4. Physical considerations and ingredients for the numerical model

The physical requirements and ingredients for the computational model employed in the present thesis are characterized in this chapter. An overview of existing approaches for the simulation of individual and multiple deformable particles immersed in a fluid is provided in section 4.1. It is discussed in section 4.2 which physical ideas and concepts should be contained in the model and which can be disregarded.

4.1. Overview of existing numerical approaches

Suspensions of rigid spheres have been simulated by Ladd [73, 74] and Aidun and Lu [75] within the framework of the lattice Boltzmann method (LBM, chap. 5). In 1996, Kraus et al. [76] have simulated, for the first time, a single deformable vesicle in an external shear flow using the boundary integral method. Two years later, Eggleton and Popel [77] combined the immersed boundary method (IBM, cf. chap. 6) [78] and a finite element method in order to simulate deformable capsules. In 2004, Feng and Michaelides [79] were the first to combine the LBM with the IBM and simulated suspensions of rigid 2D disks. Zhang et al. [68, 80] also used a combination of the IBM and the LBM for red blood cell (RBC) simulations, but still in 2D. Even in 2005, Sun and Munn [81, 82] approximated RBCs and leukocytes as rigid particles in a 2D lattice Boltzmann simulation.

A number of articles about single RBC or vesicle dynamics in external flow fields has been published in the past ten years. Noguchi and Gompper [83] studied the effect of membrane viscosity on vesicle dynamics in shear flow, taking thermal fluctuations into account. The authors combined a dynamically triangulated membrane model with the multiparticle collision dynamics in 3D. Pozrikidis published a series of articles about the simulation of RBCs in shear flow via the boundary integral method (e.g., [84, 85]). Due to its computational overhead [84, 86], the boundary integral method seems to be not suitable for the simulation of a large number of RBCs.

The simulation of deformable RBC suspensions was promoted in 2007 when Dupin et al. [87] combined the LBM and the IBM with a spring model for the RBC membranes in 3D. 200 cells with a volume fraction of 30% could be simulated. However, a larger number of particles and a higher volume fraction was not obtainable at that time. In the same year, Bagchi [88] simulated 2500 RBCs in 2D. This model was extended to 3D by Doddi and Bagchi [89] two years later. MacMeccan et al. [90] simulated deformable RBCs via a lattice Boltzmann finite element method.

Concluding, a large variety of simulation methods for particle suspensions has been proposed in recent years. Some of the methods have been implemented for 2D only, others approximate the deformable particles as rigid objects. While some of the methods are of high accuracy and mostly suitable for a small number of particles (e.g., the boundary integral method), other approaches are less accurate but more efficient and simpler (e.g., the IBM). Still, neither of these methods seems to be able to combine all of the properties required for the study in the present work: (i) 3D simulations, (ii) deformable and resolved particles, (iii) volume fractions larger than 45%, and (iv) high runtime efficiency with $\mathcal{O}(10^3)$ particles.

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4.2. Identification of the relevant physics for the present task

One of the main motivations of the present thesis is the development and application of a numerical tool for the simulation of dense suspensions of deformable particles, e.g., RBCs. Since the focus of the work lies on the investigation of collective phenomena, the ability to simulate a large number of particles is favored over high accuracy for only a few suspended objects. As a consequence, the single particle dynamics should be simplified as much as possible without losing the advantage of tracking the deformation of individual particles in the suspension. Although large progress has been made in the field of computational physics and computing power in recent years, large scale simulations of deformable particles have always required certain idealizations of the physics on the smallest resolved scales ($\approx 0.5\,\mu\text{m}$ in the present case).

In dense suspensions, the immersed particles are no passive tracers comoving with the suspending fluid. Instead, the *bidirectional* influence of the fluid and the particles is one of the key factors for successful simulations of particle suspensions. In fact, Einstein's famous expression for the viscosity of dilute suspensions, 2.6, reflects that suspended particles, deformable or not, affect the fluid rheology, even in the dilute limit. The shear thinning behavior of blood at intermediate shear rates (a few $10\,\text{s}^{-1}$), caused by the deformability of the RBCs [54], is another striking argument for the paramount importance of the bidirectional coupling of hydro- and particle dynamics. For that reason, the model has to be based on a two-way coupling: The fluid exerts stresses on the particle surfaces, and the presence of the surfaces poses a boundary condition for the fluid. Kraus et al. [76] formulated this in the following way:

> Any theory of vesicle dynamics is complicated by the fact that the boundary conditions for the three-dimensional Navier-Stokes equations have to be evaluated at the vesicle surface, which is moving with the fluid and whose shape is not known a priori.

This statement can directly be extended to any other kind of deformable particles immersed in a fluid. The IBM will be employed as efficient two-way fluid-structure coupling (chap. 6).

Since the rheology of deformable particles is of primary interest here, only the *mechanical* properties of the particles shall be considered. When RBCs are simulated, their biophysical and biochemical properties (e.g., aggregation at small shear rates or non-hydrodynamic interactions with other cells or the endothelium) are not taken into account. The deformable particles are considered as effective 2D membranes immersed in an ambient 3D fluid. A scale separation between the membrane thickness and the membrane diameter is assumed. For RBCs, this is an excellent approximation since the membrane thickness is 4 nm compared to 8 µm cell diameter [31]. Another simplification is to neglect the viscosity of the membranes. In the model, dissipation only takes place in the fluid (inside and outside of the particles), and the membranes are purely elastic. The main reason for this step is to reduce the complexity of the parameter space. Membrane viscosity may be added to the model in the future.

The deformability of RBCs is a key factor for the shear thinning behavior of blood at shear rates above a few s^{-1} [47, 54, 91]. For this reason, it shall be investigated how the deformability of suspended particles affects the viscosity of the suspension and the statistical motion of the particles. The model, therefore, should provide a controllable particle deformability. Physics happening on scales smaller than the spatial resolution of the simulations ($\approx 0.5\,\mu\text{m}$) cannot be resolved explicitly and must be put in by hand as effective ingredients. This including the elastic model for the membranes which is a consequence of its nanometer scale structure. The model for the membrane physics will be presented in chap. 7.

Membrane rearrangements are ignored in the present work, i.e., neighboring points on the membrane will always remain neighbors. This way, the numerical model for the membranes is drastically simplified since the numerical mesh topology is preserved (section 8.3). Applied to the simulation of RBCs, this simplification is still reasonable because experimental investigations

indicate that RBCs have a shape memory, i.e., the rim and the dimples of a RBC are always formed by the same patches of the membrane surface, even after deformations which are long compared to the typical advection times in the human body [92]. Thus, it can be assumed that membrane rearrangements are not important for RBCs, at least on time scales accessible by simulations.

The fluids both in the interior and the exterior of the particles are assumed to be Newtonian (which is also the case for RBCs [51, 93]). For the sake of computational efficiency, a single density and viscosity will be used for both the interior and the exterior fluids. The Newtonian fluid is modeled via the LBM as described in chap. 5. Due to the length scale separation between the fluid molecules and the RBCs, the suspending fluid does not need to be described on the kinetic level.

Thermal effects of any kind are neglected. On the one hand, a possible temperature dependent behavior of material parameters is ignored by assuming that the temperature is constant throughout the system and at all times (infinite heat conductivity). On the other hand, thermal fluctuations are not considered. The particle diameters considered in this thesis are a few micrometers or larger, thus, the particles can be considered non-Brownian [13, 94]. This is especially true for RBCs with diameters of about $8\,\mu m$. Additionally, for particles consisting of thin membranes (e.g., vesicles or RBCs), the thermal membrane fluctuations can be neglected when the energy scale for bending resistance is sufficiently large [31, 95].

The LBM (chap. 5) and the IBM (chap. 6) are efficient numerical tools. The membrane model as introduced in chap. 7 contains the physics relevant for the chosen length and energy scales, but it is not burdened with irrelevant and computationally expensive details. The resulting numerical model is highly efficient, which benefits the achievable system size and duration of the simulations.