Comparison of Different Formulas for Local Area Conservation Modulus in Spring Network Models

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***Abstract*—Modeling of elastic objects in homogeneous fluid flow can be interesting for various aims or purposes. In our case we are interested in red blood cells in flow of blood. There are five elastic moduli that model elastic behavior of objects in our model. The exact formulas for these moduli are not clear, because there are more arguments for and against different formulas. In this article we investigate three different formulas describing the elastic modulus for conservation of local area.**

***Keywords:*local area force, elastic object, object in fluid, ESPResSo**

I. Introduction

These days many scientists investigate motion of blood. Understanding physical, biological and chemical properties of blood is important for successful treatment of many diseases. Some authors consider the blood to be homogeneous fluid without regard for particular cells. This is sufficient for investigation of the impact of blood flow on vein walls. Other authors consider the blood as homogeneous fluid with elastic objects, where each object is represented by one particle. When using this type of modeling, one can not sufficiently model cell deformations. Our Cell-in-fluid research group is interested in simulations of microfluidic devices, which are used for capturing specific cells from sample of fluid. For these simulations we need model of fluid with immersed elastic objects in solid channel. For brief introduction, see [1].

II. Model

Our research group implemented the elastic moduli of immersed objects [2] as an extension of software package ESPResSo [3]. The idea of the model can be divided into three parts.

First, we have homogeneous fluid in discrete virtual points in fixed cubic mesh. The Lattice-Bolzmann method is used for modeling of fluid flow in channel with obstacles.

Second, we have elastic object with nodes in triangulation mesh on the surface of objects. Elastic behavior is due to five elastic moduli. Each node is connected in triangulation mesh with several other nodes by springs. The network of nodes covers only the surface of the object. There are acting forces in each node related to elastic moduli. Magnitude of forces depends on changes in distance between nodes, angles between neighboring triangles, areas of triangles and global area and volume of object. For each type of force we have specific elastic coefficient. The direction of forces depends on the type of force.

Fourth, we have immersed boundary method to model interaction between objects and fluid.

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III. Theoretical Analysis of Local Area Conservation Modulus

In this article we are specifically interested in local area conservation modulus. In this modulus we defined forces, which act against changes of triangle area.

In our model the acting forces are in direction from vertices towards into centroid, see Fig. 1. If triangle area increases, forces in each vertex of the triangle act towards its centroid. If area of triangle decreases, forces act in opposite direction, see Fig.1.

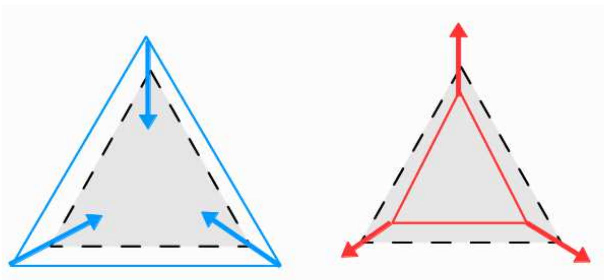

Fig. 1: Forces when triangle area increases (blue arrows) and decreases (red arrows). The gray triangle is original triangle area.

The open question is what is the best formula for local area force representation. In early attempts, we used formula from [4] in our model. There both stretching force and local area force are normalized. However, as presented in [5], we discovered that if we stretch the sphere using normalized stretching force, the experiments result in larger differences between results of stretching sphere with different number of nodes at surface than the experiments with non-normalized stretching force.

We assumed that in case of local area forces, we could obtain the same or similar results. We were looking for the better formula than normalized formula for local area forces. Our aim was to decrease dependence of results on density of mesh - number of nodes on the surface.

We compare three different formulas in basic approach to normalization - without normalization (non-normalized), normalization with representative length (length-normalized) and full normalization with representative area (area-normalized). For representative length we choose square root from original triangle area and for representative area the original triangle area. In each formula, the force acts from vertex to the triangle centroid. For simplicity we describe the forces without direction, only their magnitudes.

$$F_{al} = k_{al}\frac{(S_{ABC} - S^0_{ABC})}{S^0_{ABC}}, \quad (1)$$

$$F_{al} = k_{al}\frac{(S_{ABC} - S^0_{ABC})}{\sqrt{S^0_{ABC}}}, \quad (2)$$

$$F_{al} = k_{al}(S_{ABC} - S^0_{ABC}), \quad (3)$$

where k_{al} is elastic coefficient of local area, S_{ABC} is current area of triangle ABC and S^0_{ABC} is original area this triangle.

IV. Simulations

To analyze local area force, we performed several simulations. We modified the formula for local area force according to equations (1), (2) and (3). We wanted to investigate local area conservation modulus, so we needed to perform such experiment, in which it is sufficient to consider only local area forces. Example experiment of this type is radial stretching of the sphere. Here we applied forces in each node of triangulation on the surface and the forces act outward from middle of the sphere. In our experiments we assumed a sphere with initial radius of $4\mu m$. The sphere was located in a closed box with stationary fluid. The fluid was present only for damping of motion. At the beginning we chose a reference mesh with 1524 nodes and non-normalized formula. Next we found magnitude of applied forces increasing the sphere's radius by approximately 10%. Then we calculated product magnitude of force, which was applied in each node and number of mesh nodes. This product was taken constant for other meshes with different number of nodes, specifically for meshes with 500, 601, 727, 879, 1007, 1182, 1905, 2137, 2301 and 2600 nodes. When performing the experiment we applied the force to each node and every 100 integration steps we looked at the current radius of the sphere. For reference mesh we performed long simulation to finding relaxed state. Then we determined threshold difference between two consecutive measurements of radius to stop simulation. The value was determined experimentally to be 0.0075% of the original radius. Then we compared radii at the end of simulation for different meshes. The results for all three types of normalization are in Fig. 2. The common point of three lines in chart are results for 1524 nodes mesh. We chose acting forces to equal results for each types of normalization from reference mesh. As presented, deviations for area-normalized forces (red line, square symbol) are the largest, then next are for non-normalized forces (blue line, triangle symbol) and the smallest are for length-normalized forces (yellow line, circle symbol). When we calculated errors like sum of squares of relative deviations for all meshes for each normalization, we found that error was smaller by one order of magnitude in case of length-normalized forces compared to error for area-normalized or non-normalized forces.

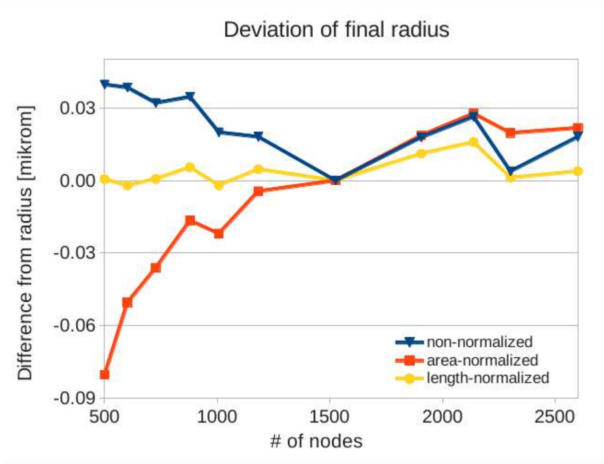

Fig. 2: Deviation of final radius for different number of mesh nodes, using area-normalized (red line, square symbols), length-normalized (yellow line, circle symbol) and non-normalized (blue line, triangle symbol) local area forces

In Fig. 3 we see a stretched sphere at three different time steps. The first is at the beginning of simulation, the second is in the middle and the last is in the end of simulation. The colors from blue to red correspond to $\mathcal{F}$ metrics, which is defined in [6]. In this special case, the colors correspond to magnitude of resulting local area forces. These are calculated as the sum of all acting local area forces in each node. Each node represents the vertex of more than one triangle. In the figure color scale is from minimum value from blue and to maximum value to red. The magnitude of local area forces are continually rising. So there are too large differences between forces acting at the beginning and at the end of simulation. Therefore the first two sphere are only blue and on the last sphere we see nonrandom distributions of local area forces. These shown results are for half-normalized forces. For other two types of normalization we obtained similar figures. The difference in simulations was in length of simulations, it means in number of steps needed to achieve relaxed state. For example, for normalized forces the simulations stopped after roughly 1000-2000 steps, for half-normalized forces they stopped after roughly 2000-4500 steps, and for non-normalized forces they stopped after roughly 5000-15000 steps. It is in line with our expectations, because acting forces between nodes in area-normalized case are larger than in length-normalized case and these are larger than those in non-normalized case. It is, of course, because the area of triangle is smaller then 1, see the eq. (1), (2) and (3).

V. Conclusion

In this work we have shown that if we increase number of nodes on surface in triangulation, the effect of acting forces is the smallest for length-normalized type of forces from the

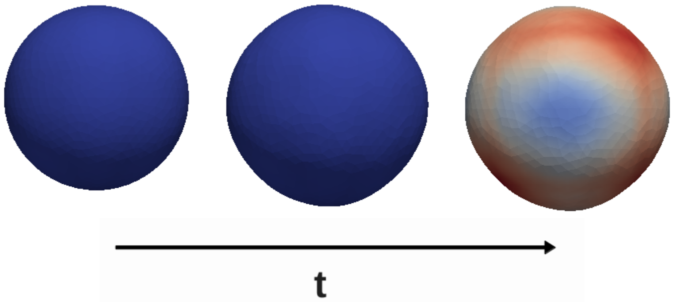

Fig. 3: Figures of spheres in experiment with length-normalized local area forces in three different time steps, from left to right. The colors correspond to magnitude of acting forces in each node from blue the smallest to red the largest. The figures were created in [7]

types above. In other words, when using this formula the dependence of simulation experiments on mesh density (on number of nodes on the surface) is the smallest from the three chosen types of local area forces. Second, the dimension of elastic coefficient k_{al} is $[N/m]$, what corresponds to physical expectation.

One open question is, whether the square root of the original triangle area is the best choice or whether we can find a better representative length.

The second open question is, if we use eq. (2) we get the same local area forces for each vertex of a triangle. We can accept this in case of equilateral triangle. Nevertheless, when stretching a triangle results in non-equilateral triangle, the distances between centroid and each vertex are different. So we should involve this difference to the formula of local area forces.

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