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3D simulation of deformable particle dynamics in channel with hydrodynamic traps

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Abstract. The importance of adequate simulation of dispersed systems in microchannels with traps is due to the need to solve applied problems arising in the design of microfluidic devices. Depending on the purposes of the devices, the geometry configuration of hydrodynamic traps and their spatial arrangement is chosen. The present work is dedicated to the study of the dynamics of dispersed particles in the viscous fluid flow in a microchannel with hydrodynamic traps. The computational approach is based on the Boundary Element Method, accelerated using the Fast Multipole Method on heterogeneous computing architectures. Simulation results and details of the method are discussed. In addition, the influence of the distance between trap rows and their spatial arrangement on the flow pattern in the microchannel has been investigated.

Keywords: Stokes equations, hydrodynamic traps, microfluidics

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3D моделирование динамики деформируемых частиц в канале с гидродинамическими ловушками

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Аннотация. Важность адекватного моделирования дисперсных систем в микроканалах с ловушками обусловлена необходимостью решения прикладных задач, возникающих при проектировании микрофлюидических устройств. В зависимости от назначения устройств выбирается геометрическая конфигурация гидродинамических ловушек и их пространственное расположение. Настоящая работа посвящена исследованию динамики дисперсных частиц в потоке вязкой жидкости в микроканале с гидродинамическими ловушками. Вычислительный подход основан на методе граничных элементов, ускоренном с помощью метода быстрых мультиполей на гетерогенных вычислительных архитектурах. Результаты моделирования показывают влияние расстояния между рядами ловушек и их пространственного расположения на характер течения в микроканале.

Ключевые слова: уравнения Стокса, гидродинамические ловушки, микрогидродинамика

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Introduction

Three-dimensional simulation of viscous fluid flow in microchannels with hydrodynamic traps is important for the design of microfluidic devices (MFDs). Currently, there is a remarkable expansion in the application of different types of MFDs. One of the applications of MFDs is the accurate manipulation of the particles in the flow, e.g. for particle fixation and sorting. At this stage of technological development, many technical approaches to particle and cell capture in microfluidic devices are known. Microfluidic devices are classified according to their functionality into the following categories: sorting or separation of particles, fixation and holding of particles, cultivation of biological objects (cells, bacteria, etc.), sample preparation or sample processing [1]. Depending on the MFD design purposes, various geometry configurations of hydrodynamic traps and their spatial arrangement are chosen. Particle trapping by arrays of microposts is a horizontal trapping method, which can be implemented by simply blocking particles whose size exceeds the distance between neighboring columns. In this approach, the distance between the posts must be adapted to the size of the target particles [2]. One problem with this type of trap, which reduces trapping efficiency, is that particles or droplets can deform and can be pushed through the gaps between the posts. Thus, it is extremely important to select the optimal geometric parameters when designing different types of MFDs.

To solve this problem and reduce the time cost of the experimental research, various numerical approaches for simulation of physical processes at the microscale are actively used. Simulation of emulsion dynamics can be carried out by different numerical approaches, for instance, the Volume of Fluid method [3], the Finite Element Method [4]. However, the high-efficiency computational approaches are required for a more detailed description of the particle deformation in the three-dimensional case in the channels of microfluidic devices. However, such problems have not been solved yet for the flow of deformable droplets in such configurations in 3D case using the Boundary Element Method (BEM). The purpose of this research is to study the efficiency of trap configurations using a numerical approach based on 3D BEM accelerated using a scalable algorithm (FMM – fast multipole method) and a heterogeneous computational architecture (CPUs and GPUs).

Problem statement and mathematical model

This study is devoted to the problem of viscous fluid flow with deformable particles in microchannels with C-shaped hydrodynamic traps under the constant volumetric flow. An array of microposts is a simple and clear method of blocking the particles in the flow. C-traps are represented as cylindrical elements of equal radius, located at equal distances from each other across the flow. Such traps are used in practice to capture of the particles. Two types of traps, symbolized as C4 and C5 (Fig. 1), are considered, as well as two spatial configurations of trap locations: in the form of a triangular array and in chess order. At a certain distance from the trap array, there are several initially spherical droplets.

The processes are considered at small Reynolds numbers under isothermal conditions. The flow of particles (index 2) in incompressible Newtonian fluid (index 1) is described by steady Stokes equations

$$-\nabla p_i + \mu_i \nabla^2 \mathbf{u}_i = 0, \;\; \nabla \cdot \mathbf{u}_i = 0, \;\; i = 1,2, \tag{1}$$

where p is a pressure, μ is a dynamic viscosity, $\mathbf{u}$ is a velocity vector.

At the interface, the velocities coincide and the difference of normal stress vectors is set

$$\mathbf{u}_1 = \mathbf{u}_2,\ \ \mathbf{f} = \boldsymbol{\sigma}_1 \cdot \mathbf{n} - \boldsymbol{\sigma}_2 \cdot \mathbf{n} = \mathbf{f}_1 - \mathbf{f}_2 = f\mathbf{n},\ \ f = 2\gamma k(\mathbf{x}) + (\rho_1 - \rho_2)(\mathbf{g} \cdot \mathbf{x}),\ \ \mathbf{x} \in \mathrm{S_d}, \quad (2)$$

where $\mathbf{f}$ is a traction, $\boldsymbol{\sigma}$ is a stress tensor, ρ is the liquid density. On the surface of the non-deformable fixed cylindrical elements forming the trap, the non-slip condition is set

$$\mathbf{u}(\mathbf{x}) = 0,\ \ \mathbf{x} \in \mathrm{S_s},\ \ \mathbf{x} \in \mathrm{S_s}, \quad (3)$$

where $\mathrm{S_s}$ is the total rigid elements surface. Droplet motion is characterized by the kinematic condition

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{u}(\mathbf{x}),\ \ \mathbf{x} \in \mathrm{S_d}, \quad (4)$$

where $\mathbf{u}(\mathbf{x})$ is the interface velocity, $\mathbf{x}$ is the radius-vector of the point, and $\mathrm{S_d}$ is the particle surface.

Three-dimensional simulation of fluid flow and dynamics of non-deformable droplets was performed using software modules based on the accelerated BEM. The basic idea of this method is as follows. The initial differential equations describing the behavior of the function inside and on the domain boundary are reduced to the integral equations that relate only the boundary values. This is one of the main advantages of the BEM, since it eliminates the need to discretize the entire 3D domain. The triangular mesh covers only the surfaces of the considering object. BEM is well suitable for describing three-dimensional particle dynamics with random deformation in domains with complex geometry, as well as in shear flows in an unbounded domain. However, it becomes more difficult to apply the standard non-accelerated BEM for large-scale problems. In this work, the standard BEM is accelerated using both a scalable algorithm (FMM) and a heterogeneous computational architecture. The description of the approach in more detail can be found in [5, 6].

Numerical results and discussion

Viscous fluid flow around the hydrodynamic traps in microchannel. Two hydrodynamic trap configurations are considered in this study (Fig. 1). The C4 trap is presented in the form of four non-deformable cylindrical elements arranged in a semicircle. The cross section of each element has a radius R. The C5 trap consists of five cylinders of the same radius, arranged similarly to the C4 trap. The main difference between the C4 and C5 trap configurations is the number of elements and their spatial arrangement relative to each other. Trap length – L_{trap_x} $6.25 \cdot R$, width – L_{trap_z} $9 \cdot R$, height – L_{trap_y} $10 \cdot R$. Reynolds number was calculated as $\mathrm{Re} = 2\rho Q/(\mu(w+h))$, where Q is the liquid volume flow rate, w is the microchannel width, h is the microchannel height. The resulting Re varied from 0.4 to 0.7.

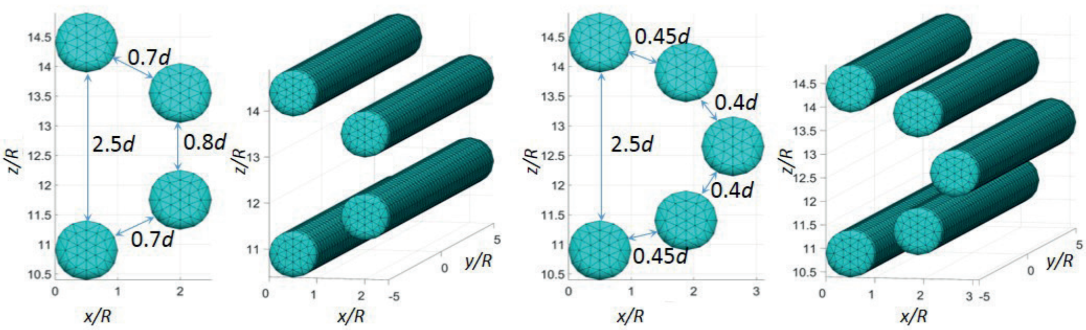

Fig. 1. C4 and C5 hydrodynamic traps configuration

One can see in Fig. 1, there is a narrow channel between the cylindrical elements of the C-trap, which is proportional to the diameter of the cylinder . Such a trap design allows for reducing hydrodynamic resistance in the microfluidic device. Simulation of creeping flows in complex three-dimensional domains consisting of similar traps was carried out in our previous work [7].

To predict the motion of droplets in the fluid flow in a microchannel with complex structure, streamlines for fluid flow without inclusions were initially obtained.

Two cases of the hydrodynamic traps arrays with different spatial configurations of C4 and C5 traps are considered. The total number of traps was 15. The distance between trap rows was $d_x = 2 \cdot L_{trap_x}$, where L_{trap_x} is the width of the trap along the Ox axis. Also, the velocity fields of viscous fluid flow in the microchannel with these spatial arrangements of the traps were calculated (Fig. 2).

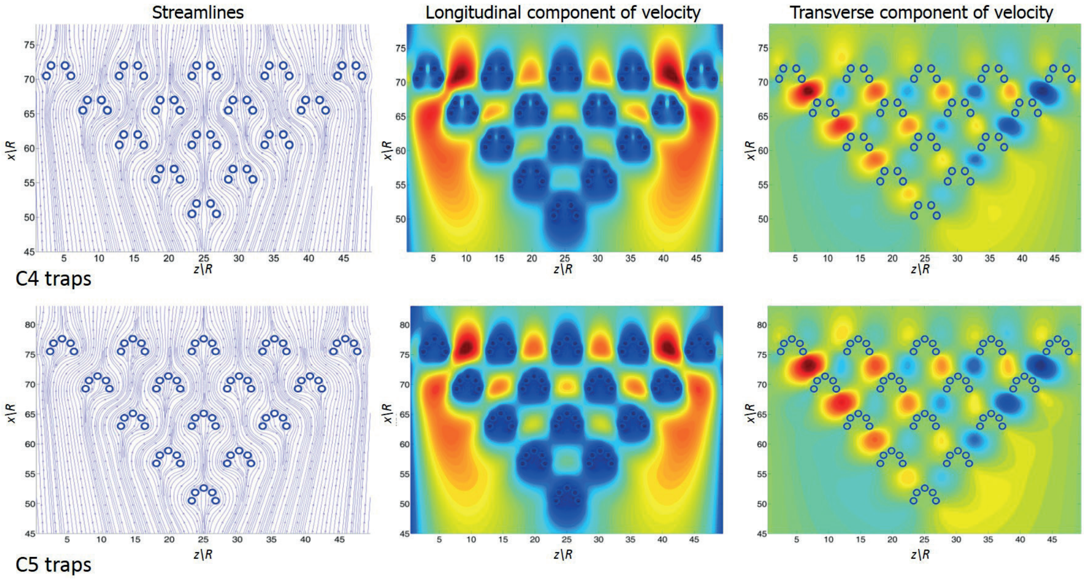

Fig. 2. Streamlines, longitudinal, and transverse components of viscous fluid flow velocity around the triangular array of traps

According to the figures, it can be seen that the greatest velocity of the fluid flow is observed near the walls of the microchannel. The cylindrical element located in the center of the C5 trap creates additional hydrodynamic resistance. This affects the velocity of the fluid flow. That is, the fluid flow velocity is minimal in the center of the C5 trap. This affects the trapping of droplets as they flow in the carrier fluid.

The next configuration consists of 22 hydrodynamic traps located in five rows across the fluid flow in a staggered pattern. The distance between trap rows was also $d_x = 2 \cdot L_{trap_x}$. Fig. 3 shows the streamlines, longitudinal and transverse components of the fluid flow velocity around the trap array, arranged in a chess order.

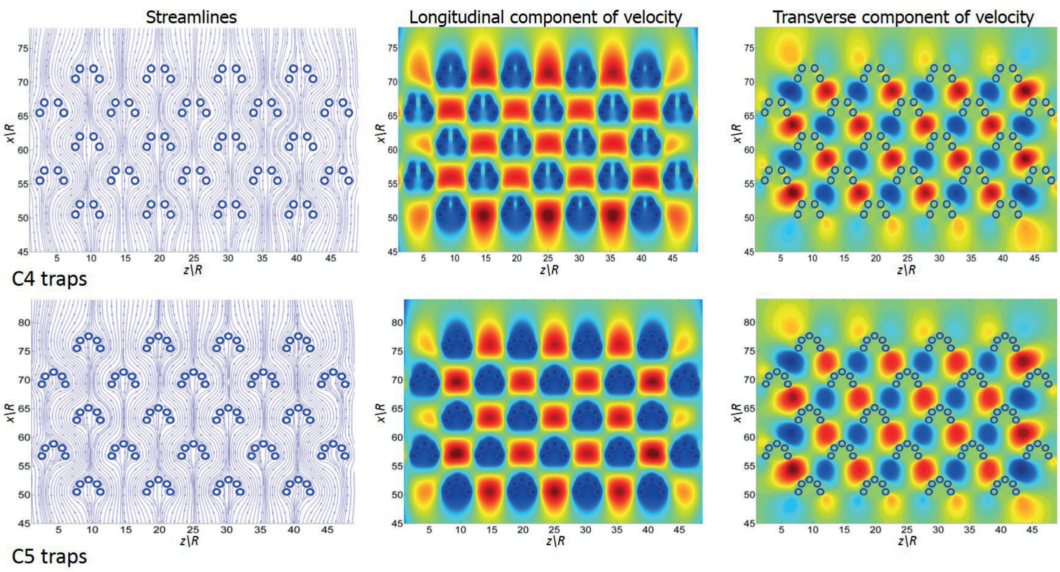

Fig. 3. Streamlines, longitudinal, and transverse components of viscous fluid flow velocity around the chess array of traps

Dispersed particles dynamics in microchannel with hydrodynamic traps. To study droplet dynamics in viscous fluid flow around hydrodynamic traps, droplets of different sizes were considered. The drop diameter ranged from $a = 0.5 \cdot d$ to $a = 1.5 \cdot d$, the distance between the drop centers along the Oz axis was $5 \cdot d$. The ratio of the droplet viscosity to the carrier fluid viscosity was $\lambda = \mu_2/\mu_1 = 10$.

There were $N = 642$ points or $N_\Delta = 1280$ triangular elements on each droplet surface. The total computational domain was covered by a triangular mesh consisting of $N_\Delta = 367800$ elements for a triangular traps arrangement and $N_\Delta = 427440$ for a chess arrangement. Thus, at each time step, the system of linear algebraic equations with more than 10^6 unknowns was solved on a workstation equipped with two Intel Xeon 5660 and one NVIDIA Tesla K20.

Initially, droplets have a spherical shape and are arranged in one row. After some simulation time in the flow, the drops are deformed and fixed in C-shaped hydrodynamic traps, moving according to the flow streamlines, or pass through the gaps between the cylindrical elements due to a change in their shape caused by deformation.

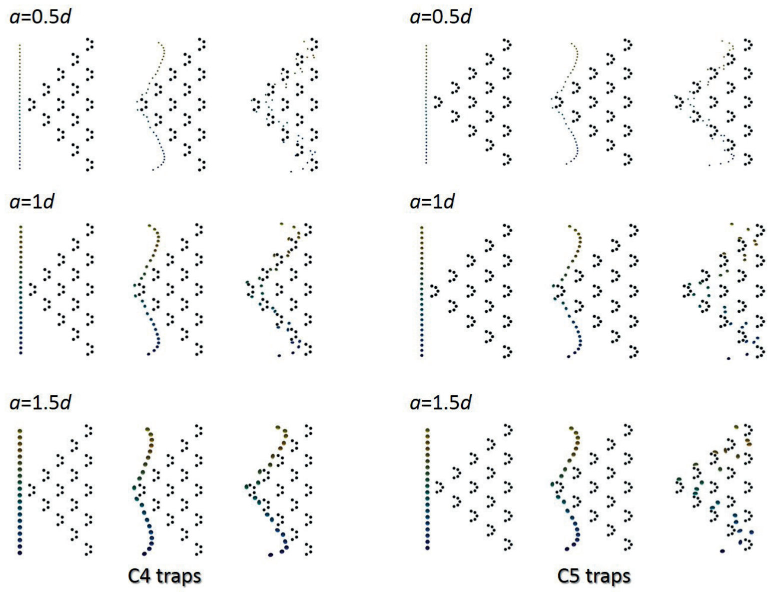

Fig. 4. Trapping of droplets of different radii (triangular array of traps) at non-dimensional time instants $t = 0$, $t = 15$, $t = 30$ (from left to right)

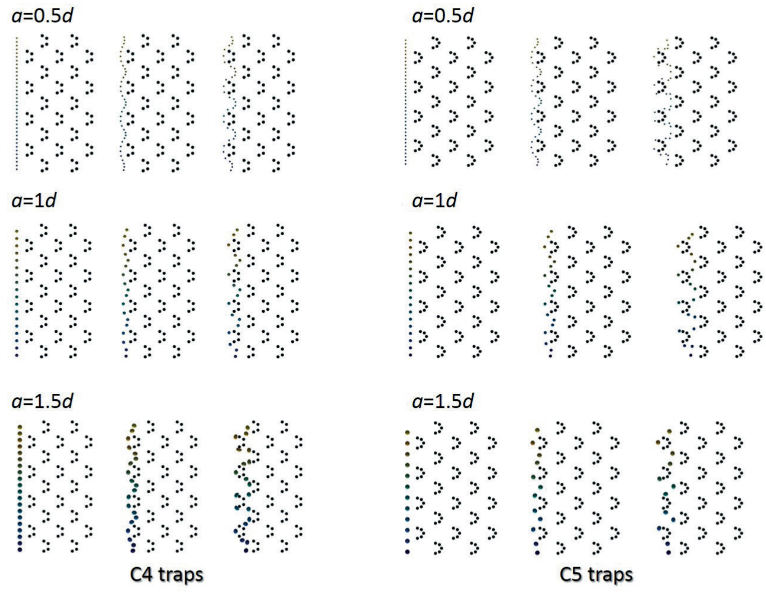

Fig. 5. Trapping of droplets of different radii (chess array of traps) at non-dimensional time instants $t = 0$, $t = 15$, $t = 30$ from left to right)

Fig. 4 shows the dynamics of droplets in a microchannel with C4 and C5 hydrodynamic traps arranged in the form of a triangle. The spatial arrangement of droplets of different radii relative to hydrodynamic traps at the time moments $t = 0$, $t = 15$, $t = 30$ is shown. Note that these computations are performed for the non-dimensional time $t = t_{non\text{-}\mathrm{dim}} = \gamma t_{\mathrm{dim}} / (\mu_1 a)$ Fig. 5 demonstrates the dynamics of trapping of deformable droplets of different radii by hydrodynamic traps arranged in a chess order at the same moments of time.

Calculation results on Fig. 4 and Fig. 5 show that droplets move faster in the case of a triangular trap arrangement, because the total hydrodynamic resistance of the channel with a trap section in the triangular case is lower than for a chess arrangement of the traps. In addition, due to significant hydrodynamic resistance, the particles tend to flow around the traps in the main liquid flow, rather than flowing into the trap. Thus, the chess arrangement of the traps is preferable because the traps in each successive row are located in the area of maximum flow velocities. The efficiency of droplet capture also depends significantly on the particle size and deformability. Larger droplets are trapped faster compared to smaller ones. The trapping of deformable particles is faster in case of the C4 trap than in case of the C5 trap.

Conclusion

The numerical approach based on the accelerated boundary element method has been applied to study the dynamics of deformable inclusions in microchannels with hydrodynamics traps in three-dimensional case. The streamlines and components of liquid flow velocity in a flat microchannel of rectangular cross section around the traps of two configurations (C4 and C5, arranged in chess order and in the form of a triangle) were obtained. The results of the simulation of the dynamics of deformable droplets of different radii in the microchannel with hydrodynamic traps have been obtained. It is revealed that with each successive row in the trap array, the efficiency of trapping of deformable droplets increases.

The results showed that the velocity components change significantly with increasing distance between the traps, which affects the dynamics of particles in the considered segment of the microchannel. From the obtained flow patterns, it can be concluded that the capture efficiency of particles with a larger distance between the traps will be higher. It is shown that for qualitative fixation of droplets, it is necessary to select the optimal size and geometry of traps, taking into account the deformability of droplets.

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