid velocity is limited to low Mach numbers and viscosity has a lower bound to ensure stability of the relaxation scheme. This limits the system size at higher \( \text{Re}_p \). Additionally, the system size itself is limited in lattice and particle size units to keep the problem computationally feasible. Therefore, with numerical simulations we cannot escape boundary effects. However, appropriate boundary conditions as proposed here can minimize such effects.

In Computational Fluid Dynamics (CFD) formulations of LEbc exist using other methods for particulate suspensions, for example a finite-element method together with a rigid-ring description of the particle \([157]\). For Lattice-Boltzmann methods (LBM) LEbc for suspensions in 3D \([158]\) were reported but unfortunately
no further details of the implementation were provided, nor answers to questions that arise when combining LEbc with lattice based models. In a recently published work [159] LEbc were used to simulate deformable particles described by a finite-element method and coupled to LBM flow. In the present work we propose a method for a consistent coupling of Lees-Edwards boundary conditions with standard LBM suspensions approaches (such as those by Ladd [144, 125] or Aidun, Lu and Ding [146, 147, 160]). In particular, we employ a corrected momentum exchange method together with a non-equilibrium refill method, both described in [151]. Throughout this section we will refer to this method as CMES.

The lattice Boltzmann method has been briefly introduced in Sec. 4.3.1. In section Sec. 4.4.2, we discuss the implementation of LEbc, while Sec. 4.4.2 is dedicated to numerical tests. First, we validate the algorithms by a simulation of a single disk crossing a LE boundary. Then, we present simulations of a dense suspension and observe flow and particle density profiles as well as $\nu_{\text{app}}$ as a function of $Re_p$.

Implementation

It what follows we present a method for suspension simulations that allows the consistent treatment of solid particles crossing the boundary between systems which move respect to each other. It is an extension of the method by Wagner and Pagonabarraga for fluid-only Lattice-Boltzmann systems [161], where fluid densities that cross a LE boundary have to undergo two steps in addition to normal periodic propagation. The first problem is the implementation of a velocity shift in a method with a fixed set of velocities of densities instead of particles with real coordinates. A Galilean transform has to be applied to the distributions, $f_{i,u_0} \rightarrow f_{i,u_0 \pm u_{LE}}$ where $u_0$ denotes the reference velocity of the computational domain, and $u_{LE} = (u_{LE_x}, 0)$ denotes the velocity shift between the system copies. Following [161] a transform rule can be derived from an approximation of (4.19),

$$f_i = f_i^{eq} + \tau (\partial_t f_i^{eq} + c e_i \nabla f_i^{eq}) + O(\partial^2). \quad (4.45)$$

All terms of order $O(\partial)$ can be skipped, because their zeroth and first moments are of negligible order $O(\partial^3)$. The $u$-dependence is kept and one arrives at a rather simple expression for the change in the boundary-crossing density due to the transform which reads

$$f_{i,u_0 + u_{LE}} - f_{i,u_0} \approx f_i^{eq}(\rho, u + u_{LE}) - f_i^{eq}(\rho, u), \quad (4.46)$$

where $\rho = \rho(f(r, t))$ and $u = u(f(r, t))$. From that we define a Galilean transform operator

$$G_{u_{LE}} f_i = f_i + f_i^{eq}(\rho, u + u_{LE}) - f_i^{eq}(\rho, u) \quad (4.47)$$

that has to be applied to all densities that cross a LEbc. The local density is conserved under this transform.

Another issue in defining a consistent LEbc for Lattice-Boltzmann systems is that the shift between the system copies $s_{LE}$ does not necessarily correspond to an integer multiple of the lattice-spacing. In practice, densities crossing a LE boundary have to be mapped to the destination lattice by an interpolation. More precisely, they have to be distributed over the two cells that partly overlap the
Figure 4.11: Illustration of the cases to be distinguished during the propagation of $f_5$ densities in a model case. Shown are some of the nodes of the upper boundary layer and a part of the lower layer at a Lees-Edwards boundary. Yellow (light gray) nodes belong to a particle crossing the boundary, blue (mid gray) are fluid nodes. $G$ denotes the application of the Galilean transform (4.47), $R$ the application of the reflection operator (4.36).

virtual destination cell. For the simple case of only fluid nodes, for the propagation of densities that are fed from nodes in a shifted reference frame, we can write

$$P_{LE} f_i(r) = s_1 G_{u_{LE}} f_i(r_1 - e_i)$$

$$+ s_2 G_{u_{LE}} f_i(r_2 - e_i)$$

with

$$s_1 = \text{mod}(s_{LE}, 1)$$

$$s_2 = 1 - \text{mod}(s_{LE}, 1)$$

$$r_1 = (x + \text{int}(s_{LE}) + 1, y)$$

$$r_2 = (x + \text{int}(s_{LE}), y).$$

Including solid-fluid interaction given by (4.35) for the propagation of densities that may cross a LE boundary we can write

$$P_{LE} f_i(r) = s_1 \begin{cases} R_{u_b} f_i'(r) & \text{if } L_1 \text{ is BL} \\ G_{u_{LE}} f_i(r_1 - e_i) & \text{else} \end{cases}$$

$$+ s_2 \begin{cases} R_{u_b} f_i'(r) & \text{if } L_2 \text{ is BL} \\ G_{u_{LE}} f_i(r_2 - e_i) & \text{else} \end{cases}.$$  

This approach is motivated by sub-grid scale boundary conditions proposed by Verberg and Ladd [140]. There also, partially covered destination nodes caused a splitting of propagated densities.

To illustrate the application of the propagation operator $P_{LE}$ Fig. 4.11 depicts the fate of $f_5$ densities which propagation vectors point outside the original domain. Density $f_5(r(1))$ is split into two parts $s_1 f_5(r(1))$ and $s_2 f_5(r(1))$ which are propagated to the two nodes of the shifted copy that partly overlap the ghost node it would go to by the application of $P$. On both parts the action of $G_{u_{LE}}$ will be applied. In the case of $f_5(r(2))$ one part, $s_1 f_5(r(1))$, is reflected by the action of $R_{u_b}$ because the according destination node belongs to the particle. In this case, $u_b$ is transformed to $u_b' = u_b + (u_{LE}, 0)$ because the particle is described by its center residing in the reference frame moving with $u_{LE}$ in respect to the original frame.
In the case of $f_3(r(3))$ both parts are reflected by $R_{u'}$. For the case the suspension model includes the description of inner fluid, the density $f_5(r(4))$ undergoes a similar procedure as $f_5(r(1))$.

**Numerical results**

**One particle crossing LEbc**  As an essential validation of the implementation of LE boundary conditions we let a single particle cross the LE boundary. No external forces are applied to the particle. Using LEbc where no solid objects are needed to drive the flow and therefore no preferred reference exists, we are able to superimpose the sheared flow with any constant velocity as long as actual lattice velocities are kept in a range where LBM is valid. Ideally, conserving Galileian invariance, the velocity of the particle should stay constant. However, serious deviations therefrom could be observed using the existing suspension methods. This led to a separate investigation and the proposal of a correction to MEA, which is addressed in Sec. 4.4.3 together with the results for the one particle crossing LEbc experiment.

**Suspension in sheared flow** Next, we simulate sheared suspensions with a solid-fluid fraction $\phi = 0.40$ using the LEbc method and the Couette scheme for comparison of the flow fields. In a squared system of size $L_x \times L_y = 259 \times 259$ lattice nodes we suspended 133 particles with a radius $R_p = 8.0$. The suspension was sheared at particle shear Reynolds numbers $Re_p = 0.005, 0.2, 1.0$ and profiles of velocity and the solid-fluid ratio were measured. Averages were obtained over a shear of $s_{LE} = 10L_x$.

Employing the Couette condition a clear deviation from the Newtonian velocity profile can be seen for $Re_p \gtrsim 0.1$, as shown in Fig. 4.12. Close to the walls an increasing slip becomes clearly detectable which lowers the velocity gradient over the bulk. This behavior could already be seen in simulations of hard-sphere suspensions [162] as well as experimental setups [155].

Fig. 4.12 shows the plot of $\phi(y)$, demonstrating that the profile deviates from the linear Newtonian profile in two aspects

(i) Especially close to the walls, particle densities oscillate with a period of slightly more than one particle width. This suggests that particles tend to align to the walls forming sheets [163]. Such structures of particles parallel to the shear velocity decrease the average inter-particle friction.

(ii) The average particle density near the wall is less than in the bulk. The presence of the wall alone causes a lift force on the particles [164] and causes a depletion zone, according to observations in experimental setups [154]. Another effect of sheet-like structures of particles is that the mobility of particles is inhibited. Particles of sheets sliding along each other mostly collide with small collision cross sections, pushing the particles back into the sheet.

Both effects lower the viscosity and therefore lead to the observed wall slip. Repeating the same experiments using LEbc’s we obtain improved behavior. Here fluid and particles experience homogeneity. Particles are free to form configurations typical for a certain shear rate all over the domain (on the right of Fig. 4.12). In fact, the plots of the profiles on the left of Fig. 4.12 show a flat distribution of
Figure 4.12: (a) Snapshot of a sheared suspension of 133 discs of radius $R = 8.0$ in a domain of $259 \times 259$ lattice sites. The particle-shear Reynolds number $Re_p \approx 1.5$. The gray scale code indicates low (dark) and high pressure (bright) areas. Note the typical particle and pressure field structures that would be inhibited by walls in a Couette scheme. (b) Comparison of profiles as obtained by application of the Couette scheme (dotted line) and Lees-Edwards boundary conditions (solid line). The local average particle density $\phi(y)$ shows strong wall effects in the Couette case. Using LEbc particles are homogeneous distributed over the system height. Both profiles were measured at $Re_p = 1.0$. The velocity profiles $v_x(y)$ as obtained using Couette boundary conditions show increasing slip effects near the wall for $Re_p = 0.1, 1.0$. Using LEbc at $Re_p = 1.0$ no systematic deviations from the Newtonian profile can be seen.
particles over the system height and no systematic deviations from the Newtonian velocity profile.

**Shear-thickening suspension** A highly relevant aspect of hard-sphere suspension rheology is shear thickening at higher particle shear Reynolds numbers $Re_p$. Already in the Stokes regime, the existence of solid particles causes a higher apparent viscosity. The increase of the relative apparent viscosity with higher solid-fluid fractions $\phi$ is best described by the semi-empirical Krieger-Dougherty relation \[165\]

\[
\frac{\nu}{\nu_f} = \left(1 - \frac{\phi}{\phi_{\text{max}}}\right)^{-[\eta]\phi_{\text{max}}}
\]

where $\phi_{\text{max}} = 0.82$ is the solid-fluid fraction in 2D at which particles are packed that dense that any particle flow is impeded and therefore the viscosity diverges. $[\eta]$ is an intrinsic viscosity of the suspension and equals 2 in 2D. It has been shown that ALD and Ladd94 methods can reproduce the Krieger-Dougherty relation in a convincing accuracy over the range of implementable fluid-solid ratios in the range of small $Re$ \[156, 149\]. In Fig. 4.13 we present measurements of the increase of $\nu_{\text{app}}$ over a wide range of solid-fluid ratios $\phi$ as obtained by CMES. The same system settings as for the simulations in the previous sections were used. The results agree well with the expected Krieger-Dougherty behavior.

For shear thickening measurements we used a system with size $259 \times 259$ and 133 suspended disks with a radius of $R = 8$, resulting in a solid-fluid ratio of $\phi = 0.40$. The density ratio was set to $\rho_s/\rho_f = 10$. We used the later value to be able to give direct comparisons with the shear-thickening simulations presented in \[149\]. To obtain the apparent viscosity we followed the method presented in \[156, 162\] which allows shear stresses to be measured in the bulk instead of measuring frictional forces at the walls. Shear stresses can be calculated along a horizontal plane as the sum over the contributions from the fluid and solid phase as outlined in \[162\]. We
obtained stresses by averaging measurements over 10 equally distributed planes and a shear of at least $10L_x$. In the case of Couette boundary conditions we took care that only bulk properties were measured by distributing the stress planes in such a manner that none of them was closer than 50 lattice sites to the wall. Looking at the profiles in Fig. 4.12 we can safely assume that direct influences of the walls are absent at this distance. Using LEbc measurements can be carried out over the whole system height. This increases the bulk area we are interested in significantly.

In Fig. 4.14 apparent viscosities are shown, normalized by the Krieger-Dougherty relation obtained for a range of $Re_p$ from 0.001 to 4.0. The maximum achievable Reynolds number is limited by stability conditions of the LBM scheme giving a lower bound for the fluid viscosity and limiting the maximum particle lattice speed. For the highest $Re_p = 4$ we used a fluid viscosity $\nu_f = 0.02$ and set the Lees-Edwards shift velocity to $u_{LE} = 0.0405$.

For comparison in Fig. 4.14 we also plotted shear-thickening measurements obtained by Kromkamp et al. with the ALD method, Couette conditions and comparable system settings [149]. Our results for the Couette case agree very well with their data. At about $Re_p = 0.01$ the apparent viscosity begins to increase and levels off at about $Re_p = 0.2$. Also at the highest $Re_p$ we could carry out stable simulation $\nu_{app}$ stayed roughly constant. We repeated the experiments using the Lees-Edwards boundary conditions proposed in this work and obtained a behavior that significantly differs from the Couette results for $Re_p > 0.1$. Instead of a saturation behavior $\nu_{app}$ shows a continued increase. The profiles in 4.12 offer a straightforward explanation for this. Using the Couette conditions we see a slip near the wall for $Re_p > 0.1$ which lowers the velocity gradient and the effective shear rate over the bulk.

A direct relation between the actual bulk shear rate and $\nu_{app}$ independent from $Re_p$ could not be found to be clearly visible over the plateau range. This may be caused by the different characters of momentum exchange events for different
slip velocities. At higher slip velocities particles may collide with much higher momentum exchange and impact on the particle structure in the bulk but, on the other hand, such events are less frequent in that regime.

When LEbc's are used these wall effects are not present and the suspension can be sheared at the actually intended shear rate enabling unbiased studies of sheared hard-spheres suspensions. The apparent viscosity obtained with LEbc shows a continued increase of $\nu_{app}$ giving rise to the assumption that shear-thickening either levels off at higher Re$_p$ or that there is a crossover to jamming behavior. There the shear rate is so high that the suspending role of the fluid becomes negligible and particles collide and jam as in a granular medium.

Using this implementation of LEbc, we could also start extended studies on cluster formation, investigating the growth of typical structures in sheared suspensions. Results will be presented in Sec. 5. Concerning the present work, we only took care that particle cluster size did not exceed system size to prevent percolation of particle clusters which would lead to a jammed suspension in a Lees-Edwards system.

For an estimation of the increase in computational effort due to the proposed implementation of LEbc, we measured the ratio between the runtime of both to be 1.06. The additional effort of 6% is still much less than the approximately 30% of the system height at the highest shear rate that cannot be used for measurements due to the bias by the wall. Increasing the distance between the walls to correct for this, as well as increasing the wall speed to maintain the same shear rate in a Couette flow simulation, would lead to a Mach number that is approximately 30% higher and would therefore lead to a potentially higher error of the LB method and to the onset of instabilities. Furthermore, LEbc do allow for simulations of systems where the typical correlation length (e.g. particle cluster size) would exceed the unbiased bulk width in a Couette flow simulation.

As a final remark, although only of technical importance, we observe that, using LEbc, the global momentum is not exactly conserved due to numerical inaccuracies of Lattice-Boltzmann schemes and the absence of solid obstacles which would define a preferred reference frame. We could improve the conservation by a correction of fluid and particle velocities equivalent to a Galilean transform of the whole system, without affecting the physics.

### 4.4.3 Corrected Momentum Exchange

We are interested in the rheology of sheared suspensions, i.e. the change in viscosity when the system is subject to an external shear flow. In such situations, it becomes useful to demand Galilean invariance of the computation of fluid-solid interactions to ensure homogeneous behavior of the particles, not dependent on the external velocity and therefore not dependent on the position in a sheared system (see Fig. 4.15).

In this section the effect of non Galilean invariance of the LBM methods on the dynamics of sheared particle-fluid systems are investigated. Selecting particular cases of one particle crossing a Lees-Edwards boundary, we show that standard

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methods for the simulations of suspension flow might lack sufficient accuracy. Using asymptotic expansion techniques, we motivate the need for a correction term and implement a possible solution. The obtained Corrected Momentum Exchange for Suspension (CMES) preserves local consistency and Galilean invariance in relevant orders.

**Asymptotic Analysis**

Using the asymptotic expansion technique [138], it can be shown that the numerical solution of (4.22) can be approximated by the expansion

\[
F_h(n, j) = f^{(0)} + h f^{(1)}(n h^2, h j) + h^2 f^{(2)}(n h^2, h j) + O(h^3)
\]  

(4.53)

with smooth and \( h = \Delta x \)-independent coefficients defined as

\[
f_i^{(0)} = w_i,
\]

\[
f_i^{(1)} = w_i c_s^{-2} c_i \cdot u_{NS},
\]

\[
f_i^{(2)} = w_i c_s^{-2} p_{NS} + \frac{w_i c_s^{-4}}{2} \left( |c_i \cdot u_{NS}|^2 - c_s^2 u_{NS}^2 \right)
\]

\[
\tau w_i c_s^{-2} c_i \cdot \nabla u_{NS} \cdot c_i,
\]

(4.54)

where \( u_{NS} \) and \( p_{NS} \) solve a Navier-Stokes problem.

From (4.54), we conclude that (4.23) yields a second order accurate velocity, while a first order accurate pressure can be obtained with

\[
p = c_s^2 \rho - \frac{1}{h^2}.
\]  

(4.55)

Similarly a first order approximation of the viscous stress tensor \( S[u] = \nu (\nabla u + \nabla u^T) \) can be extracted using

\[
S_{\alpha\beta} = -\frac{\nu}{h^2 c_s^2 \tau} \sum_i w_i \left( f_i - f_i^{eq}(f) \right) c_i \alpha c_i \beta.
\]  

(4.56)
Figure 4.16: The benchmark $D_1$: single particle crossing the boundary between different reference frames.

i.e the second order moment of the non-equilibrium part with respect to the velocity space.

The results of the analysis actually provide more than these accuracy results. They contain relevant information concerning the structure of the solution, which can be used to improve the algorithm.

**Numerical tests**

We aim on a method which resolves the dynamics of particles independently from any constant velocity superposed to the movement of local centers of mass as present in all non-trivial flow problems. In case of errors due to the violation of Galilean invariance, such errors would be amplified if the same physical problem is described using coupled reference systems, like in the application of LEbc. We used the LEbc proposed in Sec. 4.4.2 (also published as [113]) to allow simulations of homogeneously sheared systems and to superpose them with a small, constant velocity.

For the simulations presented in the following we used a system size $L_x = L_y = 128$ and a particle radius $R = 4.8$ (all numbers given in lattice units). The density ratio was set to $\rho_s/\rho_f = 10$ and the kinematic viscosity of the fluid $\nu = 1/6$.

**Single Disk ($D_1$).** We simulate a single particle in a periodic shear flow. In detail, initially a particle is placed in the midpoint of a the squared domain, with a velocity equal to the fluid velocity at that point $v_p(t = 0) = u_s(t = 0) = (u_x, 0.005)$ (Fig. 4.16). Additionally the flow is initialized and maintained at a horizontal shear $\dot{\gamma} = u_{LE}/L_y$ and the particles angular speed is accordingly initialized to $\omega(t = 0) = \dot{\gamma}/2$. With that an equilibration of near-particle fluid field and $\omega$ was reached after approximately $t = 3000$. In any case, this equilibration process is physical and should therefore be Galilean invariant, too.

Throughout the simulation we measure the vertical velocity of the particle $v_{p,y}(t)$, which should remain constant in the ideal case. However, as shown in Fig. 4.17, in the case of the ALD method a significant deviation from $v_{p,y}(t = 0) = 0.005$ can be observed already from early times on, not having reached the LEbc yet. When Ladd method is used, no deviations can be seen during that time, which finds its explanation in the fact that every error made in link-wise calculations is compensated by the use of physical inner fluid, where every momentum exchange at a boundary link has its inner inverted counterpart. Using the ALD method, e.g. applying MEA only at the outer surface, the particles feel a non-physical vertical force in situations where points at the upper surface move at a different speed than points at the lower surface.
Deviations in both methods appear when the particle crosses the LEbc. Notice that in this situation boundary links exist that connect nodes in different reference frames (in practice, different \( u_b \) are used in (4.37)). Here, errors cannot be compensated by the inner fluid. The non-Galilean effect grows linearly when varying \( u_x \). A shear rate \( \dot{\gamma} = 5 \cdot 10^{-5} \) was present in all these measurements.

Fig. 4.18 shows similar measurements. Here the curves are recorded for different \( \dot{\gamma} \) and the superposed initial velocity \( u_s = (0.05, 0.005) \) was kept constant. All the curves show similar behavior compared to the measurements in Fig. 4.17, both in absolute size and order. MEA in its form (4.37) (with \( T_{CJ} = 0 \)) leads to a non-zero force integration over the surface depending on both, the absolute particle speed as well as the difference between surface velocities at the upper half and the lower half of a particle.

**Approaching Disks (D2).** The next example aims to demonstrate the effects of combining LB fluid-structure interaction with suspension dynamics, when different flow velocities are used as background. We consider two equal particles moving toward each other, driven by a small external force (Fig. 4.19 and 4.20). The gap at time \( t = 0 \) is \( r_{1,2} - R_1 - R_2 \approx 1.19 \), in order to have at least one fluid node between the particles at the beginning. Without adaptive grid-refinement lubrication forces have to be implemented explicitly. Regarding the different suspension methods, lubrication corrections were applied as given in Tab. 4.1. For simulations using CMES we applied a lubrication correction in the form proposed in [149] for 2-dimensional systems. Such forces were invoked for gaps smaller than \( h_c = 1.0 \approx 0.21R \).

Both particles are always aligned in x-direction. To mimic the fact that particle-particle collisions happen at different locations in a shear flow, the flat (non-sheared) flow field is superposed by a constant translational velocity \( u_s \), and the experiment is repeated using different absolute values and directions of \( u_s \). The particles are always initialized with the same velocity as the fluid. Measuring the gap between the particles as a function of time, we can investigate the combined effect of force computation, lubrication corrections and nodes re-initialization.

Fig. 4.19 shows the results obtained with superimposed velocities \( u_s = (u_x, 0) \). Looking at the problem from the lattice reference frame, one particle is following the other while they get closer. In an ideal case, the lubrication-damped collision of the particles should not be affected by the absolute velocity of their center of mass. However, using Ladd’s method at higher superposed velocities the particles tend to approach themselves faster in comparison to a simulation where the center of mass is at rest (which is the usual way lubrication behavior investigations are carried out in the literature). Fluid between particles is of higher pressure than the fluid at the opposite sides of the particles. When particles move fluid nodes will turn into inner fluid. Not instantly in equilibrium with the rest of the inner fluid, such a high-pressure inside fluid causes forces that counteract lubrication forces. As an additional effect, adopting high-pressure gap nodes also leads to a kind of pumping: the following particle gains mass with the increase of inner-fluid pressure which biases the particle dynamics. The ’pumping effect’ has another consequence: When inner fluid turns into outside fluid behind the particle the increased pressure also contributes to a less damped collision behavior of the particles.

Although the last argument could also apply in the case of simulations using ALD, results obtained with this method show a better behavior. Here, by definition
Figure 4.17: The vertical speed $v_y$ of a single particle in a sheared system ($\dot{\gamma} = 5 \cdot 10^{-5}$) crossing a LEbc for different superposed velocities $u_{s,x}$. At about $t = 12300$ the particle reaches the LEbc and crosses it within a time $t_c \approx 2000$. In the ALD case the deviation from the constant velocity present from early times causes a slight shift of the minimum towards later times (also seen in Fig. 4.18).
Figure 4.18: The vertical speed $v_y$ of a single particle in a sheared system crossing a LEbc for different shear rates $\dot{\gamma}$. The particle is moving with the fluid at a superposed background velocity $u_s = (0.05, 0.005)$. 
of the model, fluid nodes always exist between the particles. As a consequence we could observe that the 'pumping effect' was less pronounced.

When particles are very close and therefore lubrication forces very sensitive we would have expected that the additional momentum exchanged when nodes are covered or uncovered lead to deviant behavior. However this seems to have little importance for the particle dynamics in these tests. Although small deviations can be seen, the action of a physical inner fluid turns out to be the most important source of errors.

In Fig. 4.20 we show the results for the case of a constant absolute superposed velocity \(|u_s| = 0.075\) but for different directions. The curves for \(\alpha = 0, \pi/6, \pi/3, \pi/2\) show only slight deviations from each other if ALD is used. In the case of active inner fluid (as in Ladd’s method), a strong angle-dependent behavior can be observed. For \(\alpha = \pi/6, \pi/3\) another effect appears. If the background velocity has an inclination \(0 < \alpha < \pi/2\) with respect to the vector \(r_{1,2} = x_{p2} - x_{p1}\), we still observe a small 'pumping'. With the broken symmetry of the problem the different properties of the two particles cause the particles to start to tumble around each other. The results in Fig. 4.20 show the results for the case a constraint \(y_{p1}(t) = y_{p2}(t)\) was applied and curves that cross the x-axis in case of tumbling.

**Galilean invariant force computations**

The previous results show that Ladd’s method and ALD have shortcomings. Using the asymptotic expansion technique it is possible to identify the main source of errors, and to derive leading order corrections to the original algorithms. Starting from (4.54), which approximates the solution of the LBM (4.22), a prediction for the momentum exchange contributions (4.37) (with \(T_{CJ} = 0\)) can be derived.

Let us consider a boundary node \(k\), and an outgoing boundary link \(i\) at \(k\). We denote with \(b_i(k)\) the intersection between the link \(c_i\) and the fluid-solid interface. Inserting ((4.54)) into ((4.37)) we obtain (dropping the time dependence for brevity)

\[
p_i(k) = p_i^{(0)}(x_k) + h^2 p_i^{(2)}(x_k) + O(h^3),
\]

with

\[
p_i^{(0)}(x_k) = 2w_i c_i
\]

\[
p_i^{(2)}(x_k) = 2w_i c_i^2 \left(p + \frac{c_s^2}{2} \left(\left|c_i \cdot u_b\right|^2 - c_s^2 u_b^2\right) - c_s^2 \nu c_i \cdot \nabla u_b \cdot c_i\right),
\]

where the quantities on the right hand sides are evaluated at \(b_i(k)\).

Using this approach, it can be proved \([152]\) that MEA yields a first order accurate approximation of the force acting on a particle \(P\),

\[
F_P(t) = \int_{\partial P(t)} (-p(x)n + n \cdot S(x))d\gamma.
\]

Beyond this general result, (4.58) provides additional useful information. We focus on the second order coefficient of (4.58), which contains a term not related to the boundary force, explicitly depending on the boundary velocity, and responsible for breaking the Galilean invariance.
Figure 4.19: Test D$_2$ a: Gap size between two particles that feel horizontal forces pushing them together for different absolute values of the superposed velocity $u_s$. The direction is $u_s \parallel r_{1,2}$. The three plots show results obtained with different suspension models.
Figure 4.20: Test D$_2$ b: Gap size between two particles for different angles \( \alpha = \angle(u_s, r_{1,2}) \). Results for the three suspension models are shown. In the Ladd case, particles (if \( y_{p1} = y_{p2} \) is not fixed) start to tumble leading to negative x-distances (dashed lines).
It must be remarked that in most cases this term produces a small global contribution [166]. However, this does not apply using Lees-Edwards BC, when the solid-fluid interaction of one particle are evaluated in different reference systems within the same time step (in practice, in this case the MEA depends on the contributions of two part of the interfaces, with different velocities).

Aware of (4.58) we can easily define a correction for the momentum exchange algorithm which reads

\[ p_i^{\text{CME}}(k) = p_i(k) - 2w_i c_i - h^2 w_i c_s^{-4} \left( |c_i \cdot u_b(b_i(k))|^2 - c_s^2 u_b(b_i(k))^2 \right) c_i. \]  

(4.60)

Together with \( p_i(k) \) in (4.37) and the summation over the particle surface in (4.38) this defines a corrected momentum exchange algorithm (CMES) for the calculation of hydrodynamical forces and the torque on the particle.

The violation of Galilean invariance by MEA, when used locally, has been already observed in [167] and cured by the introduction of additional virtual fluid nodes inside the solid domain. However, this is a special solution and care has to be taken at the implementation of such an idea when boundary links cross a Lees-Edwards boundary. The correction (4.60) offers a consistent analytical solution and, in most cases, allows an easier implementation.

**Initialization of new fluid nodes**

Reinitialization of new fluid nodes is a common task dealing with moving boundary LBM. Both Ladd’s and the ALD approach make use of inner fluid to deal with this. In general, this is justified if inner nodes hold densities which approximate the right characteristics when turning from an inner surface node to an outer surface node. This is likely only in situations where the particle acceleration is low. If a particle is accelerated the fluid directly behind the particle is typically of lower pressure while the adjacent node inside the shell would be of rather high pressure.

The problem can be solved by a more accurate initialization of LB densities according to the expansion coefficients (4.54). This can be done in an efficient way, separately approximating the *equilibrium* and the *non-equilibrium* part, as described in [166, 151]. In detail, denoting with \( k \) a new fluid node, first velocity \( u(k) \) and pressure \( p(k) \) are extrapolated using a set of available neighboring fluid node, to construct the equilibrium distribution

\[ \tilde{f}_i^{\text{eq}}(k) = E_i \left( \rho_0 + c_s^2 h^2 p(k), u(k) \right). \]

Then, a low order extrapolation for the non-equilibrium part \( \tilde{f}_i^{\text{neq}}(k) \) is added, initializing (omitting the time dependence)

\[ f_i(k) = \tilde{f}_i^{\text{eq}}(k) + \tilde{f}_i^{\text{neq}}(k). \]  

(4.61)

In practice, \( \tilde{f}_i^{\text{neq}}(k) \) can be copied from a neighboring node [151]. This approach is by definition locally consistent with the inner LB solution, and yields the same accuracy as the standard LBM [166, 151], providing a good balance between computational effort and quality of results. We remark that similar approaches, based on extrapolation techniques have been proposed in [141, 168], which also achieved accurate refill. However, these are based on more complicated extrapolations and
become less practical when dealing with the flow of dense suspensions. In practice, in case of colliding particles it might happen that not enough nodes are available in order to implement algorithm (4.61) with the required accuracy. In those cases, we have used lower order approximations for the equilibrium distribution, based on simpler averages (but still including a non-equilibrium approximation).

**Numerical Results**

Including the modifications described in the previous section, both tests D₁ and D₂ are solved more accurately.

Correction (4.60) for the momentum exchange algorithm significantly reduces non-Galilean deviations in D₁ (see figures 4.17 and 4.18) in comparison to the results obtained by standard MEA, applied only at the outer surface (ALD). Still, it can be observed that CMES does not behave as accurate as the original method by Ladd if the particle is treated in only one reference frame, but this is mainly due to additional symmetry properties of Ladd’s methods in the specific benchmark. In general, figures 4.17 and 4.18 show that the particle dynamics has significantly improved by the use of CMES when particle-surface interaction has to be treated partly in different reference frames.

The benchmark D₂ demonstrates that the use of an accurate equilibrium + non-equilibrium refill improve the resolution of particle dynamics, avoiding effects that are caused by just turning physical inner fluid nodes into outer fluid nodes and vice versa (figures 4.19-4.20).

In D₂ the ALD method also produces results almost independent of \( u_s \). However, it still requires the computation of an inner fluid. Aiming at simulations of dense suspensions the cost for this is in the order of \( \phi = V_s/V_f \). With the application of a refill procedure as proposed in this paper the computation of inner fluid can be omitted, providing a theoretical speed-up factor of \( 1/(1 - \phi) \).

**4.4.4 Initial Conditions and Observables**

When the micro-model is invoked in order to return values for the apparent viscosity \( \nu_m = \nu_{app} \) and shear-induced diffusivity tensor \( \mathbf{D}_m \), the shear rate \( \dot{\gamma}_M \) and volume fraction \( \phi \) are passed as arguments. In Fig. 4.6 it is shown that the execution of an instance of MiS is preluded by the setup of the spatio-temporal domain. As discussed in Sec. 4.2.4 we consider a two-dimensional domain of \( 72\Delta x_m \) in both dimensions at a resolution of \( \Delta x_m \) and the particle radius used was \( R = 3.15\Delta x_m \). Although this resolution of the spatial domain is smaller than that used to validate the Lees-Edwards boundaries introduced in Sec. 4.4.2, we found that this choice is a good compromise between accuracy and computational effort. Having set the solid-fluid mass density ration to \( \rho_s/\rho_f = 10 \), the measurements of the increase of \( \nu_{app} \) with \( \phi \) at \( Re \ll 1 \) and the shear-thickening behavior \( \nu_{app}(\dot{\gamma}) \), both presented in Sec. 4.4.2 could be reproduced with agreement within statistical errors. The runtime of a single MiS instance has been approximately 1 hour on a single CPU\(^5\).

\(^5\)Averaging over a strain of 100, which was the same for all values of \( \dot{\gamma} \), the number of iterations scales as \( \dot{\gamma}^{-1} \). However, with the increased resolution of the temporal scale of the suspended particles (see (4.44)), and therefore the increased computational effort to solve the particle dynamics, the total runtime of a MiS instance was approximately constant.
When the micro-model is launched the fluid velocity is initialized according to

\[ u_m(x, y, t = 0) = \frac{L_m \dot{\gamma}_m}{2} - \dot{\gamma}_m y \]  

resulting in a homogeneous shear flow field with zero velocity at the center line, \( u_m(x, y = L_m/2) = 0 \).

Initializing the suspended particles is a bit more tricky since we expect also volume fractions \( \phi \) larger than for which a random distribution of non-overlapping particles can be done. Instead, particles are placed on a hexagonal grid that fully covers the domain and satisfies the periodic boundary conditions. The grid has 10 x 12 nodes on which a maximum number of \( N_{\text{max}} = 120 \) particles can be placed. Thus, the maximum volume fraction we can reach with a fully occupied grid is \( \phi_{\text{max}} = 120 \pi R^2 / L_m^2 \approx 0.72 \). Instead of adapting the particle radius \( R \) to set \( \phi \) exactly to the value passed from MaS, \( N_{\text{max}} - N \) randomly chosen particles are removed from the grid. The number of particles \( N \) left on the grid is calculated according to

\[ N = \text{int} \left( \frac{\phi}{\phi_{\text{max}}} N_{\text{max}} + 0.5 \right) \]  

where \( \text{int}() \) truncates the real valued argument to an integer. With that we introduce a deviation from the volume fraction \( \phi \) as passed from MaS and the actual volume fraction at which the simulation is carried out is \( \phi_{\text{sim}} = N \pi R^2 / L_m^2 \). The maximum deviation from \( \phi \) is approximately 0.003, a value much smaller as the confidence range in \( \phi \)-dimension of the parameter space for which extra/interpolation are trusted to give sufficiently accurate results when values for \( \nu_{\text{app}}(\phi, \dot{\gamma}) \) and the diffusivity tensor \( \mathbf{D}(\phi, \dot{\gamma}) \) are requested from the database (see Sec. 4.6.2 for the introduction of and the discussion on such a database and confidence ranges). In any case, the values for \( \nu_{\text{app}} \) and \( \mathbf{D} \) obtained from MiS are properly added to the database for \( \phi_{\text{sim}} \) and \( \dot{\gamma} \). Through extra/interpolation \( \nu_{\text{app}} \) and \( \mathbf{D} \) will be returned to MaF and MaS, respectively, for the exact \( \phi \).

After \( N \) particles are placed on the grid their positions are randomly varied. Beginning from a maximum distance of \( d = 2R \) from the original position, in repeated attempts with random angles the particle is tried to put on a new position. When an attempt was not successful, i.e. the new position results in an overlap with another particle, the distance \( d \) is decreased and a new attempt is made with a new angle. This is repeated until a valid position is found which is at the latest satisfied for \( d = 0 \). This method could be described as “melting grid”. Particles are put in perfect order after which as much as possible disorder is introduced.

To obtain the apparent viscosity we followed the method presented in [156, 162] which allows shear stresses to be measured in the bulk instead of measuring frictional forces at the walls which can be done in Couette flow simulations. Shear stresses can be calculated along a horizontal plane \( S \) as the sum over the contributions from the fluid and solid phase as outlined in [162] according to

\[ \Sigma = \sigma_f + \sigma_s + \tau_f + \tau_s \]  

where \( \sigma \)'s refer to stresses due to pseudo-turbulent motion of the phases. The \( \tau \)'s refer to viscous stresses of the two phases, in the case of the particles it is internal elastic stress which can be calculated as \( \tau_s = (F_{pp} + F_{ip}) / A_p \). In that \( F_{pp} \)
denotes the force on a particle due to collisions with other particles, \( F_{fp} \) refers to the interaction between fluid and particle. \( A_p \) is the intersection area of \( S \) and a particle (For further explanations on the calculation of \( F_{pp} \) and \( F_{fp} \) we refer the reader to [162]). Measurement are carried out in intervals of a strain of 1/4 and averaged over a total strain of 100. The time \( t^{\text{equil}} = 1/\dot{\gamma}_m \) after initialization is considered as equilibration time needed by the system to evolve into typical flow fields and particle configurations. Only after that measurements contribute to the average of the total shear stress \( \langle S \rangle \). The apparent viscosity is then obtained by computing \( \nu_{\text{app}} = \langle S \rangle /\dot{\gamma}_m \).

### 4.5 Shear-induced Diffusion

In this work we concentrate on monodisperse hard-sphere suspensions that are relatively well understood, at least in the limit \( Re \ll 1 \) and \( \phi \ll 1 \). This also due to the tremendous theoretical work of Brady and coworkers over the last decades and the Stokesian dynamics simulations they support their theories with, and numerous experimental studies since the first publication by Eckstein, Bailey and Shapiro [169].

In the absence of external fields the transport of particles, and therefore a possible change of the local macroscopic volume fraction \( \phi(x_i) \), in a sheared suspension can be attributed to three processes. One of them is Brownian motion due to thermal fluctuations in the momentum exchange between suspended particles and the molecules of the surrounding fluid. It results in short-time diffusivity, i.e. the short-range Brownian motion which, in a dense suspension, is quickly disturbed by the interactions with the surrounding particles. A second process is the shear-induced motion of particles. Although for \( Re \ll 1 \) the interaction of two particles in a shear flow is symmetric and reversible, and might not lead to a permanent displacement (see for example [114]), for larger \( Re \) it does (see for example [170] and Sec. 5.2.1). In case of complex hydrodynamical interactions between more than two particles in a dense suspension a permanent displacement of the particles is the normal case. This leads to a shear-induced self-diffusion contribution to the total diffusivity that scales as \( D^s \dot{\gamma} \phi \) in leading order for monodisperse hard-sphere suspensions. The “standard” diffusivity induced by a gradient in the local volume fraction, i.e. \( \Delta \phi(x)/\Delta x \neq 0 \), can be well described by Fick’s law. This gradient diffusivity is defined as the proportionality factor between the concentration gradient and the resulting net flux of particles, i.e. a balancing change in the macroscopic \( \phi(x_i) \). However, assuming to be in the regime \( Pe \to \infty \), Brownian motion is disabled which would have been the driving process behind long-time diffusivity. In the limit \( \nu_f \to 0 \), where in the absence of dissipation due to hydrodynamical interaction the suspension would behave as a gas where the kinetic energy of the particles is conserved, we could define a suspension temperature and a Brownian diffusion on the particle scale. However, the suspensions we consider are at finite Reynolds numbers and any motion of the suspended particles would decay quickly if the driving process is turned off. We are therefore left with shear-induced diffusion as the only underlying process of particle transport. First experiments that showed a diffusion-like migration of particles from high-shear regions to lower shear were published by Leighton & Acrivos [171]. Also a gradient in \( \phi(x) \) provokes a gradient in the collisions
rate. This effect is also reflected in an anisotropy in the pair distribution function of the suspended particles. The net effect of these interactions is that particles will migrate from regions of high concentration to low concentration, and from regions of high shear to low shear [172]. Leshansky and Brady could show that this shear-induced gradient diffusivity $D^\nabla$, as being based on the same microstructural processes, is linear proportional to $D^s$, the shear-induced long-time self-diffusivity and can be approximated by [173]

$$D^\nabla \approx \frac{D^s}{S^{eq}(0)}. \quad (4.65)$$

Here, $S^{eq}(0)$ is the static structure factor corresponding to the hard-sphere suspension at thermodynamic equilibrium. For dilute suspensions it scales as [173]

$$S^{eq}(0) \sim 1 - 8\phi \quad (4.66)$$

based on excluded volume effects.

In the regime of larger shear rates particle migration and hydrodynamic diffusion are still not well-understood. This is due to the difficulties arising when trying to mathematically model the changing microstructure and collective behavior of the particles. Models considering single particles colliding with other particles can not be applied anymore. The scaling of the long-time self-diffusivity

$$D^s = \dot{\gamma} R^2 \tilde{D}(\phi) \quad (4.67)$$

still holds. However, $\tilde{D}(\phi)$ can be found to be a strongly increasing function of the particle volume fraction. A best fit to experimental data of sheared hard-sphere suspensions can be found as [172]

$$\tilde{D} = 0.5\phi^2 (1 + 0.09 \exp(7\phi)) \quad (4.68)$$

which, with the same functional form but with different numerical coefficients, can also be found in [174]. This is in stark contrast to

$$D^s \sim \dot{\gamma} R^2 \phi \quad (4.69)$$

derived from scaling arguments in the regime of small $\dot{\gamma}$ and $\phi$.

With the multi-scale simulations we aim for maximum flexibility of the framework in respect to the micro model, that is, we want to preset as less as possible about the behavior of the micro-model. We will make use of (4.65) and (4.66), however, not of $D^s \sim \dot{\gamma} \phi$ as this scaling can strictly only be derived under assumptions as $Re \ll 1$ and two-particle interactions. To our knowledge, no analytical derivation of $D = f(\dot{\gamma}, \phi)$ exists today which would be valid also for high shear rates where the typical microstructure differs clearly from that at low or medium shear rates. Furthermore, the linear dependence on $\dot{\gamma}$ and $\phi$ might not hold for suspended particles of non-spherical shape, if they are deformable, or in the presence of additional inter-particle forces.

At the moment we cannot model a concentration gradient in the micro-model by appropriate boundary conditions because it would make particle insertion and deletion necessary. This is a highly non-trivial task in a dynamic simulation because with the artificial deletion/insertion of particles the microstructure will be
frequently disturbed. However, we can measure self-diffusivity of single particles in the homogeneous micro-model. Doing so we are forced to make use of (4.65) and (4.66) to link the self-diffusivity behavior to the gradient diffusivity needed to describe the evolution of the particle concentration on the macro-scale. The scaling (4.66) is only valid for small $\phi$ and would give negative $S^{eq}(0)$ for $\phi > 1/8$.

As no analytically derived extension to larger $\phi$ for the effect of excluded volume on the structure factor exists, we model the structure factor as a curve

$$S^{eq}(0) = a \exp(-8b\phi) - c$$

(4.70)

where $a$, $b$ and $c$ are chosen such that $S^{eq}(0)$ itself and its first derivation in respect to $\phi$ agrees with (4.66) in the limit $\phi \to 0$. The third condition is that it should become zero for $\phi = \phi_{\text{max}}$ enforcing a divergence of $D^V$ at this volume fraction. This condition models the effect that a particle moving towards a region with maximum packing density will not find a way to enter it.

### 4.5.1 Diffusivity Measurements on the Micro-Scale

Self-diffusion coefficients can be calculated using the integral of the velocity auto-correlation function [175, 176], using the relation

$$D = \frac{1}{2R} \int_0^\infty \langle v_p(t + t_0)v_p(t_0) \rangle, \quad (4.71)$$

It could also be derived with a novel method in which use is made of the fact that an initial suspension microstructure relaxes towards the microstructure typical for long-time shearing proportionally to the gradient diffusion coefficient [175]. In the later case, averaging over a large number of initial conditions is necessary. We however want to measure the diffusivity in the same run we measure also the apparent viscosity. So instead of using an ensemble average we seek for a time-average method. In an interesting work Leshansky and Brady [173] show that the gradient diffusivity can be obtained from measurements of the dynamic structure factor of the solid phase. Based on the relaxation of the average fluctuation in particle number density the structure factor approach seem to offer a much better statistics. However, we leave the exploration of this possibility for future work and will, for now, base our computations on the “classical” direct measurements of the particle displacements in the long-time regime.

The components of the shear-induced self-diffusion tensor can be determined in a simulation by measuring the increase of the mean-square displacements with time after diffusive motion has been established according to

$$D = \lim_{t \to \infty} \frac{1}{2t} \partial_t \langle (x_p(t) - x_p(t_0) - x^a(t))(x_p(t) - x_p(t_0) - x^a(t)) \rangle \quad (4.72)$$

$$\approx \frac{1}{2t} \langle (x_p(t) - x_p(t_0) - x^a(t))(x_p(t) - x_p(t_0) - x^a(t)) \rangle. \quad (4.73)$$

Here angle brackets denote an average over all particles in the system. The affine displacement $x^a(t)$ accounts for the movement of a particle in $x$-direction with the shear flow. It has to be evaluated from the displacements at every time step and can be based on a linear shear flow assumption. The $y$-component in velocity
gradient direction is $x_y = 0$, the $x$-component is computed according to

$$x_x(t) = \sum t \left( v_{p,y}(t) - \frac{\dot{\gamma} L_y}{2} x_{p,y}(t) \right) \Delta t$$

(4.74)

where $v_{p,y}(t)$ is the $y$-component of the particles velocity at time $t$, $L_y$ is the height of the system and it is assumed that the linear shear flow is that way that $u(x, y = L_y/2) = (0, 0)$. Care has been taken in case a particle crosses a Lees-Edwards boundary in $y$-direction. The current shift of the systems copy should then be added or subtracted, respectively, from the $x$-displacement of that particle.

The preparation of the initial conditions as described in Sec. 4.4.4 aims at initial particle configurations that are very similar to configurations found at a later stage of the simulations. However, an equilibration time is needed to let the system evolve into the typical microstructure characteristic for long-time shearing. This can be also seen in measurements of the displacements $x_p(t) - x_p(0)$. In Fig. 4.21 the flow gradient component of the mean-square displacement is shown for a simulation of 42 particles in the micro systems of size $72 \times 72$ ($\phi \approx 0.25$). For very short times the increase of the displacement scales as $t^2$ characterizing the initial reordering dynamics which are different from the long-time behavior. We can not speak of short-time diffusion here, as in the absence of Brownian motion the initial dynamics of a particle are deterministic. From a strain of approximately $\dot{\gamma} t \approx 1$ the displacement curve scales as $t$ validating a diffusion description for the shear-induced movement of the particles in the long-time regime. This crossover was found to be independent of the shear rate and volume fractions. Therefore, for all micro-simulations measurements were carried out only after an equilibration time of $t_{\text{equil}} = \dot{\gamma}^{-1} = t_0$. 

Figure 4.21: Mean square displacement in $y$-direction measured in a micro pocket run with $\dot{\gamma}$ and $\phi = 0.316$. A strain of $\dot{\gamma} t \approx 1$ is needed to let the suspension evolve into typical particle configurations after the creation of the initial distribution. The reordering dynamics is characterized by a $\sim t^2$ increase of the squared particle displacements, the long-time dynamics is diffusive, i.e. the mean square displacements scale as $\sim t$. The crossover at $\dot{\gamma} t \approx 1$ defines an equilibration time $t_{\text{equil}}$ only after which measurements are carried out to determine the diffusivity tensor and the apparent viscosity.
4.5.2 Anisotropic Advection-Diffusion (MaS/LPAD)

When modeling the advection-diffusion of suspended particles to track changes of the local volume fraction $\phi(x_M)$ on the macro-scale we need a method that is capable of a wide range of Peclet numbers and space-varying anisotropic diffusivity tensors.

In general, there are two classes of methods to solve advection-diffusion problems, Eulerian and Lagrangian methods, respectively. In Eulerian approaches the problem is treated based on a mesoscopic description of the advected-diffused particles, the local concentration $c(x)$, at fixed points or volumes. PDE’s are then used to describe the evolution of $c(x)$ over time. Typically, $c(x)$ is defined on a lattice of nodes $x_i$ and finite difference methods for the iterative solution would make sense here. The Lattice-Boltzmann Method has been proven to be a suitable choice in many types of applications (see for example [177]).

However, Eulerian methods are prone to a number of problems such as the not guaranteed positiveness or the conservation of mass [178, 179] in case of large concentration gradients. Eulerian methods are also susceptible to numerical dispersion and artificial oscillations [180]. In particular, the limitation of Peclet number (see for example [181]) is the decisive factor not to use an Eulerian approach. In the present cases of a diffusivity that vanishes for very small shear rates, Eulerian methods would cause a considerable numerical diffusion, for example in a bulk flow with $\dot{\gamma} \approx 0$ and a velocity $|\mathbf{u}| \neq 0$ inclined to the lattice where we actually would expect a sharp concentration pattern not to dissolve.

Using a Lagrangian approach the dynamics of individual particles is solved. The dynamics of the particles is modeled based on stochastic differential equations which are consistent with the advection-diffusion equation. Random walk models allow to avoid a number of problems related to the Eulerian approach, and this makes them very attractive in a number of applications (see, for instance, [182, 183]).

A random walk simulation model enables the observation of phenomena on scales much smaller than the spacing of the underlying fluid grid, as well as the tracing of the movement of individual particles, thereby describing the natural processes more accurately, although we will see in this section that limits to this exist. Furthermore, information on integrated properties like residence/settling time or individual tracks can be easily obtained from the simulations. Local concentrations $c(x)$ can be directly calculated from the spatial positions of the particles and when and where required. This can be easily exploited when splitting of the temporal scale offers gain in computation speed.

The advection-diffusion equation for a concentration field $C$ reads

$$\partial_t C = -\nabla \cdot (uC - D \cdot \nabla C) \quad (4.75)$$

where the change in concentration is coupled to a velocity field $u$ and a diffusion process characterized by the diffusivity tensor $D$. Here, we only consider diagonal diffusivity tensors, e.g.

$$D = \begin{bmatrix} D_{xx} & 0 \\ 0 & D_{yy} \end{bmatrix} \quad (4.76)$$

in two dimensions. The diffusion dynamics is thus decoupled in these two dimensions. In sheared suspensions small off-diagonal elements might be found [184] due to effects of collective behavior in the presence of concentration gradients. However, we can neglect them in the present work as they are only found significant
for small $Pe$ and are dominated by Brownian contributions in $D$ which are not modeled.

Instead of solving (4.75) one can introduce a number of point particles whose local number density represents $C(x_i)$. To define the dynamics of such particle one can then reinterpret the PDE as a Fokker-Planck type of Langevin equation. We define a stochastic differential equation in the Ito sense

$$dr_p(t) = u(r_p(t))dt + \sqrt{2D}dW(t)$$

(4.77)

where $r_p(t)$ is the trajectory of a tracer particle that is subject to advection with the velocity field $u$ and a Wiener noise. We assume $W(t)$ to be Gaussian process with mutually independent values. It has a zero mean, $\langle W(t) \rangle = 0$ and a variance $E(W(t)) = \sqrt{t}I$. Note that in our case we expect $D$ to be a function of $r$ and $t$. We therefore cannot treat the terms on the right-hand side of (4.77) independently.

In order to compute a numerical approximation for (4.77) we apply the Euler scheme, i.e.

$$r(t + \Delta t) = u(r(t), t)\Delta t + \sqrt{2D}\Delta W(t).$$

(4.78)

There exist higher order approximations, e.g. those named after Milstein or Heun, the later employing a predictor-corrector step. Although offering higher accuracy, the application of such methods either involve knowledge about spatial derivatives of $D$ whose determination would be an additional source of numerical errors. Or it requires knowledge on the time evolution of $u$ for which an approximation also would lead to numerical difficulties.

The increments $\Delta W$ are computed by a random number generator that produces random numbers in the interval $[0, 1]$, which are then transformed to a Gaussian distribution using the Box-Müller algorithm [185]. We have chosen an implementation of the Mersenne Twister pseudo random number generator [186] for its speed, large periodicity and the good quality in terms of uncorrelatedness of numbers in higher dimensions.

**Mapping Macro Lattice Fields → LPAD: Interpolation**

When solving the dynamics of the Lagrangian tracer particles we make use of the advective field $u(x_M)$ and the field of diffusivity $D(x_M)$ which are both data-structures on the regular lattice of the macro scale models with a spacing $\Delta x_M$. The later fact is a consequence of running MiS and interpreting its results only at lattice sites $x_{M,i}$.

To obtain $u(x_p)$ a simple linear interpolation

$$u(r_p) = \sum_i a_i(d_i) \begin{cases} -u(x_1) & \text{if } x_i \text{ is boundary node} \\ u(x_i) & \text{else} \end{cases}$$

(4.79)

over the four nearest lattice nodes at $x_{M,i}$ is carried out. The weights $a_i$ are functions of the normalized distance vector $d_i = (r_p - x_i)/\Delta x_M$ defined as

$$a_1(d_i) = (1 - d_x)(1 - d_y)$$

(4.80)

$$a_2(d_i) = d_x(1 - d_y)$$

(4.81)

$$a_3(d_i) = d_x d_y$$

(4.82)

$$a_4(d_i) = (1 - d_x)d_y$$

(4.83)
which is illustrated in Fig. 4.22(b). This definition is always so that the particle is located in the volume around node $x_1$, the home cell. The neighbor nodes are identified from the quadrants.

This interpolation scheme is well defined in the bulk, however, at the boundaries, special care has to be taken as to the location of the real boundary where $u(x_b) = 0$. Using a Lattice-Boltzmann scheme to solve the evolution of the macroscopic flow field $u(x,t)$ with the LBGK collision operator and a no-slip bounce-back-at-the-links boundary condition we expect the hydrodynamic boundary to be located halfway between the fluid boundary node and the solid node the link points towards$^6$. To enforce the interpolated $u(r_p)$ at half the distance between fluid and solid boundary nodes, for nodes inside the solid boundary we set $u(x_b) = -u(x_1)$. When solving the particle dynamics, a reflective boundary condition is applied at half the distance between fluid and solid nodes. As the particles do not interact with each other, such a reflection boundary condition is straightforward to implement.

**Advection Test**  Testing the advection scheme, a Newtonian laminar flow through a channel confined by vertical walls was simulated and the resulting equilibrated velocity field $u(x_i)$ used to advect tracer particles which were initially ($t = 0$) randomly distributed over the volume/area of all the inlet nodes, e.g. all fluid nodes for which $x_i = 1$, with a number density of 100 particles per node. In Fig. 4.23 the particle positions after a time $t = 4 \cdot 10^4 \Delta t$ are shown. Note, that the resulting distribution of particles does not show any discretization effects. Also, the closer to the boundary the least the particles have moved, demonstrating the capability of Lagrangian particle methods to resolve even smaller scales than the spacing of the flow field lattice.

$^6$Strictly speaking, this is only true for boundaries that are aligned with the lattice. For any other inclined or curved boundary, the fluid behaves as if the boundary is slightly shifted towards the fluid by an amount that is a function of the viscosity and the angle of inclination.
Figure 4.23: Advection test 1: A distribution of tracer particles is initialized in such a way that the particles are randomly distributed over the area of all the lattice nodes at $x = 1$. Shown is the tracer particle distribution after 40000 iterations of the advection algorithm. Initially the fluid was at rest after which it was driven in positive $x$-direction using a volume force. Note that the smooth particle distribution. The gray scale corresponds to the fluid speed.

However, when repeating the test with an initially homogeneous distribution of tracer particles we see unwanted effects on the evolution of the particle distribution caused at boundaries which are not straight aligned with the lattice of the underlying LBM fluid solver. In Fig. 4.24 the positions of the particles after a time $t = 1 \cdot 10^5 \Delta t$ are shown. Downstream the corners of the confining vertical walls we see a very dense line of particles and a deserted area next to it. The width of the deserted area is clearly larger than the lattice spacing $\Delta x$ of the fluid so that this effect is also clearly visible in the integrated local density $\phi(x_i)$ which is determined on the same lattice as the fluid using a kernel of width $\Delta x$. Looking for a reason for this, we see that the particle distribution gets compressed on the upstream side of the corners. This is caused by the definition of the boundaries of the particle system to be aligned with the regular rectangular grid of the fluid model. This leads to the interpretation of volume represented by a lattice node as a rectangular shape. Solving the LBM system on a D2Q9 lattice, this is actually not true. Half of the diagonal fluid densities do actually flow “through” a corner created by a solid node. The particles, however, bounce back at the corner. They do this repeatedly with a net movement towards the tip of the corner. Downstream the corner this sweeping leaves particle-empty areas with fluid that flowed “through” a corner. When the flow expands after the constriction, the width of this area exceeds the lattice spacing.

To circumvent this, the boundary conditions of the LBM system can be modified such that also diagonal fluid densities, which actually would have a legal fluid destination node during propagation, are bouncing back. However, this is not enough. Also the interpolation scheme for $u(r_p)$ has to be modified to make a particle flow parallel to the boundary as it nears it. Using the standard interpolation scheme a particle that just entered the rectangular volume of a node adjacent to a solid node at a corner already feels the non-zero $x$-component of $u$ at the fluid node directly
Figure 4.24: Advection test 2: In this case, the particles were distributed homogeneously over the whole fluid domain. After the same number of iterations as in Fig. 4.23 the particle distribution in the bulk is still homogeneous, as expected for advection with non-compressible flow. However, we see strong deviations from the homogeneity downstream the corners as an effect of boundary conditions for Lagrangian particles. See text for discussion. The gray scale corresponds to the fluid speed.

at this corner. This can be cured by enforcing the interpolation only to be done between \( u(x_1) \) and \( u(x_2) = -u(x_1) \) in this case. However, we found that applying both of the modifications, or only one of them, it does not remove the sweeping effect sufficiently. Anyway, modifying the boundary treatment of the LBM system will lead to a relocation of the hydrodynamic boundary and might be source of instabilities. Given that the macro system in the multi-scale simulations presented in this work does only have straight boundaries aligned with the lattice, we leave the investigation of the boundary problem to future work.

Mapping LPAD → Macro Lattice Fields: Kernel Estimator

The tracer particles are used as an alternative representation of the local volume fraction \( \phi(x_i) \) which we need at the lattice nodes \( x_i \). To map the state of the Lagrangian particle system to a density function defined at the lattice nodes particle positions are integrated to a number density \( P(x_i) \), using a weight function \( K(r_p - x_i, \lambda) \) localized and symmetric around \( x_i \). In its general form it reads

\[
P(x_i) = \frac{1}{N_p \lambda^D} \sum_{p} K\left( r_p - x_i \frac{r_p - x_i}{\lambda} \right)
\]

with a bandwidth \( \lambda \). The so-called kernel function \( K(d) \) can be any function satisfying the condition of normalization, i.e. \( \int K(d)d\mathbf{u} = 1 \). In the literature \( K \) can be found modeled as a Gaussian or Epanechnikow function, amongst others [187]. However, to be consistent with the interpolation scheme (4.79) and (4.80) we use a triangular function

\[
K(d) = \begin{cases} 
(1 - |d_x|)(1 - |d_y|) & \text{if } d_x \leq 1 \land d_y \leq 1 \\
0 & \text{else}
\end{cases}
\]

(4.85)
with \( \mathbf{d} = (\mathbf{r}_p - \mathbf{x}_i)/\Delta x \), \( \Delta x \) equaling the bandwidth \( \lambda \) in (4.84). Because the kernel has a range limited to \( \Delta x_M \) in every dimension, sharp boundaries in \( \phi(\mathbf{x}_i) \) can be realized.

Depending on the average/global number density \( P_0 \) we set to represent the global volume fraction \( \phi_0 \) the local suspension volume fraction \( \phi(\mathbf{x}_M) \) is then calculated as

\[
\phi(\mathbf{x}_M) = \frac{\phi_0}{P_0} P(\mathbf{x}_M).
\] (4.86)

How many particles, i.e. what \( P_0 \), we need to represent \( \phi(\mathbf{x}_M) \) in sufficient accuracy we will estimate in the diffusion test at the end of this section.

**Flow aligned Diffusivity Tensor**

As described earlier, when mapping local quantities of macro scale fields to initial and boundary conditions of the micro scale model we make use of Galileian invariance in the sense that the reference frame of the micro-model is aligned with the flow, i.e. \( \mathbf{e}_{m,x} = \mathbf{u}(\mathbf{x}_i)/||\mathbf{u}(\mathbf{x}_i)|| \), and Galilei-transformed in such a way that the mean velocity in the micro model is zero and the velocity gradient has only an \( \mathbf{e}_{m,y} \)-component (assuming non-compressible flow). When translating \( \mathbf{D}_m \) to \( \mathbf{D}_M(\mathbf{x}_i) \), \( \mathbf{D}_m \) has to be rotated back to the reference frame of the macro scale models. Because diffusive processes are Galileian invariant the Galileian shift does not need to be reversed. In general, a transformation rule can be defined as

\[
\mathbf{D}_M(\mathbf{x}_i) = sD \cdot \mathcal{R}^{-1}(\theta) \mathbf{D}_m(\mathbf{x}_i) \quad \text{with} \quad \theta = \angle(\mathbf{u}, \mathbf{e}_{M,x}),
\] (4.87)

using the diffusivity-scale factor \( sD \). \( \mathcal{R} \) is the rotation matrix

\[
\mathcal{R}(\theta) = \begin{bmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{bmatrix}.
\] (4.88)

with the property \( \mathcal{R}^{-1}(\theta) = \mathcal{R}(-\theta) \). The transformation (4.87), involving matrix calculation with trigonometric functions as elements, is rather costly in computation. Instead, having all necessary information at hand at this stage of the computations, we can use the diagonal flow-aligned diffusivity tensor directly. The random walk is carried out in the flow aligned reference frame with the base vectors \( \mathbf{e}_{m,\|^\perp}(\mathbf{x}_i) \), and the Euler scheme (4.78) becomes

\[
r_{p,x}(t + \Delta t) = [u_x(\mathbf{r}_p(t),t) + w_{\|^\perp} \cdot e_{m,\|^\perp}(\mathbf{x}_i) + w_{\|^\perp} \cdot e_{m,\|^\perp}(\mathbf{x}_i)] \Delta t
\] (4.89)

\[
r_{p,y}(t + \Delta t) = [u_y(\mathbf{r}_p(t),t) + w_{\|^\perp} \cdot e_{m,\|^\perp}(\mathbf{x}_i) + w_{\|^\perp} \cdot e_{m,\|^\perp}(\mathbf{x}_i)] \Delta t
\] (4.90)

where

\[
w_{\|^\perp} = \sqrt{2D_{m,\|^\perp}} \Delta W_1
\] (4.91)

\[
w_{\|^\perp} = \sqrt{2D_{m,\|^\perp}} \Delta W_2.
\] (4.92)

The time step \( \Delta t \) does not necessarily correspond to the time step of MaF. The time scales can be split and a number of \( k \) sub-steps can be carried out in the interval

\[
\Delta t = \frac{1}{k} \cdot \Delta t_M.
\] (4.93)
Diffusion Test  The flow-aligned anisotropic diffusion we validate by an approximation of the solution of a well known diffusion problem, the decay of a Dirac-distributed initial concentration field with a time-independent diffusivity tensor \( D \).

The solution of the temporal evolution of the concentration field and the initial condition \( C(x, t) = \delta(x - 0) \) reads

\[
C(x, t) = \frac{1}{(4\pi t)^{3/2} \sqrt{\det D}} \exp \left( -\frac{xD^{-1}x}{4t} \right). \tag{4.94}
\]

Three otherwise similar runs of the LPAD system have been initialized with \( N_p = 10^3, 10^4, 10^5 \) particles at \( r_p(t = 0) = r_0 \), i.e. a delta distribution. The components of the flow-aligned diffusivity tensor were set to \( D_\parallel = 3 \cdot 10^{-3}, D_\perp = 5 \cdot 10^{-4} \) and it was assumed that the diffusion takes places on top of the advection in a constant homogeneous velocity field \( \mathbf{u}(x_i) = (0.05, 0.02) \forall x_i \). The LPAD model has then been run for \( 10^3 \) iterations. Plots of the resulting \( P(x_i, t) \) are shown in Fig. 4.25. As expected, the deviations from the analytical solution decrease with the number of tracer particles used. To estimate the total error we measured an error function

\[
\epsilon = \sum_{x_i} |\phi(x_i, t) - C(x_i, t)| \tag{4.95}
\]

and can confirm that the decrease of the total error behaves as \( \epsilon(N_p) \sim N_p^{-2/(D+4)} \) [187] with \( D = 2 \). Choosing a small time step \( \Delta t \), i.e. larger \( k \), to increase the accuracy of the Euler scheme does not make much sense if \( N_p \) is too small to allow for a good sampling of \( \phi(x_i) \). However, also a large \( N_p \) does not necessarily decrease the total error if the error is dominated by deviations caused by a too small \( \Delta t \). Further elaboration and practical suggestions concerning this discussion can be found in [188]. We found that for \( N_p = 10^5 \) the LPAD approximation gives a mean relative error of less than 0.015. Facing the relatively high computational costs of tracer particle systems we consider this a good approximation of the solution (4.94). Translating these findings into the application of (4.86) we estimated \( P_0 = 1000 \) and \( k = 1 \) (in (4.93)) to be a good choice to represent the advection-diffusion on the macro-scale.

4.6 A Database coupled in

4.6.1 Serial vs. concurrent coupling

Regarding the availability of data resulting from the micro-model, e.g. its solution for a sufficiently large range of parameters, as input to the macro-model one can distinguish between concurrent coupling methods [189] and serial coupling. The first case is the most common and is sometimes also referred to as “equation-free” approach [190]. In it, the communication between micro-scale and macro-scale models is “on-the-fly”, e.g. in a data-driven multi-scale model the micro-scale model is initialized, run and evaluated for specific boundary condition and parameters whenever the macro-scale model needs its input, that is, as the computation goes on. The second way of coupling is called serial coupling in which the solution of the micro-scale model is precalculated for an expected range of parameters. The coupling merely exists between the macro-scale model and a precalculated database.
Figure 4.25: Tracer particle positions (left) and number densities $P(x_M, t)$ (right) as obtained by (4.84) from the tracer particle positions $r_p$ after a time $t = 10^3$ starting from an initial distribution $r_p(t = 0) = (50, 80)$. The diffusion according to $D_\parallel = 3 \cdot 10^{-3}$, $D_\perp = 5 \cdot 10^{-4}$ took place on top of the advection with a homogeneous flow field with velocity $u = (0.05, 0.02)$ to which the diffusivity tensor was aligned to. As expected, $P(x_M, t = 10^3)$ has an inclined anisotropic Gaussian shape centered at $x = (100, 100)$. With increasing global number density $P_0$ the numerical approximations converge to the analytical solution (4.94).
and can be described as parameter passing. This is advantageous if sufficient data is already available at the beginning of the macro-scale simulation. Examples for serial coupling are the usage of data from MD simulations to define transition probabilities in Monte Carlo schemes, atomistic interaction potentials derived from quantum mechanics calculations and used in MD models, or the pre-estimation of transport coefficients later used in advection-diffusion problems. In principle, also series of data derived in experiments from a lab model which is then used in a computational model leads to the same classification. As long as the constitutive equation needed depends on only a few variables and the variable space that will be visited by the macro-model is more or less known so that precalculation can be limited to this region in variable space, serial coupling is reasonable.

At runtime of the macro-scale model the two strategies might differ only in execution time of the macro-model run. Whether the data given to the macro-scale model comes from the micro-model directly or a database in between - it is supposed to be the same.

4.6.2 A Hybrid: Database filled on-the-fly

During the course of an HMM simulation \( \left( \frac{X_M}{\Delta x_M} \right)^D \left( \frac{T_M}{\Delta t_M} \right) \) local iterations/collisions have to be carried out on the macro level and thus the same number of micro-pockets would have to be called to provide \( \nu_{\text{app}} \) and \( D_{xy} \) as collision parameters at every point \( (x_M, t_M) \). It is obvious that we, following this scheme, would repeatedly launch micro-pockets for the same set of parameters \( (\phi, \dot{\gamma}) \), or for a set of parameters that does not differ too much from a parameter set already sampled. It is clear that if we write micro-pocket results to a database and apply extra/interpolation schemes to extract \( \nu \) and \( D_{xy} \) in state-space regions we already sampled in sufficient density, we could reduce the number of micro-pockets which have to be launched by several orders of magnitude.

In doing so we combine the advantages of serial and concurrent coupling. If the needed data does already exist in the database, or can be extracted from it by extra/interpolation, we make use of precalculated data. If no data is available, a micro-pocket is run and, when terminated, a copy of the results is archived in the database. This way only as many micro-pockets are run as are needed to solve the macro-model. And we have the possibility to use solutions that already exist for a range of parameters prior to the execution of the macro-model. This data might come from precalculations with the same micro-model carried out for another study, another micro-model (e.g. for parameter ranges the first micro-model is not valid or instable for), or from experiments.

Extra- and Interpolation

Of course, the database approach makes only sense when a majority of requests can be answered through a fast interpolation between existing data points. Additionally we need an according extrapolation scheme that allows advances into unknown parameter space regions with the same step size we assume for a tolerable distance between data points as a good compromise between accuracy and speed of the simulation. Because obtaining data points is expensive we want to keep the density of data points low. On the other hand, even the best extra- and
interpolation scheme misses important characteristics if data density is too low. A certain knowledge about the smoothness of the behavior $\nu_{\text{app}}$ and $D_{xy}$ as functions of $\dot{\gamma}$ and $\phi$ is therefore necessary to set the tolerance range in $\phi$ and $\dot{\gamma}$ dimension, respectively.

We have chosen hard spheres as suspension particles because, albeit numerous open questions, its general behavior is relatively well known (see section 4.1). From the plots of $\nu_{\text{app}}(\phi)$ in fig. 4.13 we see that sampling the smooth and monotonously increasing curve can be done with a step size of $\tau_\phi = 0.25$ to capture its behavior in sufficient accuracy (what “sufficient” means remains open, see discussion on sensibility of the coupled system in section 4.8). We do not expect characteristics of the curve that are on a smaller $\phi$-scale. From the plots of $\nu_{\text{app}}(\Re(\dot{\gamma}))$ in fig. 4.14 we also see smooth and monotonously increasing $\nu_{\text{app}}$ behavior, this time on a logarithmic scale. The curve can be well represented by data points with a distance of $\dot{\gamma}_2 - \dot{\gamma}_1 = 0.25\dot{\gamma}_1$ where a factor is used to achieve equidistant points on the logarithmic scale.

One reason for not choosing an approach in which a multi-dimensional function of some form and number of degrees of freedom is fitted to the data points is, that although we know the general behavior in this particular application (hard-sphere suspension), the aim of the simulation framework is to be as general as possible. It should be possible to easily replace the micro-system MiS by another micro-model for which we do not know which behavior to expect. This will however require some adaptive accuracy control. With the functional form of the fitting function we would imply such knowledge to keep the number of free parameters small in favor of the feasibility of the regression problem. Particularly when extrapolating, a fitted curve is subject to great uncertainty since it may reflect the method used to construct the curve as much as it reflects the data. A second reason is, addressing the feasibility of the regression, that with increasing dimensionality of the problem the stability and the accuracy of the parameter-search algorithm becomes a critical question. In particular, if we increase the number of parameters to increase the flexibility of the fitting function. Also, the initial value problem would require knowledge of the behavior which should be the more complete and accurate the more free parameters we allow the function to have. For more details and description of problems in fitting functions to datasets the reader is kindly referred to appropriate literature, for example [191].

Another disadvantage of the described approaches to inter/extra-polation in more than 1 dimension is an unwanted correlation between the behavior in these dimensions. This is also true for piecewise polynomial inter/extra-polation (splines). In other words, through the indiscriminated spread of $\partial^{(0,1)}Q_j/\partial Q_i^{(0,1)}$ also in $Q_{k\neq i}$ dimension, particularly where there is only one data point neighbor in the $Q_i$ dimension, this might lead to strong over- or underestimation.

To minimize the effects addressed so far, we implemented the following approach. Let $Q_{1..q_{\text{max}}}$ be the set of $q_{\text{max}}$ given points in the $D_p + D_d$ dimensional data space, where the subspace of dimension $D_p$ is spanned by the parameters $Q_{i,p}$, i.e.

\begin{align}
Q_{1,q}^p &= \phi_q, \\
Q_{2,q}^p &= \dot{\gamma}_q
\end{align}

in the present use case with $D_p = 2$. The data subspace of dimension $D_d$ is spanned
by the data $Q_{j,q}^d$ attached to the parameter vector $Q_p$, i.e.

$$Q_{1,q}^d = \nu_{\text{app}}(\phi_q, \dot{\gamma}_q), \quad (4.98)$$

$$Q_{2,q}^d = D_{xx}(\phi_q, \dot{\gamma}_q), \quad \text{and} \quad (4.99)$$

$$Q_{3,q}^d = D_{yy}(\phi_q, \dot{\gamma}_q). \quad (4.100)$$

Figure 4.26: To obtain an estimate for $R^d$ for the given parameters $R_p$ as a point lying in the confidence range around at least one existing data point $Q_1$, in a weighted average ((4.103)) slopes $P_{ji,pq}$ are computed from the vectors $a_{qp}$ between existing database entries $Q_p$ and used to calculate $R_p$ as a point on $A$. If more than two points $Q_p$ can be found in an extended confidence range around $Q_q$, an average over all computable slopes $P_{ji,pq}$ is used.

As described above, we trust an inter/extra-polation to retrieve $R^d(R_p)$ as long as there is at least one parameter point $Q_p$ which is within confidence range, i.e.

$$\left( \sum_{i=1}^{D_p} \frac{(Q_{i,q}^p - R_{i}^p)^2}{\tau_i^2} \right)^{\frac{1}{2}} \leq 1. \quad (4.101)$$

Together with $Q_q^d$ also the slopes $P_{ji} = \partial Q_{j,q}^d / \partial Q_{i,q}^p$ are stored. This allows to compute $R^d(R_p)$ as a point on the plane $A$ from

$$R_{j,q}^d = Q_{j,q}^d + \sum_{i=1}^{D_p} P_{ji,q}(R_i^p - Q_{i,q}^p). \quad (4.102)$$

In case the condition (4.101) is met with other data points $q$, too, a simple linear interpolation is done according to

$$R^d = \frac{\sum_q (1 - \frac{1}{\tau_i}(Q_i^p - R_i^p))R_{q}^d}{\sum_q (1 - \frac{1}{\tau_i}(Q_i^p - R_i^p))} \quad (4.103)$$

with weights $(1 - ..)$ which are 0 at the boundary of the confidence area.

The slopes $P_{ji,q}$ at $Q_p^p$ can be computed if there are at least two more points $Q_{p}^p$ and $Q_{p}^p$ in a, by a factor $C$ extended, confidence range. If not then $P_{ji,q} = 0 \forall ji$. The extension by a factor of approximately $C = 1.5$ is necessary to allow the determination of $P_{ji,q}$ at points that are just outside the confidence range given by
τi in (4.101), a situation characteristic of data point distributions that are enriched on-the-fly. The slopes \( P_{ji,q} \) are determined from \( D^p \) vectors \( P_i = 1 \ldots D^p \) in the plane defined by two linear independent vectors \( a_{qp} = Q_p - Q_q \) and \( a_{qr} \), pointing from one data point to another, and the point of origin, \( Q_q \). The vectors \( P_i \) are another basis of the subspace spanned by \( a_{qp} \) and \( a_{qr} \), and the origin \( Q_q \), with the condition that \( P_{k,i} = 0 \quad \forall \ k \neq i, \ 1 \leq k \leq D^p \). Then the slope is simply \( P_{ji} = P_j / P_i \).

When searching for points \( Q^p_p \) and \( Q^p_q \), an additional condition,

\[
\frac{a_{qp} \cdot a_{qr}}{|a_{qp}| |a_{qr}|} < 0.7, \tag{4.104}
\]

is applied to make sure that \( a_{qp} \) and \( a_{qr} \) are “sufficiently” linear independent so that variations (statistical errors) in \( Q^d_j \) do not lead to great variations in \( P_{ji} \).

\[
\left( \sum_{i=1}^{D^p} \frac{(Q^p_{i,p} - Q^p_{i,q})^2}{\tau^2_i} \right)^{1/2} \leq C. \tag{4.105}
\]

Furthermore, by including another weight factor \( w_{ipq} = \frac{1}{\tau_i} (Q^p_{i,p} - Q^p_{i,q}) \) the isotropy in respect to the direction to which respect the gradient is computed is broken with the intent to minimize the correlation of \( P_{ji} \) in other directions than \( Q^p_i \).

The calculations described are rather intense and would have to be repeated every time the database is asked for some value of \( \nu_{app} \) and \( D_{xy} \). However, quite a part of the calculation is the same for a large range of \( \phi \) and \( \dot{\gamma} \) so we decided to precalculate and hold in memory lattice fields \( \nu_{app}(\phi_i, \dot{\gamma}_j) \) and \( D_{xy}(\phi_i, \dot{\gamma}_j) \) every time a data point is added to the database. A lattice spacing \( \phi_{i+1} - \phi_i \approx 0.2 \tau_\phi \) is found to be fine enough. Using a data structure based on a lattice allows for quick access of the data with the help of simple linear interpolation schemes.

In Fig. 4.27 subsets of the databases as created while running test simulations similar to those described in Sec. 4.8 are shown together with the according lattice fields for \( \nu_{app} \) and \( D_{yy} \).

**Classification of the Role of the Database**

The coupling of a database between the macro-scale models and the micro-model can be classified in different ways, depending on the role one gives the database and which component of the multi-scale system is supposed to be so smart to decide whether a micro-scale simulation has to be carried out or not.

- **One way** would be in the sense of the HMM coupling. As a part of the macro-model it could serve as the replacement for the constitutive equations needed in the collision step. Only if the macro-model is incomplete, i.e. its constitutive equations are not valid in a range of parameters, e.g. at a localized singularity, the micro-model needs to be launched to provide this information.

- **The second way** to classify the system macro-model-database-micromodel could be to understand and implement the database as a smart conduit, following the CxA idea and the functionality the MUSCLE framework provides. The macro-model does call the micro-model via the database conduit which has a memory and the functionality to process stored data into the information demanded by the macro-model.
Figure 4.27: Example database for two test runs of the multi-scale system for 
$\phi_0 = 0.3$ (crosses) and $\phi_0 = 0.5$ (stars) showing the entries of $\nu_{app}$ (top) and 
$D_\perp$ (bottom) together with the field of extra/inter-polated values points (dots) 
representing the confidence regions around data points obtained from runs of the 
micro-model.

- Another way would be to consider the database itself as the micro-model 
as it actually provides the information needed by the macro-scale model. A 
fully resolved simulation of a sheared suspension would then be considered as 
another functionality of the database agent that is employed if extra/inter-
polation can not be applied.

Parallelization?

Although spatial dependency in the macro model doesn’t allow for asynchronous 
updates of the macro fluid nodes, it might be worth to think about parallelization of 
the collision step within one iteration at $t_M$. From computational point of view the 
HMM approach leads to a coupling where the macro model functions as a master 
calling an arbitrary number of slaves, being the micro “pockets”. The later are 
independent from each other. No information has to be exchanged between pockets 
at their runtime. In this situation a farming approach as parallelization strategy 
could be applied. In that, micro pockets delivering $\nu_{app}(x_M, t_M)$ and $D_{xy}(x_M, t_M)$ 
for each macro lattice site $x_M$ and time $t_M$ could be launched in parallel running on
different processors. However, using the database coupled in between macro and micro models reduces the actual number of calls of the micro model so significantly that hardly any two sets of $\nu_{\text{app}}(\phi_{1,2}, \dot{\gamma}_{1,2})$ and $D_{xy}(\phi_{1,2}, \dot{\gamma}_{1,2})$ have to be called at the same $t_M$. Except for the first iterations, where the barn is almost empty and the biggest changes in the state of the macro model take place, only very seldom a new data point has to be added. In systems with very complicated geometries, and therefore very different local flow conditions, the number of database requests might be increased during the first time steps of the integration. However, due to the intrinsic exploitation of rotational and Galileian symmetry, the actually visited parameter space will not be much larger, and we do not expect big changes from the situation of low request density, even for problems in 3 dimensions.

![Figure 4.28: The time line of calls of the micro-model (points) and a density plot binning those events in time bins of width 1000$\Delta t_M$ illustrating the rareness in which the micro-model has to be called when a database is used to prevent redundant simulation runs.](image)

In Fig. 4.28 the number of micro pockets called are plotted over macro time steps from one of the HMM suspension runs together with a density curve measured as calls per 1000 iterations. We see that in the beginning of the simulation much more pockets have to be called in comparison to later stages of the equilibration process. Nonetheless, it happens only once that two pockets are called at the same time. A farming approach would not make sense here and was not implemented. The only parallelization strategies appropriate would be domain decomposition of the micro models which is, in principle, realizable in a straightforward manner due to Lees-Edwards boundary conditions (see Sec. 4.4.2 for discussion on that), or by extrapolation of the systems way through the parameter space and opportunistically calling a number of micro-models to fill the database in advance.

### 4.7 Other Suspension Flow Models

In this section two macroscopic suspension flow models will be briefly introduced. They will be used to discuss properties and resulting profiles together with those obtained with the multi-scale model described in this work.
4.7.1 Suspension balance model

Following [192], for the suspension as a whole and for the particle phase conservation of mass and momentum can be used to set up a balance model. Averaging these quantities over the whole domain and all phases we can write

$$\nabla \cdot \langle u \rangle = 0$$  \hspace{1cm} (4.106)

$$D_t \langle \rho u \rangle = \langle b \rangle + \nabla \cdot \langle \Sigma \rangle$$  \hspace{1cm} (4.107)

where $D_t = \delta_t + \langle u \rangle \cdot \nabla$ is the convective derivative and $\langle b \rangle$ the average over body forces acting on fluid and solid phase. Both, fluid and solid phase contribute to the stress in the suspension,

$$\langle \Sigma \rangle = -\langle p \rangle_l I + 2\eta_l \langle e \rangle + \langle \Sigma \rangle_p$$  \hspace{1cm} (4.108)

where $\langle p \rangle_l$ is the averaged pressure in the fluid, $\eta_l$ the suspending fluid viscosity, and $\langle e \rangle$ the rate of strain tensor (for the bulk). The scalar shear rate in terms of this tensor is given by $\dot{\gamma} = (\langle e \rangle \cdot \langle e \rangle)^{1/2}$.

The conservation of mass for the solid phase governs the evolution of the particle concentration $\phi$, i.e.

$$\delta_t \phi + \nabla \cdot \phi \langle u \rangle_p = 0$$  \hspace{1cm} (4.109)

where $\langle u \rangle_p$ is the average solid phase velocity. The particle flux, relative to the average suspension velocity, is given by

$$N = \phi (\langle u \rangle_p - \langle u \rangle)$$  \hspace{1cm} (4.110)

and combining it with the mass conservation,

$$\delta_t \phi + \nabla \cdot (\phi \langle u \rangle - N) = 0,$$  \hspace{1cm} (4.111)

gives

$$\delta_t \phi + \langle u \rangle \cdot \nabla \phi = \nabla \cdot N.$$  \hspace{1cm} (4.112)

With that we have an equation for the evolution of the particle concentration on the macro scale which assumes knowledge about the fluxes $N$. Thinking about where to split the scales, treating particle concentrations with help of (4.112) and measuring particle fluxes at the micro level could be one option. However, there would be the demand to explicitly model the gradient in the particle concentration on the micro level to account for the fluxes induced by it. This is not straightforwardly implementable in MiS without full knowledge of the spatio-temporal evolution of particle distributions in the surrounding areas of the pockets. We therefore need to model the concentration gradient-induced particle fluxes on the macro scale. The local diffusivity tensor is then obtained in a round-about way via the shear-induced self-diffusivity.

Following the suspension balance model into more detail we can relate the flux to gradients in the solid phase stress.

The difference between suspension velocity and solid velocity is related to the drag force on the particles. The local single particle Reynolds number in suspensions is generally low (order of $10^{-4}$) and we can assume the drag force to scale linearly with the relative velocity to the fluid,

$$\langle u \rangle - \langle u \rangle_p = M(\eta_l, a, \phi) \langle F \rangle_p.$$  \hspace{1cm} (4.113)
\( M \) is the inverse drag coefficient and accounts for the hindered mobility of an average particle due to the other particles in the suspension and is an unknown function of the fluid viscosity \( \eta_f \), the particle radius \( a \), and the particle density \( \phi \). We also assume isotropy of \( M \) here. Considering the momentum balance for the solid phase

\[
\rho_p \phi D_t^p \langle \mathbf{u} \rangle_p = \langle \mathbf{b} \rangle_p + \langle \mathbf{F} \rangle_p + \nabla \cdot \langle \Sigma \rangle_p
\]

(4.114)

where the convective derivative \( D_t^p \) is now following the average particle motion. \( \langle \Sigma \rangle_p \) is the stress in the solid phase, and \( \langle \mathbf{b} \rangle_p \) the solid body force which is \( \langle \mathbf{b} \rangle_p \) for neutrally buoyant particles. If the motion on the macro scale is also at low Reynolds number the inertial term in (4.114) can be neglected and the drag force can be written as

\[
\langle \mathbf{F} \rangle_p = -\nabla \cdot \langle \Sigma \rangle_p.
\]

(4.115)

This means, the particle flux is driven by stress gradients which is the point where micro models have to be found for.

Following the approach of Nott and Brady [192] the averaged solid-phase stress consists of the particle pressure, a deviatoric shear stress, and normal-stress differences. Later, Brady and Morris [119] could show that due to Brownian motion, short-range non-hydrodynamic particle interaction, or surface roughness, normal stresses scale linearly with the shear rate. Differences in normal stresses have the same microstructural origin as the solid-phase pressure, and therefore have the same scaling with the shear rate and volume fraction. Following [193] we can thus combine these two types of stresses into one quantity \( \Pi Z \) where \( \Pi \) is the isotropic solid-phase pressure and \( Z = I - (\eta_f/\Pi) \langle \chi \rangle \) incorporates the normal stresses. For the constitutive equation for the particle stress at small particle Reynolds number one can write

\[
\langle \Sigma \rangle_p = -\Pi Z + 2\eta_f \eta_s(\phi) \langle \chi \rangle.
\]

(4.116)

The solid-phase pressure \( \Pi \) as a function of the volume fraction and shear rate is given by

\[
\Pi = \eta_f \gamma p(\phi)
\]

(4.117)

where \( p(\phi) \) is a monotonically increasing function of \( \phi \) which can be given by

\[
p(\phi) \sim \phi^2 \left( 1 - \frac{\phi}{\phi_{\text{max}}} \right)^{-2}
\]

(4.118)

following the derivations from a microstructural model that puts the total stress in relation to the microstructure [119]. The solid phase viscosity can be modeled via the Krieger-Dougherty relation for the relative viscosity \( \eta_r \) of the suspension. In general, \( \eta_r = 1 \) for \( \phi = 0 \) and we write

\[
\eta_r = 1 + \eta_s
\]

(4.119)

Using the semi-empirical Krieger-Dougherty relation \( \eta_r \) can be modeled as (4.1).

### 4.7.2 Diffusive-Flux Model

Assuming neutral buoyancy and the absence of Brownian motion, Leighton and Acrivos [171] proposed to model the particle flux due to diffusive motion as

\[
\mathbf{N} = \mathbf{N}_\eta + \mathbf{N}_c
\]

(4.120)
with $N_\eta$ the flux due to spatial variations in viscosity and $N_c$ the contribution to the flux induced by hydrodynamical particle interaction, i.e. shear-induced diffusion. Phillips et al. [194] proposed these flux terms to be

$$
N_\eta = -K_\eta a^2 \phi (\dot{\gamma} \phi) \nabla \ln \eta 
$$

(4.121)

$$
N_c = -K_c a^2 \phi \nabla (\dot{\gamma} \phi) 
$$

(4.122)

which are based on the scaling arguments derived by Leighton and Acrivos [171]. In (4.121) $a$ is the diameter of the particles and $\eta(\phi)$ the apparent viscosity as a function of $\phi$ only. The coefficients $K_\eta$ and $K_c$ have to be determined empirically. In [193] $K_\eta = 0.62$ and $K_c = 0.42$ were used in a comparison of resulting particle concentration profiles $\phi(y)$ with those resulting from the suspension balance model and experimental works in different settings resembling viscometer geometries. Keeping the ratio $K_\eta/K_c$ constant, and varying the coefficients the time scale of the dynamics of $\phi(y,t)$ can be changed. This is one of the consequences of the conservation equation

$$
\partial_t \phi = -\nabla (N_\eta + N_c). 
$$

(4.123)

The model describes the particle concentration field $\phi(x,t)$ as resulting from the particles moving from regions of high interaction frequency to regions of lower interaction frequency [172]. This is analogous to a statistical gas model and in that similar to the modeling of the particle flux in this work (see Sec. 4.5.2). The main difference is the flux $N_\eta$ due to a gradient in the viscosity. This is motivated by the fact that the strength of hydrodynamic interactions increases with the viscosity $\eta$ analogous to an increased effective cross section in the collision dynamics of two approaching particles. In this, the diffusive-flux model is based on an assumption we do not make in our multi-scale model where a fully resolved micro-model is used. In a micro-model with traceable particles this effect will be included in the measured shear-induced diffusivity $D$.

The diffusive-flux model was successful in predicting particle concentration profiles in several benchmark problems [195]. However, its profiles do not satisfactorily agree with those seen for cone-and-plate and parallel plate geometries. In [193] a possible explanation for this is given pointing out that the interaction-induced flux $N_c$ is isotropic. The fact that the component of the shear-induced diffusivity tensor in direction of the shear gradient is only approximately half the other components might indeed have an impact on the dynamics of $\phi(x,t)$ in curved geometries. In our micro-model the components of the flow aligned diffusivity tensor are measured independently, not simplifying diffusion to an isotropic process. In [193] Fang et al. introduce a flow-aligned diffusivity tensor into the diffusion-flux model. However, also with this modification the diffusive-flux model does not predict particle concentration profiles as good as the suspension balance model.

### 4.8 Simulations and Results

To test the concept of the HMM model for suspensions we applied it to the simulation of the pressure driven flow of a 2-dimensional hard-sphere suspension through a straight channel. As we apply periodic boundaries in $x$-direction, instead of a pressure difference at the in- and outlet we mapped $\Delta p$ to a volume force according to $G_x = \Delta p / L_x$ which is used in (4.19) and (4.27). We carried out simulations with
volume forces of different magnitude $|G| = G_x = 1 \cdot 10^{-14}, 1 \cdot 10^{-13}, 1 \cdot 10^{-12}, 1 \cdot 10^{-11}$ to drive the flow parallel to the channel axis. Furthermore, we repeated this series of simulations for global volume fractions of $\phi_0 = 0.3$ and $\phi_0 = 0.5$.

The macro-models are initialized with the fluid at rest, i.e. $u(x_M, t_M = 0) = 0$ for all $x_M$, and a random but homogeneous distribution of tracer particles of the MaS model. More specifically, a number of 1000 tracer particles are randomly distributed over the volume of each node around $x_M$, for both cases of global volume fraction $\phi_0$. This results in a homogeneous volume fraction field $\phi(x_M, t_M = 0)$ with small variations of less than 2% (see Sec. 4.5.2 for a discussion on that).

We measured not only the volume fraction and velocity profile that are typically accessible by experiment and the primary result of models for the macroscopic flow of suspensions. We also measured shear rate profiles $\dot{\gamma}(y)$, the diffusivity component $D_\perp$ perpendicular to the flow direction, and kept track of the viscosity profile $\nu_{\text{app}}(y)$ to be able to gain insight into the coupling of those quantities and their dynamics.

As discussed in Sec. 4.6.2 the database approach allows to re-use any knowledge on the micro-model prior to the multi-scale simulation by putting it into the database in appropriate format. We defined a minimum shear rate $\dot{\gamma}_{\text{min}} = 5 \cdot 10^{-14}$ which is small enough to assume that viscosity and diffusivity will assume values close enough to their values for $\dot{\gamma} = 0$ and inserted data points sampling the semi-empirical Krieger-Dougherty relation for the increase of $\nu_{\text{app}}$ with $\phi$ (see (4.1)) and components of the diffusivity tensor $D_\parallel = D_\perp = 0$ which equals the zero-shear limits for shear-induced diffusivity. The lower shear-rate limit was not hit again after the equilibration phase.

### 4.8.1 Profile Development Dynamics

Starting from a homogeneous volume fraction $\phi(x, t = 0)$ over the channel and zero velocity, the system of coupled flow and diffusion needs an equilibration time $t_{\text{equil}}$ to fully develop the profiles. Only for $t \geq t_{\text{equil}}$ averages over the fluctuating profiles can be taken. Actually, the total equilibration dynamics consists of the dynamics of flow and diffusion, and we can distinguish between a $t_{\text{equil,flow}}$ and $t_{\text{equil,diff}}$. Over all ranges of the shear rate and all volume forces applied we find for the ratio of the characteristic time scales

$$\frac{\nu_{\text{app}}}{D} \gg 1 \quad (4.124)$$

and therefore $t_{\text{equil,diff}} \gg t_{\text{equil,flow}}$. The velocity profile develops from a flat zero profile within a few thousand $\Delta t_M$. The diffusive dynamics of the volume fraction, however, is much slower, a behavior also found in experiments [196]. To illustrate this behavior and the effects associated with it in Fig. 4.29 the shear rate and volume fraction profiles for two distinguished times in the development of one system is shown which had a global volume fraction of $\phi = 0.3$ and was driven with a volume force $G_x = 1 \cdot 10^{-11}$. At this highest volume force the shear rate close to the walls reaches values corresponding to shear Reynolds numbers $\text{Re}_p > 1$ where the micro-model shows the onset of shear-thickening. At $t_1 = 7000\Delta t_M \approx t_{\text{equil,flow}}$ the volume fraction profile does not yet differ much from the homogeneous initial distribution. The velocity profile, however, has fully developed by then and shows the characteristics of a shear-thickening fluid, i.e. a higher curvature around the
center than in the rest of the channel a fact also reflected in the slightly steeper $\dot{\gamma}$-profile in this region. Over the time to $t_{\text{equil,diff}}$ the volume fraction profile develops the typical maximum at the center of the channel, seen in profiles for $t_2 > t_{\text{equil,diff}}$. In this course the shear rate profile changes from a form typical for shear-thickening fluids to that of a shear-thinning fluid due to the stronger increase of the viscosity with $\phi$ as with the shear rate $\dot{\gamma}$.

This difference in the time scales of diffusion and momentum transport also influences the way the system moves through the parameter space during equilibration. In Fig. 4.31 the sampled regions in the parameter space are shown as recorded in the databases for the different simulation runs.

Nott and Brady have shown [192] that an estimation for the total length $L_{\text{equil}}$ the suspension needs to travel before equilibration is established can be given by

$$\frac{L_{\text{equil}}}{H} \sim \frac{1}{12 \hat{D}(\phi)} \frac{H^2}{R}$$  \hspace{1cm} (4.125)

where $H$ is the width of the channel $H = L_M$, and $\hat{D}(\phi)$ is the scaling of the self-diffusivity with $\phi$ (see (4.68)). Whether the maximum velocity or a mean velocity based on the total flux has to be taken as a reference $v_{\text{ref}}$ for a calculation of $L_{\text{equil}} = t_{\text{equil}} v_{\text{ref}}$ is not clear but might make a difference since the velocity profiles change for the different settings of volume force and global volume fraction. In Fig. 4.30 the equilibration times $t_{\text{equil}}$ are plotted for the different simulation settings that were obtained in test runs prior to the actual runs that were used for the measurement and averaging of profiles and that therefore were much longer. In the plot we see that indeed the equilibrium time behaves as

$$t_{\text{equil}} \sim \frac{1}{v_{\text{ref}}(G_x) \hat{D}}$$  \hspace{1cm} (4.126)

Using the assumption $v_{\text{ref}} \sim G_x$ here, we find that the mean velocity $v_{\text{ref}}$ does approximately linearly increase with the applied volume force despite the presence
of shear-thickening for the highest-shear regions in the runs at maximum volume force.

We have made use of this relation of $t_{\text{equil}}$ to $G_x$ and $\phi_0$ and scaled the diffusivity in such a manner that $t_{\text{equil}} \approx 10000$. With that we could accelerate the diffusive dynamics and reduce the runtime of the macro-model by a factor of almost four orders of magnitude in case of $\phi_0 = 0.3$ and $G_x = 1 \cdot 10^{-14}$ without violating the temporal scale separation of flow and diffusive dynamics during equilibration. This can also be seen in the chronology of the entries in the database. In the beginning points with increasing $\dot{\gamma}$ are added without deviations from $\phi = \phi_0$. Only after that the maximum shear rate for $\phi = \phi_0$ is reached the diffusive dynamics leads to a widening of the distribution of entries in the $\phi$-dimension.

### 4.8.2 Equilibrium Profiles: Results and Discussion

In Fig. 4.32 and Fig. 4.33 the equilibrium profiles are shown for $\phi_0 = 0.3$ and $\phi_0 = 0.5$, respectively. They all were obtained by averaging them over at least $N = 300$ independent samples at times separated by an autocorrelation time $t_{\text{corr}} \approx 5000$ estimated from the exponential decay of the correlation function $C(\delta t)$ for measurements of the suspension velocity $v_x(x_M)$ at times $t_1$ and $t_2 = t_1 + \delta t$ (averaged over all $x_M$ and $t_1$). The error bars on the data points show the average fluctuation of the considered quantity over the measurement time instead of the statistical error which would be a factor $\sqrt{N}$ smaller. Fluctuations in the profiles have their origin in the random nature of the Lagrangian model for the macroscopic advection-diffusion of $\phi(x_M)$. In that it might be similar to the measurements on real suspensions that have a finite particle number and are also averaged over a finite time. However, because the non-interacting tracer particles in MaS have a different dynamics these two types of fluctuations cannot be directly related here.

In favor of a better understanding of how the features of the profiles develop in a suspension that is driven through a straight channel, how one quantity influences the other, and the feedback loops that exist in the coupled system Fig. 4.34 shows
Figure 4.31: Shown are the entries to the database in the parameter space spanned by $\phi$ and $\dot{\gamma}$ together with the confidence range around the entries. Every point corresponds to a run of the micro-model. Starting from the top left plot the successive enrichment of the database is shown with each simulation run under different conditions of global volume fraction $\phi_0$ and volume force. All runs started from a zero velocity, i.e. zero shear profile $\dot{\gamma}(y)$, and flat $\phi(y)$ profile. Before the first run (4.1) was used to prepare the viscosity entries for a minimal $\dot{\gamma}_{\text{min}} = 5 \cdot 10^{-14}$. The diffusivity for those entries were set to $D_\parallel = D_\perp = 0$. 

Figure 4.32: Equilibrium profiles of local volume fraction $\phi$, diffusivity component $D_\perp$ in shear gradient direction, velocity $v_x$ (normalized to a total flux of 1), shear rate $\dot{\gamma}$, and viscosity $\nu$ for $\phi_0 = 0.3$. All in macro-scale lattice units.
Figure 4.33: Equilibrium profiles of local volume fraction $\phi$, diffusivity component $D_\perp$ in shear gradient direction, velocity $v_x$ (normalized to a total flux of 1), shear rate $\dot{\gamma}$, and viscosity $\nu$ for $\phi_0 = 0.5$. All in macro-scale lattice units. A straightforward explanation for the secondary peaks for the highest $G_x$, also seen for $\phi_0 = 0.3$ in Fig. 4.32, we cannot offer at this stage of the research. However, we also find similar effects in the experimental results by Lyon and Leel [123], for comparison shown in Fig. 4.35.
Figure 4.34: Illustration of the coupling of the local quantities.

With $a \rightarrow b$ we denote the positive coupling between $a$ and $b$. More precisely, $b$ is a monotonously increasing function of $a$. With $a \rightarrow b$ we denote the fact that $b$ will decrease when $a$ increases. A number of feedback loops can be identified. With $\Gamma$ we denote the flux of particles away from the considered volume element as a result of the local $D$. The coupling between the considered quantities in an abstract manner.

The general shape of the volume fraction and velocity profiles resulting from our simulations agree quantitatively well with those predicted by the diffusive flux model, the suspension balance model and the experimental results by Lyon and Leal which are reproduced for comparison in Fig. 4.35 and Fig. 4.36. In all cases of global volume fraction $\phi_0$ and applied volume forces $G_x$ the suspended particles tend to move to the center region of the channel. This can be explained by the positive coupling $\dot{\gamma} \rightarrow D$ whereby particles from high-shear regions near the wall diffuse much stronger than those in the lower-shear regions at the center which leads to an effective flux towards the center. This tendency is enhanced through the viscosity $\nu_{app}(y)$ which increases with $\phi(y)$ and lowers the shear rate $\dot{\gamma}(y)$. This positive feedback loop can be found as coupling $D \rightarrow \Gamma \rightarrow \phi \rightarrow \nu \rightarrow \dot{\gamma}$ in Fig. 4.34. The effective flux between positions $y_1$ and $y_2$ will vanish if $D(y_1)\phi(y_1) = \Gamma_{1 \rightarrow 2} = \Gamma_{2 \rightarrow 1} = D(y_2)\phi(y_2)$, expressed as the negative feedback $D \rightarrow \Gamma \rightarrow \phi \rightarrow \nu \rightarrow \dot{\gamma}$ in Fig. 4.34. Since $\nu_{app}$ is a monotonously increasing function of $\phi$ the viscosity in the center region is much higher than in the rest of the channel. This coupling is depicted as $\phi \rightarrow \nu$ in Fig. 4.34. The higher viscosity leads then to a smaller shear rate in the center region ($\nu \rightarrow \dot{\gamma}$) resulting in blunted velocity profiles. The negative feedback $\nu \rightarrow \dot{\gamma} \rightarrow \nu$, for shear rates large enough for shear-thickening exists but does not play a prominent role as discussed below.

The global volume fraction $\phi_0$ has a clear effect on the equilibrium profiles. In general, we find that for $\phi_0 = 0.3$ the profile of the local volume fraction over the channel width has a much more pronounced maximum at the center of the channel. This is in agreement with the experimental results by Lyon and Leal which have been included in Fig. 4.36 for comparative purposes. This tendency is also immediately clear from the plots of the diffusivity Fig. 4.32(b) where we find a much more pronounced valley within the central region of the channel for $\phi_0 = 0.3$ in comparison to that for $\phi_0 = 0.5$. Comparing the velocity profiles in 4.32 and 4.33 we see that for $\phi_0 = 0.3$ the profile only slightly differs from a Newtonian velocity profile for the lowest volume force whereas the profiles for $\phi_0 = 0.5$ are equally strongly blunted for all applied volume forces. Also Lyon and Leal find this
Figure 4.35: Experimental results for the velocity and the volume fraction profiles as obtained by Lyon and Leal [123] together with the equilibrium profiles as predicted by the diffusive flux and the suspension balance models. (Pictures taken from Fang et al. [193]). On the left the results for $\phi_0 = 0.3$ are shown, on the right for $\phi_0 = 0.5$.

Figure 4.36: Experimental results by Lyon and Leal comparing profiles of different global volume fractions $\phi_0 = \phi_{\text{bulk}}$. (Taken from [123])
influence on the global volume fraction. All their experiments were carried out at very small particle Reynolds numbers of the order of $10^{-6}$. The particle Reynolds numbers of the lowest volume force applied in our work compare well with that and so do the profiles for $G_x = 10^{-14}$.

Comparing the profiles for different volume forces $G_x$ applied we find a strong dependency in the case of $\phi_0 = 0.3$. The overall shape of the profile $\phi(y)$ stays approximately the same except for secondary peaks for the highest $G_x$, for which we cannot offer a consistent explanation here. However, we also find similar effects in the experimental results by Lyon and Leal [123]. Comparing the profiles for different volume forces $G_x$ applied we find a strong dependency in the case of $\phi_0 = 0.3$. The overall shape of the profile $\phi(y)$ stays approximately the same. However, the difference of the local volume fraction at the center $\phi(x_{\text{center}}) - \phi(x_{\text{wall}})$ is a clearly increasing function of $G_x$. This is not so prominent for $\phi_0 = 0.5$ where volume fraction profiles are more compressed. The dependence on $G_x$ is in clear contrast to the predictions by the diffusive flux and the suspension balance model which both result in profiles independent from the total flux. We find this dependency also for shear rates for which no shear-thickening could be observed which actually agrees with the Newtonian flow assumption in both models. The reason for this must therefore be a much stronger shear-rate dependency of the diffusivity resulting from our micro-model. In both other models the shear rate is a linear function of $\dot{\gamma}$, with an additional dependency on the viscosity gradient in case of the diffusive flux model.

One of the most obvious differences in all the profiles measured by Lyon and Leal is that in their measurements the volume fraction in the outer 20% of the channel width drops down to zero at the wall for almost all settings of flow speed, global volume fraction and the ratio $H/R$. However, Lyon and Leal themselves believe that this is an artifact of their experimental setup namely a lower signal-to-noise ratio that is an intrinsic property of the measuring technique (LDV) they were using. In later comparative measurements with optical microscopy they indeed found higher volume fractions near the walls and confirmed this assumption on the shortcoming of LDV. Although presented for bidisperse suspensions, and therefore strictly speaking not comparable to the monodisperse systems discussed here, regarding the values near the wall the profiles in [124], the local volume fractions near the wall obtained by optical microscopy are much more similar to those presented here and the predictions of the diffusive-flux and suspension balance models.

Lyon and Leal also investigated the influence of the ratio $H/R$ on the profiles but could not find changes larger than the experimental uncertainty for the particle and channel sizes they used. Also the diffusive flux model results in profiles that do not know a dependence on the particle size. On the other hand, the suspension balance model has an explicit dependency on the ratio $H/R$. However, this dependency is relatively weak and based on this model we can estimate that changes would hardly be distinguishable from the fluctuations in our simulations. The suspension balance model contradicts the results from Lyon and Leal regarding the $H/R$ dependence of the velocity fluctuations and is therefore reason for discussion. Also, the influence of the particle size on the profiles vanishes for $H/R \to \infty$ which matches very well the HMM modeling approach based on the separation of the scales of the micro and the macro-dynamics. As described in Sec. 4.2.4 the choice of the models on the micro and macro-scale puts strong limits on the range of parameters we
can investigate, so investigating the influence of the spatial scale separation is not straightforward with our setup and the reason for differences found in the results will be hard to track down since with the spatial scale separation other scalings will change as well.

The Reynolds numbers in the experiments by Lyon and Leal, taking the maximum channel velocity as a reference, were no larger than $10^{-5}$. Even when these are converted to particle shear Reynolds numbers we find $Re_p \ll 1$. That means, no shear-thickening will have occurred in their experiments. For the used particle size Brownian motion was negligible as well, so no significant dependence of the apparent viscosity on the shear rate can be expected at all. In our simulations presented here we deliberately also applied volume forces which resulted in particle shear Reynolds numbers larger than 1 where the suspension began to thicken. However, for the highest volume force applied, $G_x = 10^{-11}$ (macro-scale lattice units), also the difference in particle concentration $\phi(x_{\text{center}}) - \phi(x_{\text{wall}})$ was maximized and the influence of $\phi$ on $\nu_{\text{app}}$ was stronger than that of $\dot{\gamma}$. As a consequence, no clear effect of shear-thickening could be observed in the equilibrium profiles. The differences in the profiles with increasing volume force can be attributed to the increase of the shear-induced diffusivity which was stronger than the decrease caused by the $\nu_{\text{app}} \rightarrow \dot{\gamma} \rightarrow D$ feedback. To investigate this behavior the application of even higher volume forces would be desirable. In the current micro-macro coupling, however, the limits of the micro-model, both, in terms of maximum $\phi$ as well as $\dot{\gamma}_m$ were reached.

Most prominent for the simulations of the suspension with a global volume ratio $\phi = 0.3$, we find a dependency on the flow rate, i.e. volume force the suspension is driven through the channel. This is already true for flow rates that do not lead to shear-thickening ruling out this phenomenon for an explanation. It suggests that the functional dependence of $\nu_{\text{app}}$ on on the volume fraction, and the functional form of $D$ in dependence on shear rate and volume fraction are of a form that lead to different equilibrium profiles in contrast to the equilibrium profile resulting from diffusive-flux or suspension balance model which predict no dependence on the flow rate. With the numerous micro-model runs at different combinations of $\dot{\gamma}_m$ and $D_m$ we, in principle, have enough data collected to discuss these dependencies. However, as the primary intent of this work was to present the computational side of the multi-scale model a discussion in appropriate level of detail is postponed to a future, more physics related work.

A discussion on the error in the presented results proves difficult. As the dynamic coupling of the field quantities $\phi(x)$, $D(x)$, $\nu(x)$ and $\dot{\gamma}(x)$ themselves form a highly sensible feedback network, an estimation of the total error is a highly non-trivial task. Besides that, a sensitivity analysis with respect to the spatio-temporal resolution of the macro-model could not be carried out because changing $\Delta x_M$ and $\Delta t_M$ would change the scaling between micro- and macro-models and the error associated with it. Too many variables change in an almost unpredictable way when one of them is varied. Although we deliberately reduced the dimensionality of the macro-model to exclude phenomena that are related to the break of such enforced symmetries, the coupled system has to be approached almost like an experimentalist approaches his subject of study. That is, it is not always possible to fix one degree of freedom to study the other under pure conditions. Additional tricks, as that of using a database, also come with the trade-off of errors related to
Of course, a main shortcoming of the simulations in this chapter is the fact that it all has been modeled in only two dimensions. The functional dependence of $\nu_{\text{app}}$ on $\phi$ and $\dot{\gamma}$ will be different in three dimensions where suspended particles can avoid high stresses by moving in the extra dimension. The same is true for the shear-induced diffusivity where hydrodynamical particle-particle interactions induce a movement of the particles in the extra dimension and therefore smaller components in the first two. The functional form of the dependencies won't change. Coefficients and exponents might, however, and will lead to a different equilibrium on the macro-scale. The profiles resulting from the 2D model in this work nevertheless show the same features of those obtained in experimental channel flow proving that the behavior in 2D is very similar to that in 3D. Another aspect is that in the experiments by Lyon and Leal and the two models the macroscopic flow is assumed to be laminar and fluctuations in the volume fraction are small in size. In this case, the 2D flow as modeled in this work is equivalent to the 3D flow between two plates.

4.9 Outlook

We are convinced that the multi-scale model and the simulations carried out so far summarized in this chapter offers a good base for the extension to other problems. While building the software care has been taken of the flexibility to include other micro-models and to extend the coupling between micro and macro-models.

As mentioned in the preceding discussion the current model was reduced in dimensionality in several aspects. Besides the obvious need to replace the 2D micro-model by a 3D version to more realistically model apparent viscosity and particle diffusivity of a real suspension, the extension of the dimensions of the macro-model offers the ability to study additional phenomena. When the periodic simulation box of current 2D channel is extended from 1 lattice node to a length comparable or larger than the channel width, non-laminar flow can be studied on the macro-scale. In case of a density ratio $\rho_s/\rho_f \neq 1$ the suspended particles will feel an additional centrifugal acceleration in curved flow. It would make it necessary to model this additional coupling of the macroscopic curvature to a particle force. The result will be an altered apparent viscosity and shear-induced diffusivity due to the non-zero average fluid flux through the array of moving particles. The centrifugal or -petal (depending on $\rho_s/\rho_f$) particle drift will lead to a break of the left-right symmetry of the advection-diffusion dynamics of $\phi(x_M)$ perpendicular to the flow lines. Phenomena like or similar to the clustering of particles in turbulent aerosols, i.e. due to the sweep-stick mechanism, will be possible to investigate based on a realistic modeling of the dynamics of the microstructure.

Another possible extension goes back to the original intent of the suspension model, namely the simulation of blood flow on the cell level. The complex rheology of blood is the result of the many degrees of freedom of the cells suspended in the plasma and their various ways to interact. With a hematocrit of approximately 45% blood is a rather dense suspension. Most of the “solid” phase volume red blood cells (RBC) account for. RBC’s are shaped as biconcave disks, with a dumbbell-shaped cross section and a torus-like rim. This distinctive shape has large influence on the flow in large blood vessels where it can optimize the flow properties of blood,
e.g. stabilization of laminar flow at higher Reynolds numbers and minimization of platelet scatter, which suppresses their positive influence on the formation of atherosclerosis in those large vessels. In large blood vessels, RBC’s sometimes form rouleaux’s, i.e. stacks of RBC’s flat side next to flat side. This occurs more or less often in dependence on levels of certain serum proteins, e.g. during inflammation. Furthermore, the deformability of RBC’s lets the blood adapt to flow effectively through tiny capillaries with less resistance than plasma by itself. As a comparison, if all human hemoglobin were free in the plasma rather than being contained in RBC’s, blood would be too viscous for the cardiovascular system to function effectively. The deformability is also dependent on chemical factors, as is the attractive interactions between RBC’s that causes RBC’s to stick together, with negative effects on the capacity to transport oxygen due to the reduction of their free surface. Modeling of the blood’s microstructure under consideration of such additionally triggered interactions and coupling this to a continuum model as described in this chapter could offer a great tool to study blood flow properties under variation of certain proteins, chemical factors etc.

The multi-scale coupling with the use of the database as described in Sec. 4.6.2 could also offer great improvement in the simulations of hemodynamics in complex geometries. As the parameters shear rate $\dot{\gamma}$ and $\phi$, and other scalar quantities, are invariant under the scale transformation (except for a constant scale factor), results can be re-used in a running simulation although the absolute velocity of the flow at the macro point $(x_M, t_M)$ and its direction might be different. This Galileian and Rotational invariance reduces the actual calls of the micro-model considerably, also in very complex flow geometries.

Besides RBC’s, other important constituents of blood are white blood cells, or leukocytes, and platelets. Leukocytes make up for only 0.7% of the blood volume and might therefore be negligible in bulk flow, however, they have considerable influence on the flow along the vessel walls and therefore particularly on the flow through narrow vessels [197, 198]. Leukocytes tend to stick to and slowly roll along the endothelium driven by the momentum exchange with the remaining blood. In a HMM type of multi-scale simulation a micro-model for the boundary could include leukocytes and therefore resolve their influence on the flow, an effect difficult to model at the continuum level.

Platelets, or thrombocytes, are small (2-3$\mu$m), irregularly-shaped anuclear cells with an average lifespan of normally just 5 to 9 days. Platelets play a fundamental role in hemostasis (and therefore thrombosis, see also Sec. 3.4.1) and are a natural source of growth factors that play a significant role in the repair and regeneration of connective tissues. Platelets have the feature that they can be activated, i.e. brought into a state in which they aggregate and adhere to collagen that is exposed by damaged endothelial tissue. This activation is triggered, besides by stimulation through inflammatory products, by shear stress they experience in the flow. In a HMM type of multi-scale simulation a platelet concentration field and an additional scalar activation field could transport platelet properties over the macro-scale. On the micro-scale, single platelets are modeled and their activation and adhesion to walls simulated. The formation of platelet deposit in arbitrary complex geometries could be studied.

All the above mentioned extensions will introduce additional parameters necessary to describe the states of the particles with increased degree of freedom. Also
their representation in macroscopic fields that show advective and/or diffusive dynamics will have to be tracked, e.g. a field describing the probability density to find an activated platelet or the average strength of activation of the platelets in a volume $\Delta x_M^3$. In principle, they will be treated similarly to the field of particle concentration, i.e. local volume fraction, as demonstrated in this work. With the increase of complexity of the micro-model, reflected in the increase of the number of parameters, the coupling using an intermediate database with inter/extra-polation functionality will show its strength because with every new dimension in the parameter space the actually sampled parameter space will tend to be much smaller than the full hypercube which corners are defined by the minimal and maximal values of each parameter. The effective speedup of the multi-scale computation will therefore increase with the number of parameters.

### 4.10 Conclusion

As a proof of concept we demonstrated that the described multi-scale model is capable of the simulation of the macroscopic flow of a suspension of hard spheres that are several orders of magnitudes smaller than the channel width. The profiles of the local volume fraction $\phi(y)$ and the velocity $v_x(y)$ resulting from the simulations at volume forces varied over four orders of magnitude not only show the same general trend as the diffusive-flux and the suspension balance model. They also show tendencies that can only be found in measurements of real suspensions. Moreover, we find a dependency on the flow rate, i.e. volume force used to drive the suspension through the channel on the profiles which is not present in the diffusive flux and suspension balance model. Whether this is a behavior also found for real suspension is not clear from the literature known to us.

We could show that the application of the HMM idea to the macroscopic suspension flow using a fully resolved micro-model as a replacement for the constitutive equations for $\nu_{app}(x_M)$ and $D(x_M)$ in the macro-models not only reduces the computational effort by several orders of magnitude. It is clear that by exploiting of Galileian invariance the HMM approach enable that type of simulations in the first place.

We also could show that with the use of a database and extra/inter-polation functionality in a confidence range around data points the actual number of micro-model calls could be reduced to a maximum of 30 for each multi-scale simulation carried out. This limited the total runtime of the multi-scale simulation to 2 days on a single CPU. Without the database, e.g. at every macroscopic point in space-time $(x_M, t_M)$ a micro-model would have to be executed to be able to carry out collision steps in the macro-models, a standard HMM type of multi-scale simulation for the considered suspension system would be infeasible.

Besides the main spatio-temporal scale separation between the macro-models and the micro-model leading to the HMM multi-scale modeling approach we identified further scale separations that were exploited in a more technical manner to either increase the numerical stability or to accelerate the dynamics. First, in the micro-model the dynamics of particles in close approach has to be resolved on a much finer spatio-temporal scale to maintain stability of the numerical integration of their trajectories. The fluid was assumed to be constant at the sub-time steps the particle dynamics was solved at. With that, we could increase the applied
shear rates by almost an order of magnitude allowing us to study shear-thickening
in a larger region of particle Reynolds numbers with the fully resolved micro-model.
The other scale separation we made use of is the separation of the time-scales of the
slow diffusive dynamics in $\text{MaS}$ from the fast fluid dynamics modeled in $\text{MaF}$. We
identified how this separation scales with the volume fraction $\phi_0$ and the volume
forces applied to the macro fluid and made use of it by accelerating the diffusive
dynamics.