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Lattice-Boltzmann Simulation of Particle Suspensions in Shear Flow

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Inclusion of short-range particle–particle interactions for increased numerical stability in a lattice-Boltzmann code for particle-fluid suspensions, and handling of the particle phase for an effective implementation of the code for parallel computing, are discussed and formulated. In order to better understand the origin of the shear-thickening behavior observed in real suspensions, two simplified cases are considered with the code thus developed. A chain-like cluster of suspended particles is shown to increase the momentum transfer in a shear flow between channel walls, and thereby the effective viscosity of the suspension in comparison with random configurations of particles. A single suspended particle is also shown to increase the effective viscosity under shear flow of this simple suspension for particle Reynolds numbers above unity, due to inertial effects that change the flow configuration around the particle. These mechanisms are expected to carry over to large-scale particle-fluid suspensions.

KEY WORDS: Suspension; lattice Boltzmann; parallelization.

1. INTRODUCTION

Particulate matter suspended in a carrier fluid is transported in many industrial processes. Mixtures of fluid and particles are also met in various natural processes, important examples including blood flow and soil transport by rivers and winds. Even if the carrier fluid itself were Newtonian, inclusion of the solid particles results in a variety of non-Newtonian behavior. One of its more striking effects is shear thickening that is especially pronounced in suspensions of high solid-volume fraction under

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large shear rate. Abrupt increase in shear viscosity can have unpredictable effects, e.g., in industrial processes, which often decrease their efficiency.[1]

In spite of being a long-lasting research topic, there probably are more open than resolved issues in the rheology of suspensions. The origin of the shear-thickening behavior, e.g., is still largely unknown. The most probable explanation so far seems to involve formation of particle clusters which act as channels for momentum transfer, but the mechanism by which they are formed has not been clarified. Another phenomenon related to shear thickening, which however has attracted less attention, seems to be inertial effects that become noticeable for particle Reynolds numbers above unity.

The rheology of suspensions can be studied by experiments and theoretical models, and recently also by computer simulations. To get a realistic picture of the complex mesoscopic dynamics of the suspensions, three-dimensional systems with large numbers of particles are however needed. Continuous development of computing power has made it possible to meet this requirement, but to this end parallel computing must be used.

Several methods have been developed to simulate suspension flows. So far the largest and maybe the most realistic suspension simulations have been performed with the lattice-Boltzmann (LB) method (cf. ref. 2) that appears to be efficient for simulating various multiphase-flow problems.[3] One of the main advantages of the LB method is the spatial locality of the algorithm, which makes it ideal for parallel computing. Inclusion of large, in comparison with lattice spacing, solid particles unfortunately diminishes the spatial locality of the method, and thereby complicates its parallelization. Shared memory would be quite simple to implement, but an efficient code capable of utilizing a large number of processors requires the use of message passing.

In this paper, we first discuss the application of the LB method to suspension simulations. Then, parallelization of the LB algorithm is discussed together with the resulting scaling properties of the code. Next we demonstrate that large-scale simulations of a suspension predict correctly its viscosity. Then we discuss in more detail two simple test cases in which the effect on shear stress of a single cluster of particles, and the inertial effects due to a single suspended particle, are respectively analyzed. Finally we summarize and discuss our results.

2. LB METHOD FOR SUSPENSION SIMULATIONS

The LB model most widely used is the Lattice Bhatnagar–Gross–Krook (LBGK) single-relaxation-time model. This model is based on a

discrete Boltzmann equation that is usually solved on a regular lattice. The dynamics of the method is given by the LB equation

$$f_i(\mathbf{r}+\mathbf{c}_i, t+1) = f_i(\mathbf{r}, t) + \frac{1}{\tau}\left[f_i^{\mathrm{eq}}(\mathbf{r}, t) - f_i(\mathbf{r}, t)\right], \tag{1}$$

in which f_i is the distribution function of the fluid particles moving in the $\mathbf{c}_i$ direction, and $f_i^{\mathrm{eq}}(\mathbf{r}, t)$ is the equilibrium distribution towards which the distribution functions are relaxed. This relation Eq. (1) is characterized by the relaxation time τ. The density ρ and velocity $\mathbf{u}$ of the fluid are determined at each lattice node from the first and second velocity moments of the distribution function f_i, respectively. We use the three-dimensional 19-velocity model (D3Q19) in our simulations.[4] An attractive feature of the LB model is the easy computation of the deviatoric stress tensor from the non-equilibrium parts of the distribution functions by

$$\sigma'_{\alpha\beta} = \left(1 - \frac{1}{2\tau}\right)\sum_i \left[f_i(\mathbf{r}, t) - f_i^{\mathrm{eq}}(\mathbf{r}, t)\right] c_{i\alpha} c_{i\beta}. \tag{2}$$

We utilize this property in our stress analysis of suspensions in Section 4.

One of the advantages of the LB method is the easy implementation of the fluid–solid no-slip boundary condition by using the heuristic bounce-back rule. This approach is usually accurate enough regarding the other sources of error inherent in typical multiphase simulations. The bounce backs of the distribution functions are usually performed on the lattice links, i.e., the distributions are reflected at the midpoints between the fluid and solid nodes in the advection phase of the LB algorithm.

A pioneering work on applying the LB method to suspension simulations was that by Ladd,[5] who generalized the bounce-back rule for moving boundaries,

$$f_i(\mathbf{r}, t+1) = f_{-i}(\mathbf{r}, t) + \frac{2\rho t_i}{c_s^2}(\mathbf{u}_w \cdot \mathbf{c}_i). \tag{3}$$

Here $-i$ denotes the link opposite to i in the lattice, $\mathbf{u}_w$ is the local velocity of the moving boundary, t_i is a weight factor related to direction i,[4] and c_s is the speed of sound. Equation (3) makes the simulation of moving particles straightforward. It does not only describe the action of the particles on the fluid, but can also be used to compute the hydrodynamic forces and torques acting on the particles at a very small computational cost. When these two quantities are known, the velocities, angular velocities, and positions of the particles can be computed by using methods

familiar from molecular dynamics.[6] In the original Ladd model particles were considered as solid shells filled by the LB fluid.[5] An alternative scheme without the interior fluid has been proposed by Aidun and Lu,[7] and we use this scheme here in our simulations.

When two particles are close enough to each other, there are no fluid nodes left between them. As a result of this, an unphysically low pressure appears between the particles if a suspension model without the interior fluid is used. To eliminate this problem, we have added 'virtual' fluid links (cf. Fig. 1) between the particles, which are obtained from the relevant equilibrium distribution function in which the velocity of the fluid–solid boundary and the average fluid density have been used. Virtual-fluid links are only used when forces on adjacent particles in close contact are calculated. After the bounce back, all virtual links remain inside the particle, so the related virtual-fluid populations do not escape into the real fluid as they are not connected to fluid nodes.

It is obvious that the LB method is incapable of giving correct hydrodynamic (lubrication) forces between particles in close contact.[8,9] It is therefore necessary to add a lubrication-force correction to this kind of particle pairs. We have used the correction scheme proposed by Nguyen and Ladd[8] in which an extra two-body force of the form

$$\mathbf{F}_{\mathrm{lub}} = \begin{cases} -6\pi\mu \frac{a_1^2 a_2^2}{(a_1+a_2)^2} \left(\frac{1}{h} - \frac{1}{h_N}\right) \mathbf{U}_{12} \cdot \hat{\mathbf{R}}_{12} \hat{\mathbf{R}}_{12}, & h < h_N \\ 0, & h > h_N \end{cases} \tag{4}$$

is used. Here μ is the dynamic viscosity of the fluid, a_1 and a_2 are the radii of the two particles, h is the shortest distance between the surfaces of two adjacent particles, h_N is a cut-off distance below which correction

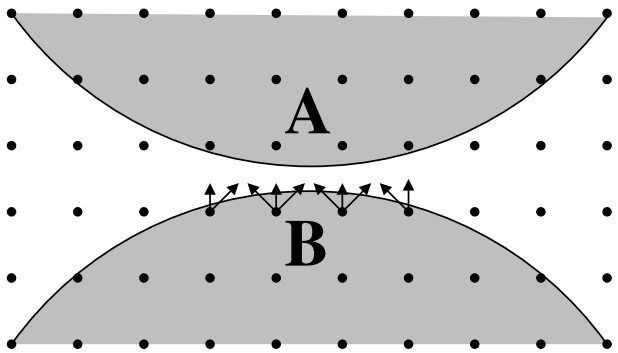

Fig. 1. An illustration of virtual-fluid links in a two-dimensional case. The virtual links inside particle B, which are seen by particle A, are shown.

is used, $\mathbf{U}_{12} = \mathbf{U}_1 - \mathbf{U}_2$ is the velocity difference between the particles, and $\hat{\mathbf{R}}_{12}$ is a unit vector from the center of particle 1 to that of particle 2. At small interparticle distances this divergent correction can, however, lead to high accelerations and velocities and thereby to numerical instability, if the force is explicitly applied on the particles. On the other hand, an implicit updating of particle velocities also leads to numerical problems as it has the complexity of $\mathcal{O}(n^3)$.[8] We have solved this problem by adding the lubrication correction in an explicit manner, but have also set an upper limit to the force. In this way we can prevent problems arising from too large particle accelerations. Also, the rules of elastic collision are used if the particles come in near contact. With these manoeuvres only, particle overlaps may however occur.[10] To this end we added a small short-range velocity-independent repulsive force. This force is needed mainly for dense suspension, especially when flows with high shear rates are simulated. In other cases particle configurations hardly ever evolve such that this force needs to be added. The actual value of the force depends on the simulation parameters, but an acceleration of the order of 10^{-3} (in lattice units) is typically enough to keep all particles separated.

3. PARALLELIZATION

Suspension simulations with large numbers of particles require large computational grids and thus a lot of memory. Also, hundreds of thousands time steps are needed before the system has reached the steady state, and has as well been monitored over several characteristic time scales to ensure statistical reliability of the results. To keep the simulation times reasonable and to meet the memory requirements set by the system size, simulations are typically executed on parallel systems.

The fluid phase is easily parallelized by dividing the computational grid into cuboid subdomains, each handled by a processor dedicated to this purpose. Due to the spatial locality of the LB algorithm, information exchange is only needed between nodes at opposite sides of a boundary between two subdomains, and the computational overhead is thus small.[11] Unfortunately, inclusion of solid particles in the LB fluid complicates the implementation of the method for parallel computers. In a three-dimensional space composed of cuboid subdomains, e.g., a particle can be partially located in eight different subdomains. Special care is therefore needed to ensure that the good scalability of the LB method is preserved.

We have parallelized our suspension code using the message passing interface (MPI). Every particle has its dedicated control processor according to the subdomain where the center of the particle is located. If the particle is partially located in other subdomains, its replica is sent to the

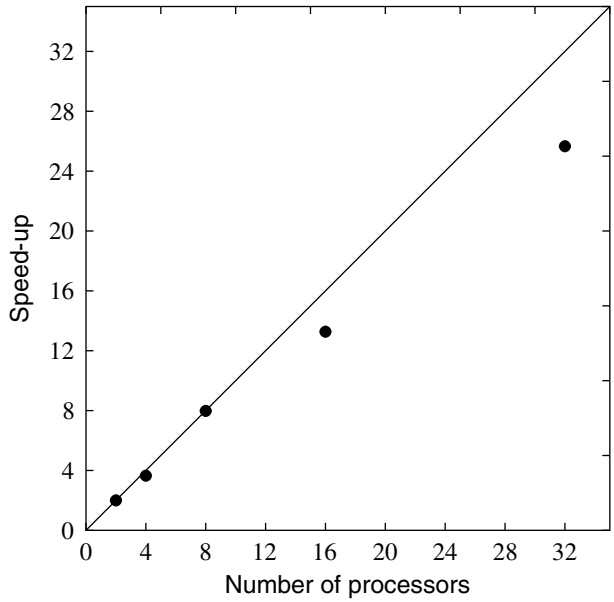

Fig. 2. Scaling behavior of a system of 129^3 grid nodes and 5385 particles.

processors dedicated to these subdomains.[12] Every processor computes the forces and torques acting on all the particles located at least partly in its subdomain. Then the forces and torques determined for the replicas are sent to the control processors of the particle. Finally, each processor updates the velocities, angular velocities, and positions of the particles that are under its control. If the center of a particle crosses the boundary of two subdomains, the control of this particle is handed over to the corresponding processor.

We tested the scaling behavior of our code on a 129^3 grid with 5385 particles (diameter six lattice units). This is a typical number of particles in our simulations in which good discretization of the particles is needed for our momentum-transfer analysis. Test runs were done on an IBM p690 system with IBM Power4 processors. The scaling results for one-dimensional cartesian topology (slice decomposition) are shown in Fig. 2. It is evident that they are rather good: for the highest number of processors the efficiency is still 0.80, and an even better scaling was found for three-dimensional decomposition topologies. We have also performed a preliminary scaling test for 50,000 small particles with a clearly lower resolution than the one used otherwise in this work, and the scaling behavior of the code remained equally good in this case. Notice finally that a paralleliza-

tion of a LB suspension code similar to ours has also been reported by Wolffe *et al.* in ref. 13.

4. RESULTS

All simulations presented in this section were performed in a plane Couette geometry for non-Brownian spherical particles. Suspensions were confined between parallel plates, and a shear flow was created by moving the plates in opposite directions with equal speeds. Periodic boundary conditions were imposed in the other two directions.

For validation of the code, we determined the relative viscosity of the suspension as a function of the solid-volume fraction. Simulations were performed in the Stokes regime, and the number of simulated particles (diameter 12 lattice units) varied from 200 to 2000 depending on the solid-volume fraction. As is evident from Fig. 3, the result is in excellent agreement with the semi-empirical Krieger–Dougherty relation[14] for this system.

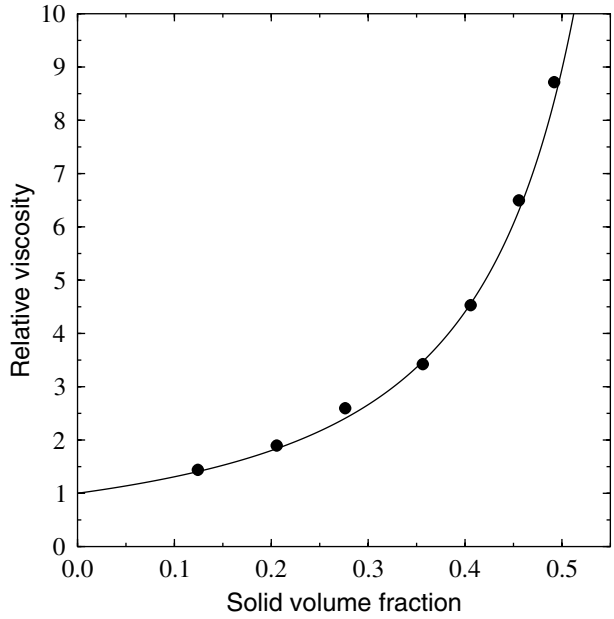

Fig. 3. Relative viscosity of a Stokesian suspension of spherical particles as a function of solid-volume fraction. Circles denote the simulated data and the solid line is the Krieger–Dougherty relation.

For our subsequent analysis we need to determine the shear stresses in the fluid and solid phases. The total momentum tensor can be expressed in both phases in the form

$$\Pi_{\alpha\beta}(\mathbf{r}, t) = \rho u_\alpha u_\beta - \sigma_{\alpha\beta}, \tag{5}$$

where ρ is the density, $\mathbf{u}$ the velocity, and $\sigma_{\alpha\beta}$ the stress tensor of the phase in question. The first term on the right-hand side of Eq. (5) gives the convective stresses. For the fluid phase the second term can be written as

$$\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} + \sigma'_{\alpha\beta}. \tag{6}$$

Here the first term on the right-hand side gives the contribution of pressure, and the second term that of viscous stresses, to the total fluid stress. Thus, the total shear force acting on an arbitrary plane in the suspension is a sum of the solid phase stresses, which are composed of convective and internal stresses, and fluid phase stresses, which are composed of convective and viscous parts. Previous two-dimensional studies of momentum transfer in particle suspensions have shown that convective stresses are negligible in Couette flow at small and moderate Reynolds numbers.[15] We have made the same observation in our three-dimensional simulations, and these stresses will be neglected in the following. The viscous fluid stresses can be directly determined from Eq. (2), and the internal particle stresses due to pressure and viscous forces can be determined by integrating the fluid stress tensor over the surfaces of the particles.[15] We show below our results for the relative stresses that are the actual stresses divided by the stress for the fluid alone.

Changes in the microstructure of the suspension appear to play a significant role in the rheology of the suspension. An interesting phenomenon related to these microstructural changes is the formation of chain-like clusters of particles, which rotate while being advected in the shear flow.[16] We now demonstrate the effect on the total shear stress of an idealized rotating chain-like cluster. The artificial cluster considered consists of seven spherical particles (cf. Fig. 4), the size of the system is $50 \times 160 \times 111$ (vorticity, flow, and gradient directions, respectively), the diameter of the particles is 14 lattice units, the wall speed is 0.003 lattice units, and the BGK relaxation parameter is 1. After the particles are placed in their initial positions their motions are determined as explained in Section 2.

During the whole simulation the shortest distances between the particles remain larger than one lattice spacing, and the lubrication-force correction Eq. (4) is not needed. As the model suspension is sheared, the

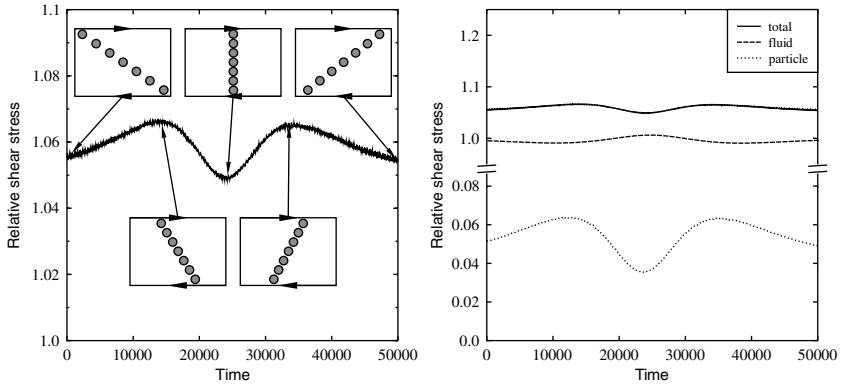

Fig. 4. In the left panel the relative wall stress is shown as a function of time for an idealized cluster of suspended particles. The average relative shear stress for a random configurations of the same particles is 1.03. The insets show the orientation of the cluster at different instants of time. In the right panel the shear stress of the fluid and of the particle in the middle plane of the system are shown.

chain-like array of particles rotates, and the shear forces acting on the particles bring them closer together when the orientation of the array changes from horizontal to vertical (see Fig. 4). There after interparticle distances begin to increase when the array continues to rotate further, and the cluster may eventually break up. During this process, the relative shear stress stays clearly above that for a random configuration of the same particles. This stress increase results from increased internal stresses of the particles and the high fluid stresses created between them (see Figs. 4 and 5). We expect that a qualitatively similar mechanism is behind the shear-thickening behavior of many real suspensions.

As the last example we consider the shear-thickening behavior of the simplest possible suspension consisting of only one particle in the middle of the system. (Notice, however, that there are periodic boundaries.) Due to its initial position, the particle does not move during the simulation, but it can rotate. The size of the system is 50^3 and the diameter of the particle is 22 lattice units. Simulations were done by using a fixed value for the viscosity and increasing the shear rate. Our simulations show (see Fig. 6) that a small but detectable shear thickening is seen even in this very simple system, when the particle shear Reynolds number exceeds unity. On the other hand, in simulations with linear equilibrium distribution functions (i.e. Stokes flow), this effect is absent. Stress analysis in the middle plane shows that now shear thickening mainly results from increased particle stress due to pressure forces.

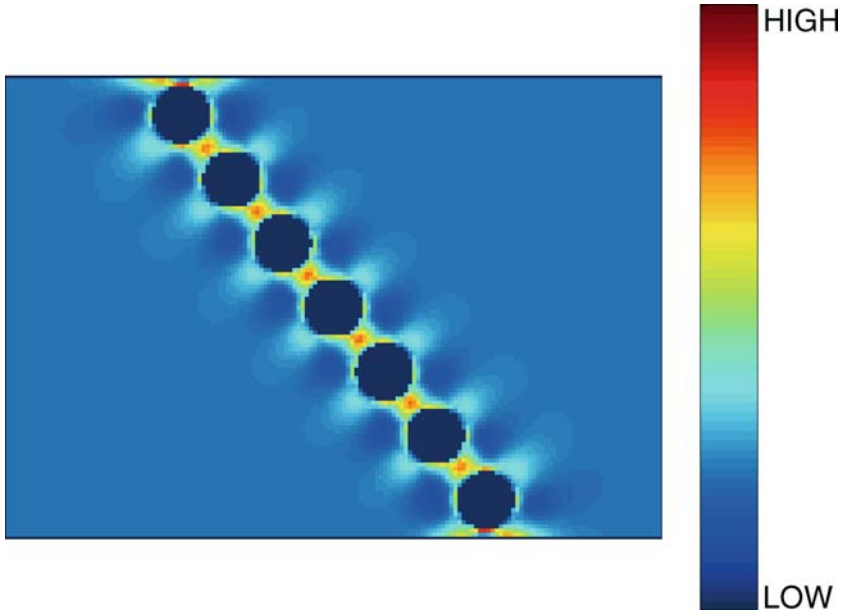

Fig. 5. Instantaneous fluid shear stresses in a planar cross section of the system with an idealized cluster.

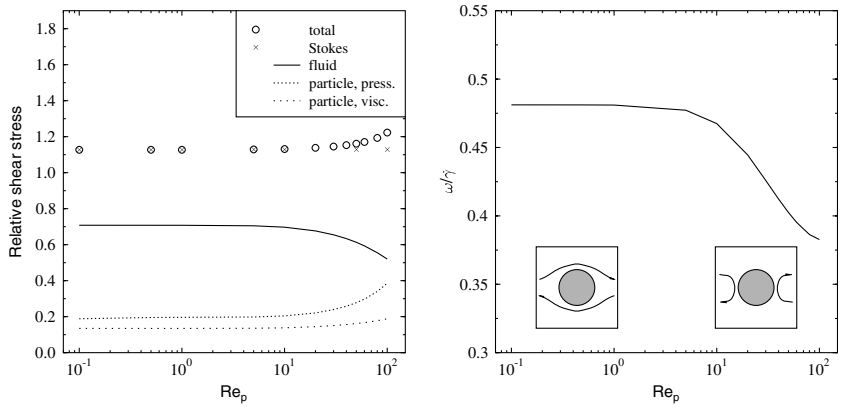

Fig. 6. In the left panel the relative shear stress of the suspension is shown as a function of particle Reynolds number (defined as $\dot{\gamma}d^2/\nu$ with $\dot{\gamma}$ the shear rate and d the particle diameter). Also shown are the results for the Stokes flow simulations and the different components of the stress in the middle plane of the system. In the right panel the angular velocity of the suspended particle scaled with the shear rate is shown as a function of particle Reynolds number. The insets in the right panel show schematically the change in the flow field as Re_p increases.

Simultaneously with shear thickening, a change in the flow field around the particle is also observed. For small shear rates fluid flows smoothly through the gaps between the particle and the walls. When the shear rate increases, streamlines begin to increasingly bend in front of (and behind) the particle, finally making a complete 'U-turn'. This behavior leads to a situation in which the fluid speed in the gaps is (relatively) decreased, and the angular velocity of the particle is also reduced (cf. Fig. 6). Similar observations for a single suspended particle have been made in two dimensions by solving the Navier–Stokes equation with a finite element method.[17] Notice also that in two-dimensional LB simulations, a reduction in the angular velocity of particle clusters has been observed to be connected with the shear thickening of the suspension.[18]

5. CONCLUSIONS

The basic LB algorithm can very effectively be parallelized, but inclusion of solid particles suspended in the fluid complicates parallelization with message passing. We showed that good scaling behavior of a parallelized suspension code can however be obtained if the particle phase is properly treated. Handling of the particle–particle interactions at very short distances so as to increase the numerical stability of the code was also discussed. For validation purposes we simulated the shear flow in Couette geometry of a non-Brownian suspension, and found that, as a function of the solid-volume fraction, in the Stokes regime the simulated viscosity of the suspension agrees well with the semi-empirical Krieger–Dougherty relation.

In terms of two simple examples we showed how the LB method in combination with detailed stress analysis can be used to effectively study the origin of the observed non-Newtonian behavior of particulate suspensions. First we considered the effect of a single artificial cluster of suspended particles on the solid-volume fraction dependence of the viscosity of this suspension, and, in search for inertial effects, analyzed then the shear-thickening behavior of the simplest possible suspension consisting of a single suspended particle.

A chain-like cluster of suspended particles rotating in the shear flow was found to increase the momentum transfer between the channel walls in comparison with random configurations of particles. This behavior indicates that increased formation of particle clusters for increasing solid-volume fraction of the suspension will contribute to the related increase in its viscosity. In the case of the single-particle suspension, inertial effects that become detectable for particle Reynolds numbers above unity, change

the flow field around the particle so as to increase the shear stress of the system.

The stress analyses presented here are by no means restricted to small systems. In our future work we will extend these analyses to large-scale suspensions. As already indicated by the results reported here for simplified systems, detailed analyses of stresses of individual particles and spatial distributions of fluid stresses, are expected to give us new insight into the complex rheology of real suspensions.

REFERENCES

1. H. A. Barnes, J. F. Hutton, and K. Walters, *An Introduction to Rheology* (Elsevier Science Publishers, Amsterdam, 1989).
2. N.-Q. Nguyen and A. J. C. Ladd, Microstructure in a settling suspension of hard spheres, *Phys. Rev. E* **69**:050401 (2004).
3. S. Chen and G. D. Doolen, Lattice Boltzmann method for fluid flows, *Annu. Rev. Fluid Mech.* **30**:329–364 (1998).
4. Y. H. Qian, D. d'Humières, and P. Lallemand, Lattice BGK models for Navier–Stokes equation, *Europhys. Lett.* **17**:479–484 (1992).
5. A. J. C. Ladd, Numerical simulations of particulate suspensions via a discretized Boltzmann equation. Part 1. Theoretical foundation, *J. Fluid Mech.* **271**:285–310 (1994); Numerical simulations of particulate suspensions via a discretized Boltzmann equation. Part 2. Numerical results, **271**:311–339 (1994).
6. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon Press, Oxford, 1987).
7. C. K. Aidun and Y. Lu, Lattice Boltzmann simulation of solid particles suspended in fluid, *J. Stat. Phys.* **81**:49–61 (1995).
8. N.-Q. Nguyen and A. J. C. Ladd, Lubrication corrections for lattice-Boltzmann simulations of particle suspensions, *Phys. Rev. E* **66**:046708 (2002).
9. E.-J. Ding and C. K. Aidun, Extension of the lattice-Boltzmann method for direct simulation of suspended particles near contact, *J. Stat. Phys.* **112**:685–708 (2003).
10. R. C. Ball and J. R. Melrose, Lubrication breakdown in hydrodynamic simulations of concentrated colloids, *Adv. Colloid Interface Sci.* **59**:19–30 (1995).
11. D. Kandhai, A. Koponen, A. G. Hoekstra, M. Kataja, J. Timonen, and P. M. A. Sloot, Lattice-Boltzmann hydrodynamics on parallel systems, *Comput. Phys. Commun.* **111**:14–26 (1998).
12. T. Suviola, Parallelization of a lattice Boltzmann suspension flow solver, *Proceedings of PARA 2002*, June 15–18, 2002, Espoo, Finland, J. Fagerholm *et al.* eds., Lecture Notes in Computer Science, Vol. 2367, pp. 603–610 (2002).
13. G. Wolffe, J. Oleszkiewicz, D. Cherba, and D. Qi, Parallelizing solid particles in lattice-Boltzmann fluid dynamics, *Proceedings of PDPTA '02*, June 24–27, 2002, Las Vegas, USA, H. R. Arabnia ed. (CSREA Press, 2002), pp. 2016–2022.
14. I. M. Krieger and T. J. Dougherty, A mechanism for non-Newtonian flow in suspensions of rigid spheres, *Trans. Soc. Rheol.* **3**:137–152 (1959).
15. A. Shakib-Manesh, P. Raiskinmäki, A. Koponen, M. Kataja, and J. Timonen, Shear stress in a Couette flow of liquid-particle suspensions, *J. Stat. Phys.* **107**:67–84 (2002).
16. P. Raiskinmäki, J. A. Åström, M. Kataja, M. Latva-Kokko, A. Koponen, A. Jäsberg, A. Shakib-Manesh, and J. Timonen, Clustering and viscosity in a shear flow of a particulate suspension, *Phys. Rev. E* **68**:061403 (2003).

17. N. A. Patankar and H. H. Hu, Finite Reynolds number effect on the rheology of a dilute suspension of neutrally buoyant circular particles in a Newtonian fluid, *Int. J. Multiphase Flow* **28**:409–425 (2002).
18. P. Raiskinmäki, Dynamics of multiphase flows: liquid-particle suspensions and droplet spreading, PhD Thesis (University of Jyväskylä, 2004).