# The analysis of fluid discretization and its impact on elastic object immersed in fluid*

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**Abstract:** In our simulation model of fluid flow we have investigated the influence of fluid discretization on the simulation results. Proper discretization of fluid and objects is very important for quick and correct results. Coarser spatial grid for fluid discretization causes inaccuracies in simulation results. These inaccuracies can be partly corrected by change of the simulation settings. The size of spatial step of fluid discretization greatly affects computational time, especially in case with fewer objects in simulation box.

## 1 Introduction

In our research group, we develop a simulation model of blood flow in microfluidic devices. The model is implemented in the open source software ESPResSo as Object-in-fluid framework [1]. It allows us to simulate the blood. It is modeled as fluid (blood plasma) with objects (mainly red blood cell) immersed in it. The velocity profile of fluid is calculated by the lattice-Boltzmann method [2] and deformation and movement of elastic objects are calculated by our model described in [3]. The shape of objects is described by triangulation of their surface. The model does not contain any randomness.

Correct discretization of fluid and object in simulation model is very important for computational time and accuracy of results. In section 2, we discuss the influence of fluid discretization on the behaviour of elastic object. Coarser spatial grid causes inaccuracies and they can be partly corrected by changing the simulation settings, as

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we describe in section 3. In section 4, we analyze dependence of fluid discretization on the computational complexity. The influence of density of blood on computational time is presented in the last part of this paper.

# 2 Behaviour of fluid flow and objects in different spatial grids

We investigate influences of different fluid discretizations on the behaviour of fluid flow and objects. Especially, we compare two spatial grids with $1\mu m$ step and $2\mu m$ step. At the beginning the only one simple basic test was performed. We designed the simulation box $30\mu m \times 30\mu m \times 18\mu m$ with periodic boundaries along the $x$-axis and $y$-axis with solid walls on the top and on the bottom. A red blood cell was seeded in the center of the channel in $y$ and $z$ directions as we see in Fig. 1, 2. The flow direction was along the x-axis. In the lattice-Boltzmann method, we use an external force per unit of volume to simulate the pressure drop. During the simulation, we have recorded three quantities: Volumetric flow rate between the walls and velocities of horizontally and vertically seeded cell.

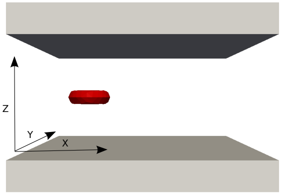

Figure 1: The design of the simulation box with horizontally seeded of cell.

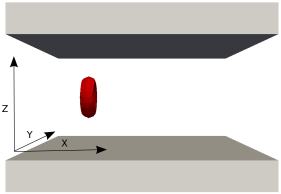

Figure 2: The design of the simulation box with vertically seeded of cell.

Table 1: The simulation results of the channel with width $18\mu m$ and external force $0.01\ nN$.

| | grid 1 | grid 2 | $\frac{\text{grid 1}}{\text{grid 2}}$ |
|---|---|---|---|
| volumetric flow rate $[\frac{\mu m^3}{\mu s}]$ | 82.110 | 67.680 | 1.213 |
| velocity vertical $[\frac{\mu m}{\mu s}]$ | 0.227 | 0.196 | 1.162 |
| velocity horizontal $[\frac{\mu m}{\mu s}]$ | 0.237 | 0.206 | 1.151 |

As steady state, a Poiseuille flow [4] develops in our simulation box. The velocity in the middle between walls is the greatest and the velocity at the walls equals zero.

Lattice-Boltzmann method calculates the velocity in the fixed vertexes of grid [5]. If we use a spatial grid with $2\mu m$ step, it causes inaccuracies in our model.

Tab. 1 shows a comparison of recorded values for spatial grids with $1\mu m$ step and $2\mu m$ step. There are differences between results in these two simulation setups. The recorded values are smaller in case of spatial step $2\mu m$ than in case of spatial step $1\mu m$. This is caused by discretization of the flow. The flow with finer spatial discretization describes parabolic shape more precisely than the flow with coarser discretization. The illustration of this problem is depicted in Fig. 3.

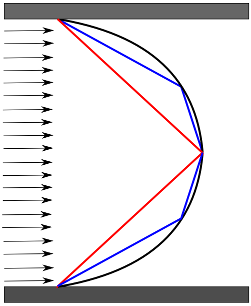

Figure 3: An illustration of the discretization coarse-graining. Black line represents the real velocities of fluid in channel with walls on the top and on the bottom. The blue line and the red line represent differences for two fluid discretization.

The ratios $\frac{\text{grid 1}}{\text{grid 2}}$ in Tab. 1 present differences between two different fluid discretizations. These ratios are different for each recorded parameter.

Next, we investigated values of these ratios for different widths of the channel and for different external forces. We see the values of ratios rounded to the third decimal place for channel width $18\mu m$ and $24\mu m$ and for external force $0.01\ nN$ and $0.02\ nN$ in Tab. 2. Each ratio decreases with increased width of channel. Different external forces do not influence it.

Table 2: The ratios of setups with spatial grid with $1\mu m$ step and $2\mu m$ step for volumetric flow rate, velocity of vertically seeded cell and velocity of horizontally seeded cell.

| | grid 1 / grid 2 | | | |
|---|---|---|---|---|
| | width $18\mu m$ | | width $24\mu m$ | |
| external force | $0.01\ nN$ | $0.02\ nN$ | $0.01\ nN$ | $0.02\ nN$ |
| volumetric flow rate $[\frac{\mu m^3}{\mu s}]$ | 1.213 | 1.213 | 1.150 | 1.150 |
| velocity vertical $[\frac{\mu m}{\mu s}]$ | 1.162 | 1.160 | 1.108 | 1.108 |
| velocity horizontal $[\frac{\mu m}{\mu s}]$ | 1.151 | 1.151 | 1.107 | 1.107 |

# 3 Correction of inaccuracies caused by discretization of fluid

The problem caused by different discretizations of fluid could be corrected by changing the external force. We run simulations with greater external force for spatial grid with step 2 $\mu m$. It was set as ratio from Tab. 1 multiplied by the original external force $0.01$ $nN$. This was done for volumetric flow rate and velocities of horizontally and vertically seeded cells. Tab. 3 shows the change of external force for different discretizations of fluid corrected with respect to the chosen. The main problem of this kind of correction is that there is a different ratio for different observations.

Table 3: The simulation results of the channel with width $18 \mu m$ with external force $0.01$ $nN$. Volumetric flow rate, velocity of vertical cell and velocity of horizontal cell were recorded. The ratio is the proportion between the values of grid 1 and values grid 2.

| | grid 1 | grid 2 |
|---|---|---|
| external force | $0.01000\ nN$ | $0.01213\ nN$ |
| volumetric flow rate $[\frac{\mu m^3}{\mu s}]$ | 82.110 | 82.080 |
| external force | $0.01000\ nN$ | $0.01162\ nN$ |
| velocity vertical $[\frac{\mu m}{\mu s}]$ | 0.227 | 0.228 |
| external force | $0.01000\ nN$ | $0.01151\ nN$ |
| velocity horizontal $[\frac{\mu m}{\mu s}]$ | 0.237 | 0.237 |

The basic rule for simulation with different spatial grid is to keep the same volumetric flow rate. It is simple, when we know ratio between their volumetric flow rate. Coarser spatial discretization causes inaccuracies which we see in the ratios of velocities. This problem may be caused by changing of ratio between average length of object edge and spatial step of fluid discretization and will be the subject of further research.

# 4 Computational complexity

In this section we show the influence of fluid discretization on the computational time. We have designed two experimental simulations. The first one is a simple periodic simulation box with dimensions $30 \mu m \times 30 \mu m \times 30 \mu m$ without any obstacles and walls. The second one is the same simple box with wall on the top and on the bottom. The size of the box was chosen as the smallest simulation part used for parallel computing in our model. We have chosen five different sizes of spatial step ($0.5 \mu m$, $1 \mu m$, $1.5 \mu m$, $2 \mu m$, $3 \mu m$) and six different cell counts(0, 1, 5, 10, 20, 40). For the each combination of design of the box, discretization step and number

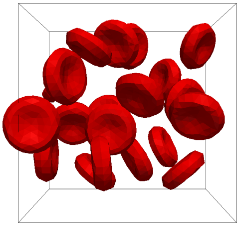

Figure 4: The design of simulation box without walls with 20 cells.

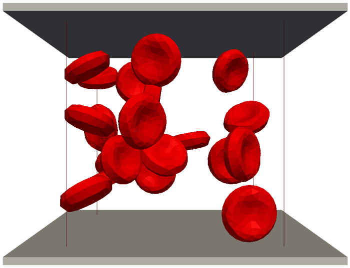

Figure 5: The design of simulation box with walls with 20 cells.

of cells, 10 simulations were performed with random seedings of cells. The computational time was recorded and averaged over each set of simulations. We see the design of boxes with seeded 20 cells in Fig. 4 and 5

Table 4: Computational time in seconds for the simulation box with walls.

| **Grid** | **Number of cells** | | | | | |
|---|---|---|---|---|---|---|
| | **0** | **1** | **5** | **10** | **20** | **40** |
| **0.5** | 9.71 | 10.15 | 10.62 | 11.41 | 13.07 | 17.94 |
| **1** | 1.35 | 1.68 | 2.14 | 2.79 | 4.45 | 9.15 |
| **1.5** | 0.40 | 0.78 | 1.22 | 1.88 | 3.51 | 8.15 |
| **2** | 0.18 | 0.54 | 0.98 | 1.63 | 3.27 | 7.91 |
| **3** | 0.06 | 0.40 | 0.83 | 1.47 | 3.10 | 7.71 |

Table 5: Computational time in seconds for the simulation box without walls.

| **Grid** | **Number of cells** | | | | | |
|---|---|---|---|---|---|---|
| | **0** | **1** | **5** | **10** | **20** | **40** |
| **0.5** | 9.97 | 10.55 | 10.95 | 11.78 | 13.21 | 17.77 |
| **1** | 1.28 | 1.42 | 2.08 | 2.68 | 4.19 | 8.64 |
| **1.5** | 0.34 | 0.43 | 1.10 | 1.66 | 3.12 | 7.47 |
| **2** | 0.14 | 0.22 | 0.88 | 1.44 | 2.89 | 7.23 |
| **3** | 0.05 | 0.12 | 0.75 | 1.31 | 2.75 | 7.05 |

These simulations ran for 2500 time steps and were performed on one processor (Intel(R) Xeon(R) CPU E5-2609, 2.40GHz). The average time of the simulation is in Tab. 6 and 7. These tables show a little bit longer durations for simulations with walls, because collisions with it have to be computed. Simulations with spatial step $0.5\mu m$ are exceptions, because computation of fluid has a major effect and computation of collision with walls has negligible impact.

The dependence of computational complexity on the hematocrit is showed in Fig. 6 and 7. Here we see speed-up of computational time in percent for the spatial grid with step $1.5\mu m$, $2\mu m$ and $3\mu m$ compared to spatial grid with $1\mu m$ step.

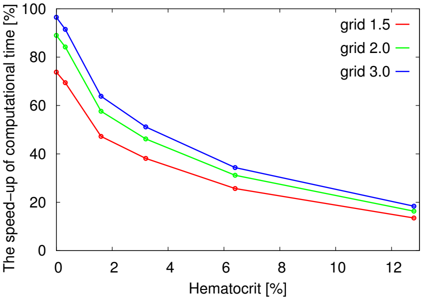

Figure 6: The speed-up of computational time in percent for simulation box without walls.

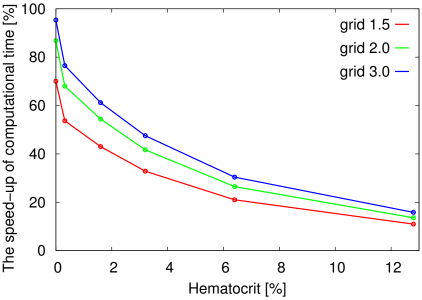

Figure 7: The speed-up of computational time in percent for simulation box with walls.

## 5 Conclusion

We have analyzed the behaviour of fluid discretization by spatial grid with step $1\mu m$ and step $2\mu m$. We have investigated three parameters: Volumetric flow rate and velocities of vertically and horizontally seeded cell. The measured parameters were smaller in case with larger spatial step than in case with smaller spatial step. In simulation with different spatial grids the most important thing is to keep the volumetric flow rate constant. We presented a way to modify external force to obtain the same volumetric flow rate. Large size of spatial step may cause inaccuracies which we saw in different ratios for our three analyzed parameters. The problem of velocities of cell can be caused by coefficient of immersed boundary method. It depends on ratio between average length of object edge and spatial step of fluid discretization but it is a topic of further research.

In the second section of this work we have presented the dependence of spatial step on the computational time. We have performed a simulation test with different values of hematocrit. The speed-up of computational time decreases with hematocrit increasing. In this case, the computation of fluid has only a minor effect. The main part of computational time is used for the computation of objects.

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