

# Development of a hybrid lattice Boltzmann-molecular dynamics code for coarse-grained hemodynamics simulations

Bridging the gap between continuous and high-resolution particulate blood models

Florian Janoschek,<sup>1,2</sup> Federico Toschi,<sup>2</sup> and Jens Harting<sup>1,2</sup>

<sup>1</sup>*Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany*

<sup>2</sup>*Dept. of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands*

## I. MOTIVATION

The particulate nature of blood, which in first approximation may be treated as a suspension of highly deformable red blood cells (RBCs) in blood plasma, makes it difficult to find appropriate models and pushes the amount of computational resources needed for simulation. While on large scales like in arteries, blood behaves as a continuous or even Newtonian fluid [1], these assumptions are surely invalid in smaller vessels. On the other hand, there are treatments of deformable cells in capillaries [2, 3], but these models are computationally too demanding to apply them to considerably larger systems.

Our work follows an intermediate approach: we keep the particulate nature of blood, but try to simplify the description of each single cell as far as possible. Our ultimate goal is to perform large-scale simulations that enable us to connect bulk properties like the effective viscosity to effects at the single RBC level.

## II. MODEL

To couple fluid and particles efficiently, we use a method similar to the one described in [4] and [5] implementing rigid particles of finite size. Physiological RBCs, however, are deformable and assume the shape of biconcave disks in the absence of external stresses [6]. We thus choose a simplified ellipsoidal geometry and add phenomenological pair potentials to account for the more complex behavior of real RBCs. We start with the repulsive branch of a Hookian spring potential

$$\phi(r_{ij}) = \begin{cases} \varepsilon(1 - r_{ij}/\sigma)^2 & r_{ij} < \sigma \\ 0 & r_{ij} \geq \sigma \end{cases} \quad (1)$$

since this is the most simple way to describe (elastic) deformability. With respect of the disk-shape of the particles, we follow the approach of Berne and Pechukas [7] and choose the energy parameter

$$\varepsilon(\hat{\mathbf{o}}_i, \hat{\mathbf{o}}_j) = \frac{\bar{\varepsilon}}{\sqrt{1 - \chi^2 (\hat{\mathbf{o}}_i \hat{\mathbf{o}}_j)^2}} \quad (2)$$

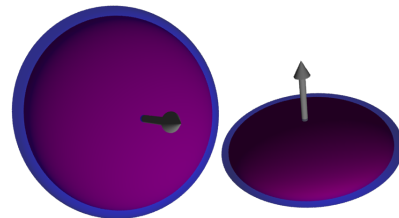


FIG. 1: Schematic outline of the model. Depicted are two model-cells with their respective ellipsoidal volumes defined by the cell-fluid (purple) and the cell-cell interaction (blue). Also shown are the unit vectors  $\hat{\mathbf{o}}_i$  and  $\hat{\mathbf{o}}_j$  parallel to their axes of rotational symmetry.

and the range parameter

$$\sigma(\hat{\mathbf{o}}_i, \hat{\mathbf{o}}_j, \hat{\mathbf{r}}_{ij}) = \frac{\bar{\sigma}}{\sqrt{1 - \frac{\chi}{2} \left[ \frac{(\hat{\mathbf{r}}_{ij} \hat{\mathbf{o}}_i + \hat{\mathbf{r}}_{ij} \hat{\mathbf{o}}_j)^2}{1 + \chi \hat{\mathbf{o}}_i \hat{\mathbf{o}}_j} + \frac{(\hat{\mathbf{r}}_{ij} \hat{\mathbf{o}}_i - \hat{\mathbf{r}}_{ij} \hat{\mathbf{o}}_j)^2}{1 - \chi \hat{\mathbf{o}}_i \hat{\mathbf{o}}_j} \right]}} \quad (3)$$

as functions of the orientations  $\hat{\mathbf{o}}_i$  and  $\hat{\mathbf{o}}_j$  of the particles and their normalized center displacement  $\hat{\mathbf{r}}_{ij}$ . We achieve an anisotropic potential with a zero-energy surface that is approximately that of ellipsoidal disks. Their half-axes  $\sigma_{\parallel}$  and  $\sigma_{\perp}$  parallel and perpendicular to the symmetry axis enter (2) and (3) via

$$\bar{\sigma} = 2\sigma_{\perp} \quad \text{and} \quad \chi = \frac{\sigma_{\parallel}^2 - \sigma_{\perp}^2}{\sigma_{\parallel}^2 + \sigma_{\perp}^2} \quad (4)$$

$\bar{\varepsilon}$  determines the potential strength. The zero-energy surface and the smaller surface defining the particle-fluid interaction are depicted in FIG. 1.

## III. PRELIMINARY RESULTS

We investigate the effects of all model parameters by measuring the effective viscosity as a function of the shear rate for plane shear flow of a homogenous suspension of cells. In general, shear thinning is visible. Increasing  $\bar{\varepsilon}$  leads to a higher yet more constant viscosity which is qualitatively consistent with experiments on suspensions of artificially hardened cells [8]. FIG. 2 shows our currently best fit to literature data for physiological blood. We are thus able to produce quantitative agreement for high shear rates but the absence of attractive effects leads

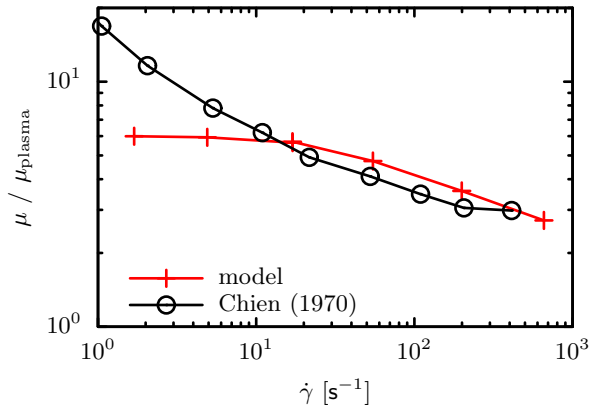


FIG. 2: Shear-rate dependent effective viscosity both for our simulations and for real blood as measured in [8]. Our model still does not account for attractive interactions that become important at low shear rates.

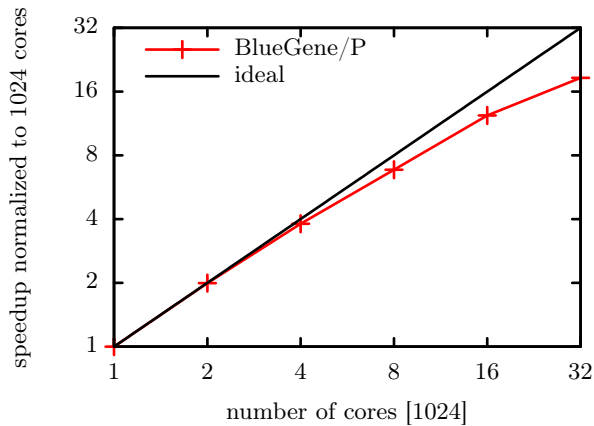


FIG. 3: Speedup during strong scaling benchmark for the BlueGene/P. The system contained  $512^3$  lattice sites and  $2.5 \times 10^5$  particles.

to increasing discrepancy at low shear rates where aggregation is dominant.

Despite its simplifications, the model is computationally demanding due to the spacial resolution of the fluid ( $\sim 10$  lattice sites per cell diameter). Thus systems that are small in physical units still require parallel supercomputers which makes the scalability of the code crucial. FIG. 3 shows the parallel speedup on the BlueGene/P for a homogenous suspension of approximately  $0.04 \text{ mm}^3$ . Around 8192 cores a significant performance degradation sets in. However, the code is not yet specially optimized for this architecture and, for 32768 cores, each computational domain contains only 4096 lattice sites.

#### IV. CONCLUSION

The results make clear that our model scales well and bears the potential to reproduce the behavior of blood quantitatively at high shear rates. This justifies further investigations in improvements of the parallel performance and in attractive potentials to cover also the region of low shear rates.

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