SIMULATION OF FLUID MOTION IN COMPLEX CLOSED SURFACES USING A LATTICE BOLTZMANN MODEL

V. Kuzmych, M. Novotarskyi

CFD (computational fluid dynamics) modeling is used to determine the distribution of pressure, velocity, and other movement parameters of liquids or gases. Simulation of a fluid flow in a complex closed surface has become demandable in many scientific, medical, and industrial areas. The lattice Boltzmann model is an efficient numerical scheme for modeling fluid flows. In this paper, we investigate nonstationary hydrodynamic processes in closed surfaces using the Boltzmann lattice model to simulate fluid flow in the human stomach.

Keywords: *hydrodynamics, lattice Boltzmann model, simulation*

Introduction

Simulations are widely used in several advanced engineering studies. A suitable numerical method is crucial to obtain accurate results in fields such as fluid flow, thermal transfer, or mechanical engineering.

Today, it is necessary to use an adapted numerical method in complex systems and fields that would be too expensive, dangerous, difficult, or even impossible to study by direct experimentation. Gastrointestinal surgery is a field of study where natural experiments or measurement of various properties of objects or treatment is costly, complex, and unsafe in some cases.

Computational fluid dynamics (CFD) is a branch of hydromechanics that uses numerical analysis and data structures to analyze and solve problems related to the movement of fluids. Computers are used to perform the calculations required to simulate the free flow of a fluid and the interaction of a fluid (liquids and gases) with surfaces defined by boundary conditions. Large and complex problems can be solved with the use of high-speed supercomputers. Modern software provides the accuracy and speed of modeling complex scenarios with transonic or turbulent flows. The first experimental verification of such software is carried out using a wind tunnel, and the final confirmation is carried out during full-scale tests, for example, flight tests.

The gastrointestinal tract is a system such that the health of the whole organism depends on its state. It is known that a disturbance in the balance of proteins, fats, carbohydrates, vitamins, and microelements causes many diseases. All those substances enter into an organism with food. But even the most helpful food products do not become a source of health if the functioning of the gastroenteric tract is violated. In this case, the necessary substances are not assimilated. Therefore, it is essential to pay significant attention to the support of proper functioning of the gastroenteric tract. This problem acquires a particular meaning when dealing with diseases requiring surgical intervention. Among such conditions, the critical place is occupied by the oncologic diseases of parts of the gastroenteric tract, gunshot injuries of the peritoneal cavity, and other illnesses which require reconstruction-recovery operations.

Reconstructive surgery on the human digestive tract can cause negative consequences. These effects were manifested in the appearance of unwanted deformations, so-called "blind bags," which arose due to the formation of zones of high pressure after changes in the geometry of hollow objects of the digestive tract during reconstructive surgery. For this reason, developing a mathematical fluid flow model on the closed surface has become crucial in recent years.

Literature review

We developed the first series of in vitro systems to analyze human digestion [1, 2] at the beginning of the 1990s. Despite the sizeable amount of human and animal digestive tract data, conflicting results have been obtained [3]. The main limitation of this method is the difficulty of reproducing the geometry and motility of the digestive tract. Unfortunately, developing an in vitro system capable of accurately producing the fluid mechanical forces that promote digestion is complicated.

Singh et al. presented an advanced fluid dynamics program that offers a promising technique to characterize the mechanisms promoting digestion [4]. It is possible to use computational fluid dynamics for numerical simulation of the flow of gastrointestinal contents during digestion using knowledge of the motor response of the digestive tract and the physicochemical properties of luminal contents. Pal et al. initially attempted to simulate the gastric flow during digestion [5, 6]. Still, the computational effort required to reproduce the geometry and motility of the stomach prevented an excellent characterization of the system.

Such parameters play the reconstruction-recovery operations, a significant role in the pressure distribution and the field of velocities in the region under study. The mathematical models describing the motion of fluid under the action of peristaltic oscillations are represented most frequently by a system of equations that includes the Navier–Stokes equation and the equation of continuity of a flow [12]. Such an approach is sometimes called "top-down" technology. In this case, fundamental properties of the fluid are used to calculate specific physical parameters. The boundary-value problems, which are formed based on such a system of equations, require significant expenditures of computer time and computational resources for their solution.

Today, modeling fluid flow in a volume with closed-moving surfaces, such as the human digestive tract, requires significant computing resources. Using a probabilistic approach will reduce costs for determining the fluid velocity field. Therefore, this article investigates the possibility of using the Lattice Boltzmann Method (LBM) in fluid flow simulation inside biological objects.

LBM is one of the currently popular methods of computational fluid dynamics, which has been successfully applied to fluid flows through porous media [13], multiphase fluid flows [14], non-Newtonian particle flows [15], and even medical technology [16]. This method differs from traditional CFD methods, such as the finite element method (FEM) and the finite volume method (FVM), which aim to solve boundary value problems based on the Navier-Stokes equation numerically. The mentioned boundary value problem considers a continuous fluid flow. The fundamental difference of LBM is that, in this case, the fluid flow is considered as the movement of particles with elementary fluid volumes. These particles collide in the moving process, changing the parameters of the velocity vector under physical laws.

Our work is devoted to the application of LBM for the simulation of fluid flow processes on complex closed surfaces based on the experience obtained by comparing the properties of fluid flow in different closed complex geometries.

Methodology

The lattice Boltzmann method is a numerical method to solve the Boltzmann equation on a discrete lattice:

$$v \cdot \nabla_x f + F \cdot \nabla_p f + \frac{\partial f}{\partial t} = \hat{\Omega}(f), \tag{1}$$

where F – an external body force, ∇_x, ∇_p, is the gradient in position and momentum space, and $\hat{\Omega}(f)$ is the collision operator. The Boltzmann equation describes the dynamics of a fluid from a microscopic point of view: particles, each with velocities v_i, collide with a certain probability and exchange momentum among each other. For ideal collisions, total momentum and energy are conserved in the collisions. The Boltzmann equation expresses how the probability $f(x, v, t)$ of finding a particle with velocity v at a position x and at time t evolves with time.

Assuming $F = 0$, equation (1) will be next:

$$v \cdot \nabla_x f + \frac{\partial f}{\partial t} = \hat{\Omega}(f). \tag{2}$$

For the sake of simplicity, the collision operator is taken in the most frequently used form:

$$\hat{\Omega}(f) = \frac{1}{\tau}\left(f - f^{(eq)}\right). \tag{3}$$

In (3), τ is a constant defining the time scale, which is necessary for the establishment of local equilibrium, and $f^{(eq)}$ is the density distribution function (so-called Maxwell—Boltzmann distribution function).

Thus, we get the Bhatnagar-Gross-Krook-model (or BGK-model) [7]:

$$v \cdot \nabla_x f + \frac{\partial f}{\partial t} = \frac{1}{\tau}\left(f - f^{(eq)}\right). \quad (4)$$

We make discretization of this model in the space of velocities on a finite set of vectors $\{v_k\}$ with regard for the conservation laws [8]. As a result, we get the system composed of Q equations:

$$\frac{\partial f_k}{\partial t} + v_k \nabla f_k = \frac{1}{\tau}\left(f_k - f_k^{(eq)}\right), k = 0,1,2,\ldots,Q-1, \quad (5)$$

where $f_k(x,t) = f(x, v_k, t)$ is the density distribution function associated with the direction of a velocity vector v_k, $f_k^{(eq)}$ is the equilibrium density distribution function corresponding to the vector v_k.

We executed the full discretization of (5) with a time step of Δt and a spatial step of $\Delta x_k = v_k \Delta t$ [13], in order to simplify computer realization:

$$\frac{f_k(x_k + v_k\Delta t, t + \Delta t) - f_k(x_k + v_k\Delta t, t)}{\Delta t} + \\ + \frac{f_k(x_k + v_k\Delta t, t) - f_k(x_k, t)}{\Delta x_k} = \frac{-f_k(x_k, t) - f_k^{(eq)}(x_k, t)}{\tau}.$$

Setting $\Delta x_k = \Delta t = 1$, we get the Boltzmann lattice equation

$$f_k(x_k + v_k\Delta t, t + \Delta t) - f_k(x_k, t) = \frac{-1}{\tau}\left(f_k(x_k, t) - f_k^{(eq)}(x_k, t)\right), \quad (6)$$

where x_k is a point in the discretized physical space.

According to the BGK-model, Eq. (6) can be solved with the use of two steps.

1. Collision-related step:

$$\tilde{f_k}(x_k, t + \Delta t) = f_k(x_k, t) - \frac{1}{\tau}\left(f_k(x_k, t) - f_k^{(eq)}(x_k, t)\right) \quad (7)$$

2. Flow-related step:

$$f_k(x_k + v_k\Delta t, t + \Delta t) = \tilde{f_k}(x_k, t + \Delta t) \quad (8)$$

In (7) and (8), the distribution function $\tilde{f_k}$ describes a post-collisional state of the elementary volume of a fluid or the particle of a substance at the point of the discrete space x_k. In the BGK model, the collisions are considered as oscillations of elementary volumes of a fluid relative to the positions of local equilibrium.

The values of elements of the set $\{v_k\}$ are determined in view of the dimension of a model and the number of connected nodes forming the lattice basic element.

The mesoscopic and macroscopic levels of the modeling are connected by means of the following formulas:

$$\rho = \int_{-\infty}^{\infty} f(x, v, t)dv = \sum_{k=0}^{Q} f_i = \sum_{k=0}^{Q} f_k^{(eq)} \quad (9)$$

$$u = \frac{1}{\rho}\int_{-\infty}^{\infty} v \cdot f(x, v, t)dv = \frac{1}{\rho}\sum_{k=0}^{Q} v_k f_k \frac{1}{\rho}\sum_{k=0}^{Q} v_k f_k^{(eq)} \quad (10)$$

where u is the velocity vector of a flow in the fluid, and ρ is the mass density of a flow in the fluid.

Experiments

In order to achieve the practical significance of analysis of fluid flow properties in complex closed surfaces, we prepared two 3D models of the stomach in two different states – a normal state and an anastomosis state. We used Blender software [11] to construct these models. They are displayed in Fig 1-2.

To apply LBM we discretized each model into a square mesh with the size of $120 \times 78 \times 142$. Parameters of LBM itself are the following: $\Re = 1000$, $\rho = 1000$. We introduced boundary value in the top as a constant flow directed to the bottom, with a velocity equal to 0.1 m/s.

We choose the D3Q19 lattice scheme [10] due to its faster performance in comparison to larger schemes while maintaining acceptable accuracy. The velocity scheme with all v_k vectors is displayed in Fig. 3. This cubic lattice D3Q19 is defined by the following velocities:

$$v_0 = (0,0,0)$$
$$v_{1,2}, v_{3,4}, v_{5,6} = (\pm 1,0,0), (0,\pm 1,0), (0,0,\pm 1)$$

$$v_{7,\dots,10} = (\pm 1,\pm 1,0)$$
$$v_{11,\dots,14} = (\pm 1,0,\pm 1)$$
$$v_{15,\dots,18}, = (0,\pm 1,\pm 1)$$

All experiments were performed on a PC with Ryzen 7 5800X CPU and 32 GB RAM, using the Pylbm python library [9].

We measured the magnitude of fluid velocity field distribution at modeling times t = 2.5 sec and t = 5.0 sec. Fig.4-5 show the distribution for the normal state, fig. 6-7 shows the anastomosis state of the human stomach.

Results

Results demonstrated higher velocity magnitude near the bottom part of the stomach in case of anastomosis than in the normal state. In addition, the anastomosis model shows the increased fluid velocity in the “blind bag” under the stomach. In real situations, it can cause the development of negative consequences.

We investigated the relationship between average velocity inside the stomach area and modeling time in the states mentioned above. Fig.8 shows this relationship. During all modeling periods, the average velocity in the normal state is higher than in anastomosis. Due to this outcome and previously mentioned results, we can conclude that the velocity field in the anastomosis state is irregular in comparison to the normal state of the stomach.

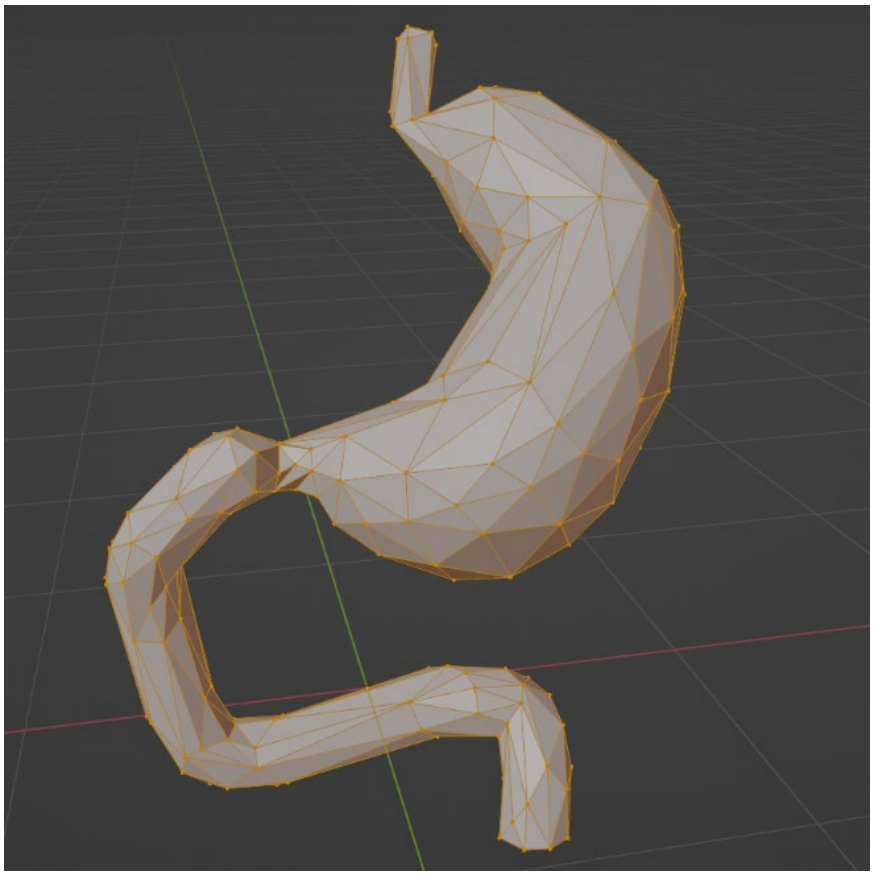

Fig.1. Normal stomach

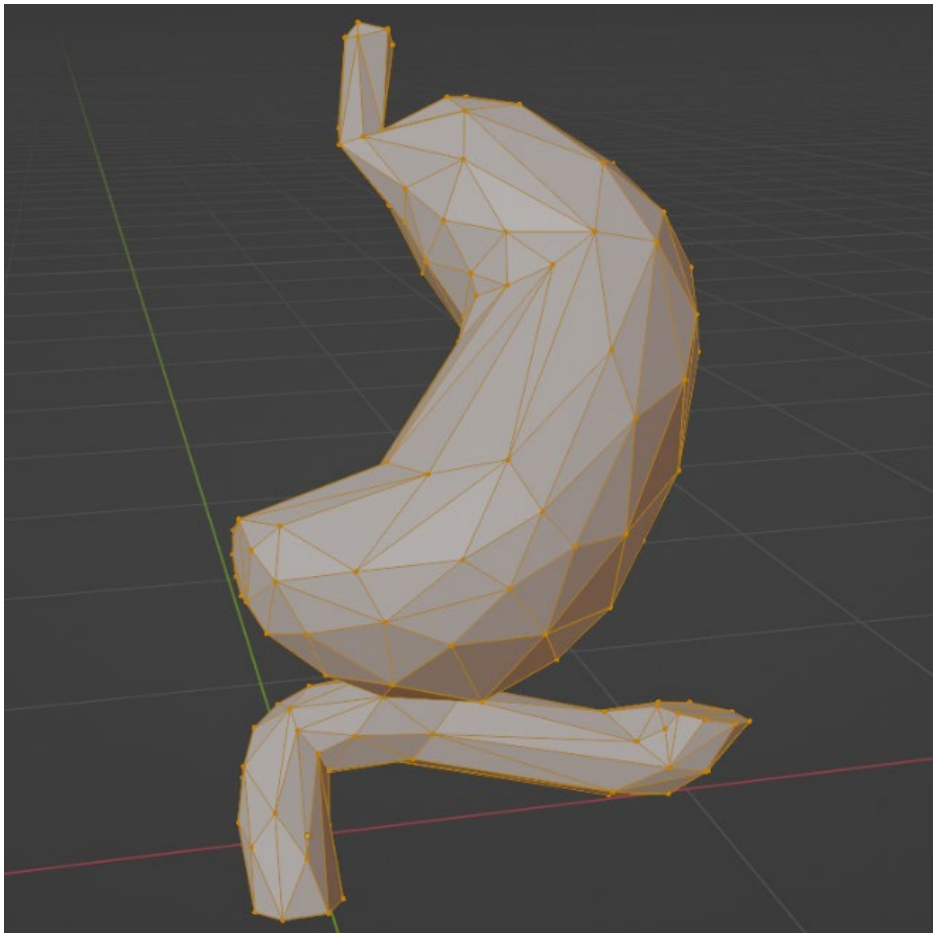

Fig.2. Anastomosis state of the stomach

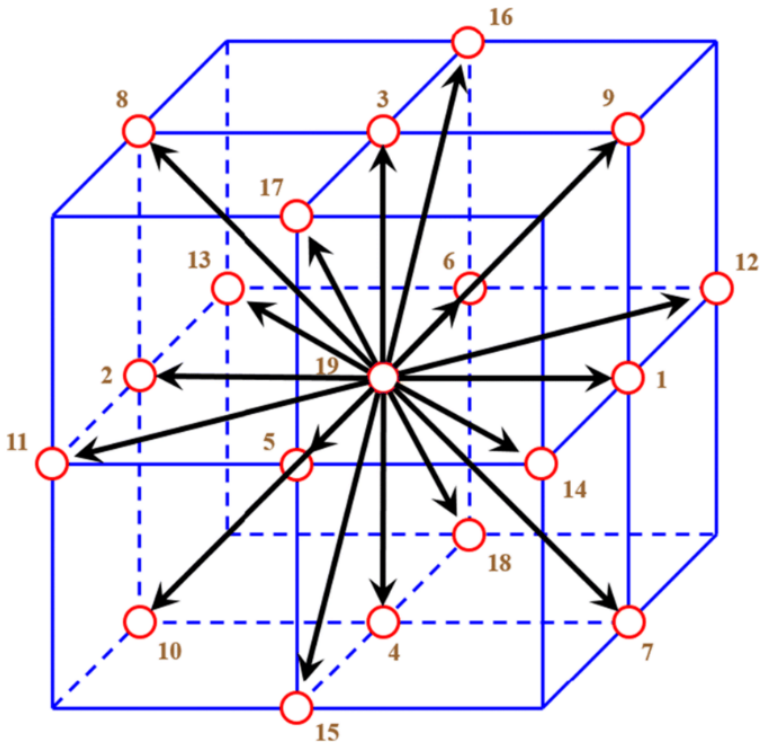

Fig.3. D3Q19 scheme

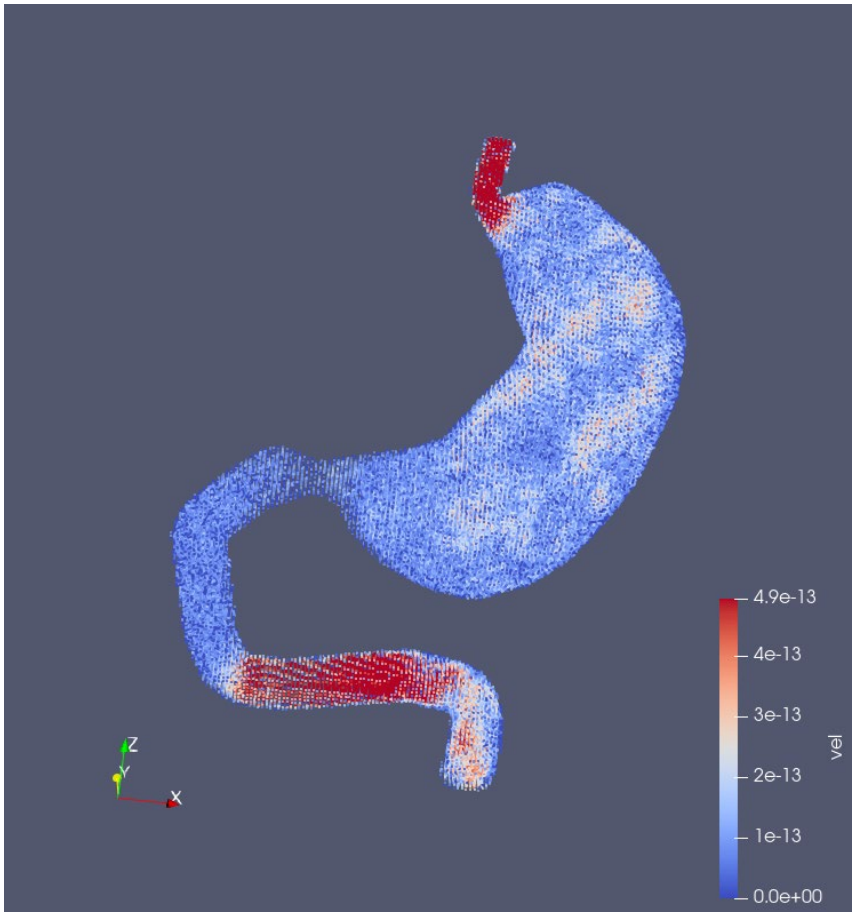

Fig 4. Velocity field distribution in a normal state at time 2.5 sec

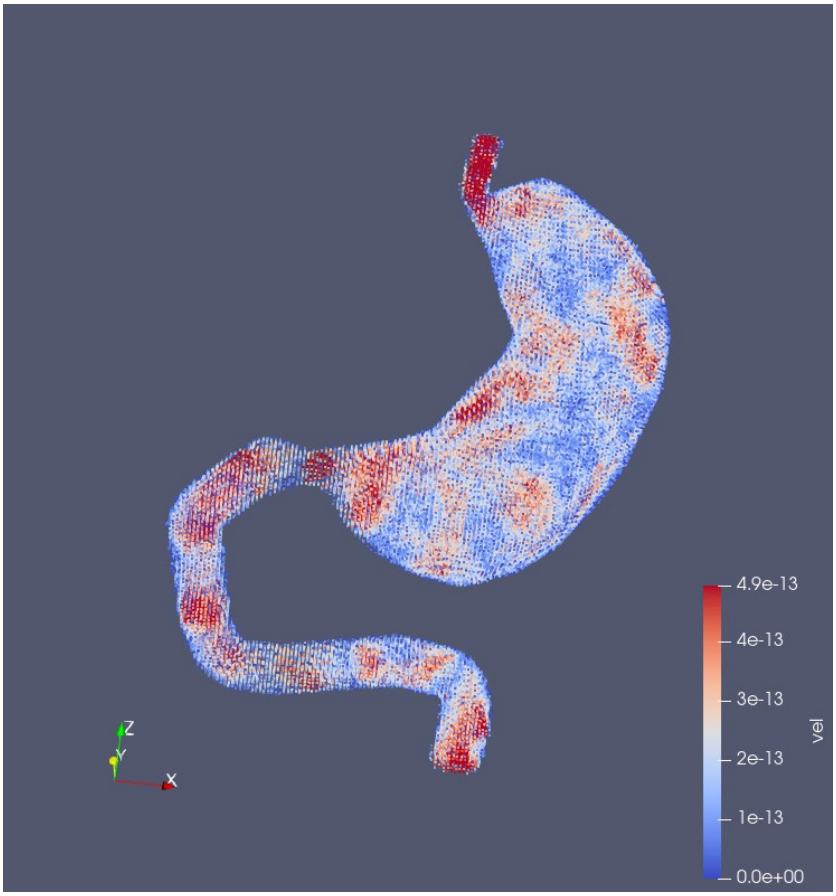

Fig 5. Velocity field distribution in a normal state at time 5.0 sec

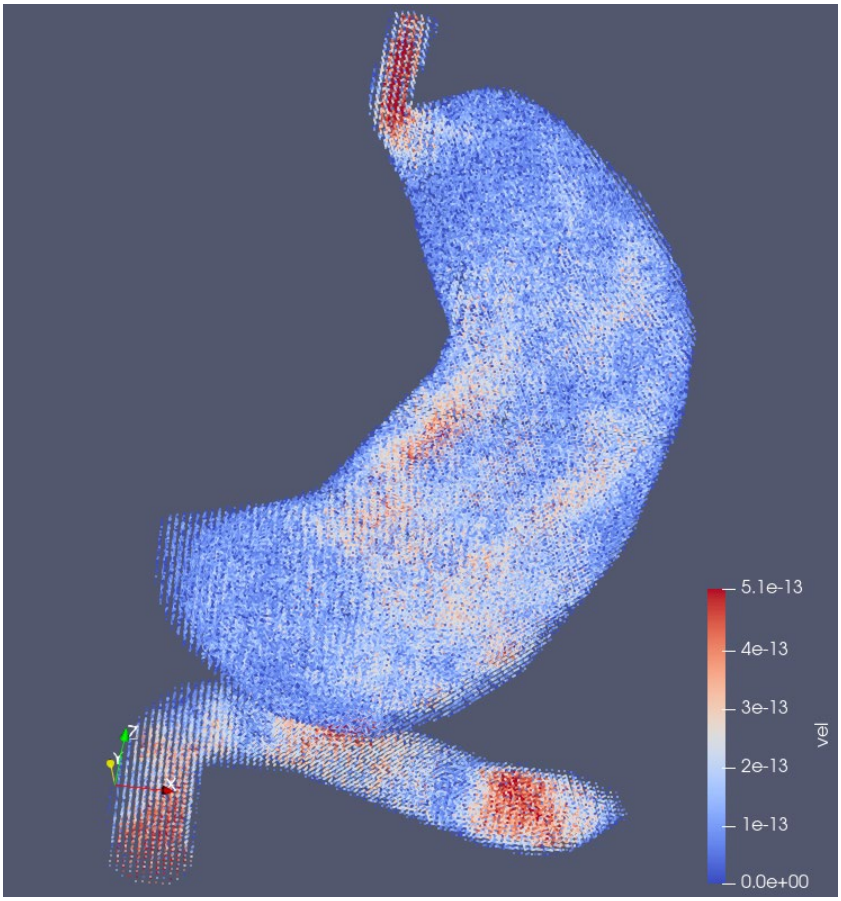

Fig 6. Velocity field distribution in anastomosis state at time 2.5 sec

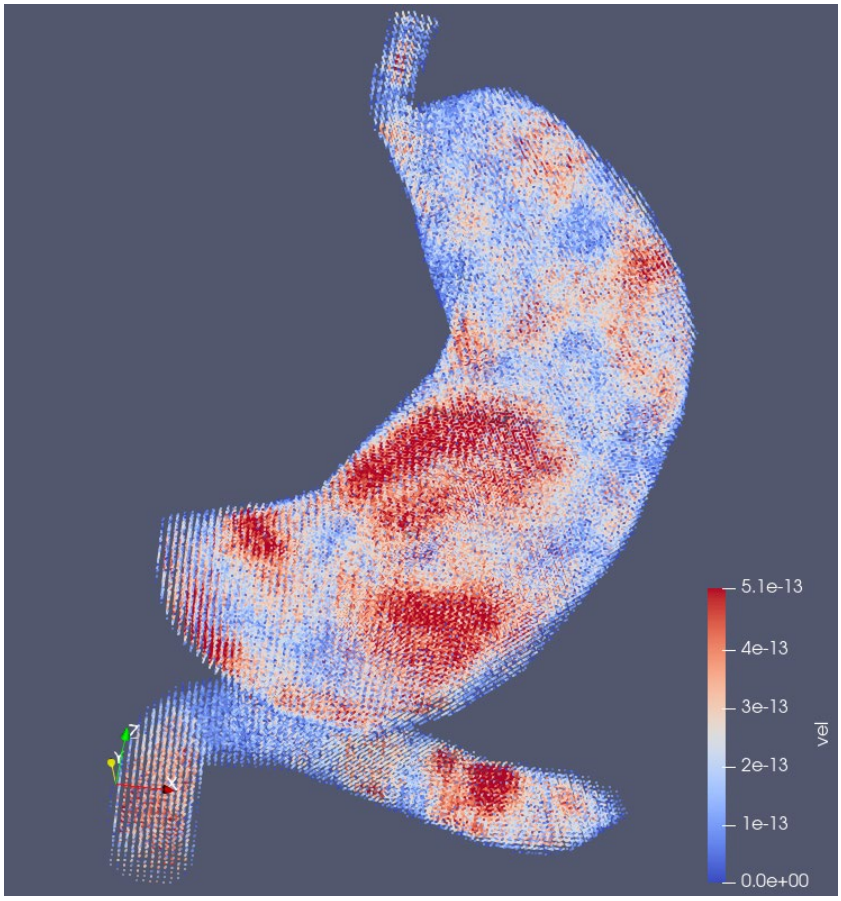

Fig 7. Velocity field distribution in anastomosis state at time 5.0 sec

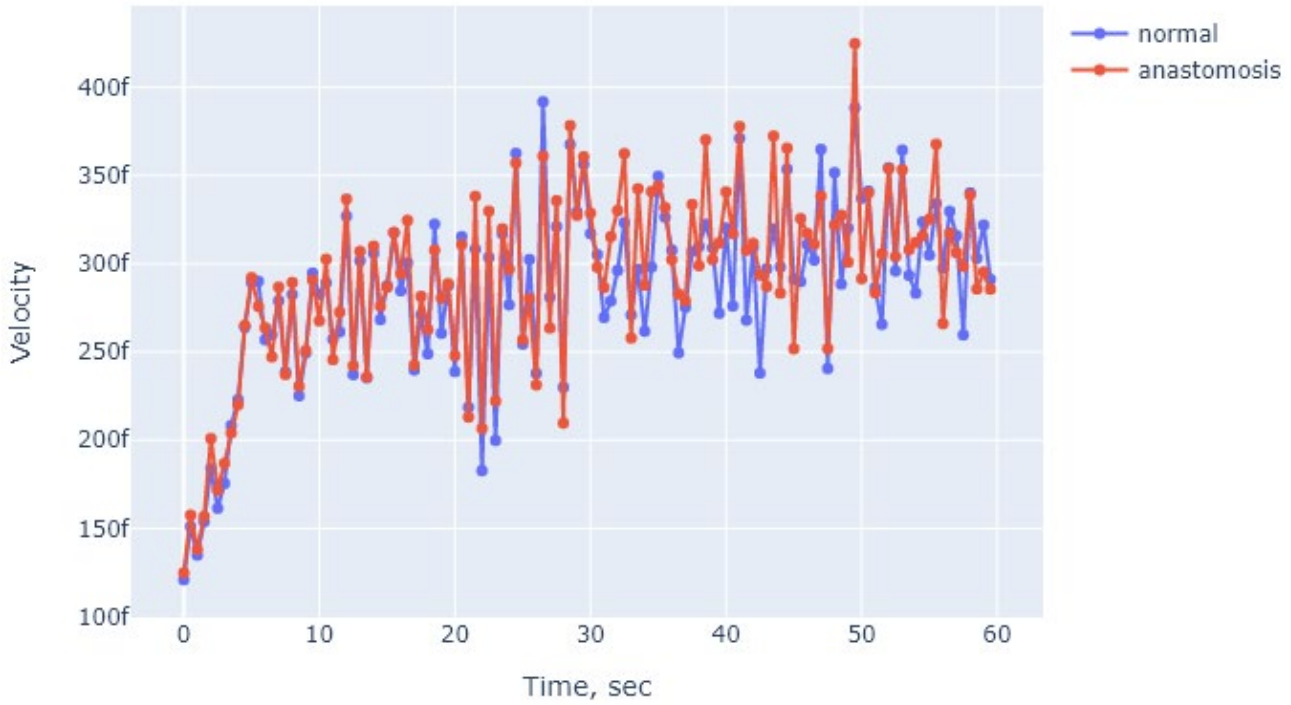

Fig.8 Average velocity during modeling

Conclusions

This paper studies the principles of simulating with the lattice Boltzmann models in fluid motion simulation on closed surfaces. The human digestive tract was chosen as an appropriate example of a closed surface due to the practical significance of this model.

This article studies the principles of using the lattice Boltzmann model for simulating the movement of fluid in objects with closed surfaces. Modeling is implemented on the example of the closed surface of the human digestive tract. Such studies are of great practical importance as they increase the results of reconstructive operations on the human digestive tract.

The developed simulation model provided a unique insight into the fluid dynamics of gastric contents. The conducted experiments show a clear difference in simulated behavior between the normal state of the stomach and the state of anastomosis. This result indicates the practical significance of our work. In addition, the proposed approach made it possible to analyze the processes in the digestive tract in dynamics by visualizing the pressure distribution and changes in the velocity field along the entire modeling geometry.

One of the possible implementations of the investigated method is detecting regions in the gastrointestinal tract where values of concerned fluid flow properties are higher or lower than some critical thresholds. It can help for better planning of surgery operations. The second possible application can be real-time monitoring of the gastrointestinal tract during the process or post-operation. All those implementations require accurate diagnostic tools, which can show the inner structure and geometry of the patient's gastrointestinal tract. There is a possibility of transforming into a 3D model that can be handled by simulation software.

The presented approach to the dynamic simulation of fluid flows in closed surfaces of a complex shape has a particular drawback, which is associated with insufficient accuracy in determining changes in the pressure distribution. A further research direction is the application of machine learning technologies to increase this accuracy.

References

1. Aoki S. Evaluation of the correlation between in vivo and in vitro release of phenylpropanolamine HCl from controlled-release tablets /. Aoki S,
2. Molly K. Development of a 5-step multi-chamber reactor as a simulation of the human intestinal microbial ecosystem / Molly K, Vandewoestyjne

3. Yoo JY. GIT physicochemical modeling-a critical review / Yoo JY, Chen XD // Int J Food Engr, 2006 - 2(4), Art. 4
4. Singh SK. Fluid flow and disintegration of food in human stomach // University of California, Davis, CA: Biological Systems Engineering, 2007.
5. Pal A. Gastric flow and mixing studied using computer simulation / Pal A, Indireshkumar K, Schwizer W, Abrahamsson B, Fried M, Brasseur JG. // Proc R Soc Lond B, 2004
6. Pal A. A stomach road or ‘‘Magenstrasse’’ for gastric emptying. / Pal A, Brasseur JG, Abrahamsson B. // J Biomech, 2007
7. Bhatnagar P.L. A model for collision processes in gases. I: Small amplitude processes in charged and neutral one-component system / Bhatnagar P.L., Gross E.P., Krook M. // Physical Review.– 1954. – Vol.94, №3 – P.511–525.
8. He X. Theory of the lattice Boltzmann equation: from Boltzmann equation to lattice Boltzmann equation / He X., Luo L-S. // Physical Review E.– 1997.– Vol. 56, №6.– P.6811–6817.
9. https://github.com/pylbm/pylbm
10. T. Kruger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva, and E. M. Viggen, The Lattice Boltzmann Method: Principles and Practice (Springer International Publishing, 201
11. https://www.blender.org/
12. Rast M.P. Simultaneous solution of the Navier-Stokes and elastic membrane equations by a finite element method / M.P. Rast // International Journal for Numerical Methods in Fluids.– 2005.– Vol.19, No. 12.– P.1115–1135.
13. Inamuro, T.; Yoshino, M.; Ogino, F. Accuracy of the lattice Boltzmann method for small Knudsen number with finite Reynolds number. Phys. Fluids 1997, 9, 3535–3542.
14. Deen, N.G.; Annaland, M.V.S.; Kuipers, J.A.M. Detailed computational and experimental fluid dynamics of fluidized beds. Appl. Math. Model. 2006, 30, 1459–1471.
15. Basagaoglu, H.; Harwell, J.R.; Hoa, N.; Succi, S. Enhanced computational performance of the lattice Boltzmann model for simulating micron- and submicron-size particle flows and non-Newtonian fluid flows. Comput. Phys. Commun. 2017, 213, 64–71
16. Tarksalooyeh, V.W.A.; Zavodszky, G.; van Rooij, B.J.M.; Hoekstra, A.G. Inflow and outflow boundary conditions for 2D suspension simulations with the immersed boundary lattice Boltzmann method. Comput. Fluids 2018, 172, 312–317