Three-dimensional modeling of the viscous fluid flow and the dynamics of dispersed systems in microstructures using the boundary element method

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Abstract. Direct simulation of viscous fluid flow and dispersed flow at low Reynolds numbers in microstructures with complex geometry is needed for a wide range of industrial applications associated with the porous materials. The numerical approach is based on the boundary element method (BEM) for 3D problems accelerated both via an advanced scalable algorithm (FMM), and via utilization of a heterogeneous computing architecture (multicore CPUs and graphics processors). This enables direct large scale simulations on a personal workstation, which are confirmed by demo computations. In present work, the hydrodynamic flow of viscous liquid around the rigid structures with various configurations is studied. Also, the numerical approach is successfully applied for modeling the dynamics of deformable dispersed inclusions in the flow around microstructures. The results of the research may be used for the solution of problems related to microfluidic device construction, the theory of the composite materials production, and are of interest for computational hydrodynamics as a whole.

1. Motivation

Nowadays, micro models and microfluidic devices are widely used as effective equipment for quantitative and qualitative analyses of the features of fluid flow and other processes taking place in different porous materials at milli-, micro- and even nano-meter scales. Studying the processes in porous media is a difficult problem due to the large number of parameters affecting fluid flow in complex pore networks. The structure geometry is another factor that should be taken into account in micro scale simulations. Researchers have successfully applied various types of microscale models representing the connected networks of channels designed to study a specific phenomenon and two-dimensional porous medium representations, in which flow of fluids, particles, and solutes are visualized and studied.

Direct simulations of Stokes flows in various domains of complex geometry are essential for investigation of the effects arising in nature and engineering. For example, the manufacturing of composite assemblies is performed by infiltration of a liquid matrix into a thin porous medium made from a fiber assembly. Entrainment of air bubbles may accompany this process. So, the direct three-dimensional numerical simulations of single-phase or two-phase viscous flows around complex structures are of interest for this technology. Nowadays there is a wide range of works dedicated to two-phase flows in composite manufacturing including experiments [1] and computations [2, 3]. Nevertheless, the development of efficient numerical approaches for the detailed study of the dynamics of deformable dispersed inclusions in the domains of complex geometry remains relevant.
Present work is dedicated to the 3D numerical simulation of Stokes flow around the fixed rigid structures. Despite the fact that the formulation of the corresponding mathematical problems is carried out within the framework of the classical equations of mechanics and physics, modern computational methods and hardware are used to solve them.

2. Problem formulation and numerical implementation

The viscous fluid flow around the fixed non-deformable structures and the dynamics of deformable inclusions (index 2) in a viscous fluid flow (index 1) around non-deformable objects in Cartesian coordinates are studied. It is assumed, that the processes are considered in isothermal conditions, at low Reynolds numbers, without taking into account the van der Waals forces. Then liquid motion is described by the Stokes equations. On the surface of the inclusions, the equality of the velocities inside and outside is considered, and the traction is known. On the surface of non-deformable fixed structures, the non-slip condition is considered. The problem statement in more details is represented in [4].

The numerical approach is based on the boundary element method (BEM). The BEM has been successfully applied for simulation of Stokes flow (see general overview and details of the BEM in the monograph of Pozrikidis [5]), but its application to simulation of large non-periodic systems is very limited. As each considered object is covered by triangular mesh, in case of complex structures or a large number of the simulated objects, a number of computational points may reach several million. Thus, the key here is the acceleration of the BEM both via advanced scalable algorithms, particularly, the fast multipole method (FMM), and via utilization of advanced hardware, particularly, graphics processors (GPUs) and multicore CPUs [6]. We developed and applied this technique to study the 3D emulsion dynamics and viscous fluid flow in various domains [7, 8] and bubble dynamics at low [9] and large [10] Reynolds numbers. In our previous works example computations were successfully conducted for 3D dynamics of systems of tens of thousands of deformable drops and systems of several droplets, with very high discretization of the interface in a shear flow [7]. The features of the boundary integrals calculations for considered problem are described in more detail in our previous work [4].

3. Results

All program modules, except multi-level FMM, are implemented in Matlab. The computations were performed on workstations equipped with CPU Intel Xeon 5660 and GPUs NVIDIA Tesla K20, 5 GB of global memory (Kepler architecture).

First of all, a numerical study of the features of viscous fluid flow patterns around cylindrical elements in the presence of solid walls has been carried out. This part of computer design in this work is motivated by the need to study viscous binder fluid flow around reinforcement fibers in the manufacture of composite materials. At the initial step of this research, we consider that the walls of the preform are located far enough so that their influence can be neglected, also when the fibers are located across the cell, they can be considered infinitely long.

![Figure 1. Geometry of considered rigid structure, in the plane y = 0.](image)

Calculations were carried out for the flow around structures with the uniform flow velocity at the infinity $U_\infty = (u, 0, 0)$. The configuration of the fixed structure, shown in figure 1, consists of four planes that set up as a closed domain of rectangular cross-section, and cylindrical filaments with radius $R$ with different positions in space frozen into the medium. The surface of each element was covered...
by a mesh with \( N_\Delta = 13720 \) triangular elements, on the surface of each flat plane \( N_\Delta = 387200 \) approximately. As a result, the total problem size was \( N_\Delta = 428360 \) and the size of the computation matrix was \( N_\Delta = 1285080 \). For the best convergence of the solver, particular attention was paid to the mesh quality and more precisely to such parameters as the ratio of the maximum and minimum sides of the triangles, the ratio of the triangle areas to the lengths of their sides, the ratio of angles in the triangle, and the valence of the nodes.

Calculations were conducted to investigate the effect of the location of fibers on the stagnation zone formation between the fibres for the case of cylindrical elements. It is important because the bubbles and other dispersed inclusions can be trapped and remain in the vortex. The distance between the fibres was varied as follow \( \Delta x = 0.25 R, 0.5 R, 2 R, 3 R, 4 R \). The obtained flow patterns are presented in figure 2 in the domain \( 15 R \leq x \leq 35 R \), \( 5 R \leq z \leq 10 R \) in the plane \( y = 0 \). The streamlines in figure 2 show that stable, more significant vortices are formed when the distance is approximately equal to the radius of the fibres themselves or may be slightly larger or slightly smaller \( \Delta x = R \). In the case when the distance exceeds the radius, for example two times or more, the formation of stagnant zones is not observed. Similar results were obtained for cases where the distance is much smaller than the radius \( \Delta x = 0.25 R, 0.5 R \). All the results were obtained for \( \text{Re} = 0.45 \).

![Figure 2. Streamlines for the flow around the structures for different distance between the cylindrical fibres \( \Delta x = 0.25 R, 0.5 R, 2 R, 3 R, 4 R \) (from the left to the right) in the domain \( 15 R \leq x \leq 35 R \), \( 5 R \leq z \leq 10 R \) in the plane \( y = 0 \), \( \text{Re} = 0.45 \).](image)

The series of calculations were conducted for the case of the dynamics of dispersed inclusions in a viscous fluid flow in the flow around fixed structures, based on the FMM-accelerated version of the boundary-integral formulation. Figure 1 shows the configuration with the following geometrical parameters of the surrounding box of flat planes: length along \( x \) \( L_x = 30 \cdot R \), width along \( y \) \( L_y = 5 \cdot R \), width along \( z \) \( L_z = 8 \cdot R \), \( \Delta x = R \). Simulations were carried out for \( \text{Re} = 0.4 \).
The dynamics of single and several dispersed inclusions for $\lambda = 1.5$, where $\lambda = \mu_2 / \mu_1$ is the ratio of the viscosities of the liquids, with a different initial position was considered. Cases were simulated for different position of the initially spherical drop along the axis $z$ at the level of the domain center line $z_0 = 4 R$, above $z_0 = 4.5 R$, below the center line $z_0 = 3.5 R$ and $z_0 = 3.75 R$, $a = 0.75 R$, $x_0 = 5 R$, $y_0 = 0$. The number of triangular elements on each drop surface $N_\Delta = 1280$. The dynamics of a dispersed inclusion (red line) around the fixed elements (blue line) is presented in figure 3 and figure 4 and in plane $y = 0$.

![Figure 3](image1)

**Figure 3.** Dynamics of deformable inclusion (red line) with initial position of mass center $(5R; 0; 4R)$ (on the left) and $(5R; 0; 4.5R)$ (on the right) in the flow around the structures (blue line).

The part of computational domain $2R \leq x \leq 20R$, $0 \leq z \leq 8R$ in the plane $y = 0$, $\lambda = 1.5$, $Re \approx 0.4$.

![Figure 4](image2)

**Figure 4.** Dynamics of deformable inclusion (red line) with initial position of mass centres $(5R; 0; 3.75R)$ (on the left) and $(5R; 0; 3.5R)$ (on the right) in the flow around the structures (blue line). The part of computational domain $2R \leq x \leq 20R$, $0 \leq z \leq 8R$ in the plane $y = 0$, $\lambda = 1.5$, $Re \approx 0.4$.

Further, the dynamics of several deformable dispersed inclusions was considered. In figure 5 a demonstration calculations of viscous fluid flow is presented with three initially spherical droplets of equal radius $a = 0.75 R$ located in the same positions with respect to $x$ and $y$, $x_0 = 5 R$, $y_0 = 0$, but different to $z$ in $z_0 = 1.75 R$, $z_0 = 4 R$, $z_0 = 6.25 R$. The dynamics of smaller inclusions was also considered. The calculations were performed with the same physical parameters, but for the droplets with radius $a = 0.05 R$. Figure 6 shows the simulation results for 19 drops at different dimensionless time $t = t_{\text{non-dim}} = \gamma \text{dim} / (\mu \text{dim})$, where $a$ is the droplet radius, $\gamma$ is the surface tension, $\mu_1$ is the viscosity of carrier fluid.
Figure 5. The dynamics of 3 dispersed inclusions (red line) in the flow around the structures (blue line). The part of computational domain $2R \leq x \leq 20R$, $0 \leq z \leq 8R$ in the plane $y = 0$, $\lambda = 1.5$, $Re \approx 0.4$.

Figure 6. The dynamics of 19 dispersed inclusions (red colour) in the flow around the structures (grey colour) in different time $t = 0$, $t = 4$, $t = 6$, $t = 8$. The part of computational domain $2R \leq x \leq 20R$, $0 \leq z \leq 8R$ in the plane $y = 0$, $\lambda = 1.5$, $Re \approx 0.4$.

It is shown that, while approaching the structures inclusions significantly deform and move according to the streamlines. This can lead to the breakup and fragmentation of dispersed inclusions, but in this problem formulation the modeling of the object topology changing has not been considered yet.

Conclusions
The represented efficient numerical approach was applied for the study of flow patterns around rigid structures of different configurations and for the research of the dynamics of deformable dispersed inclusions in viscous flow in the domains with nontrivial geometry. The information obtained from case studies and analysis of parametric dependences can be useful for the development of tools for efficient
simulation, prediction, and control of multiphase flows in microstructures. Further improvement of the performance of the current numerical approach can be of interest for practical applications.

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