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

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.

Keywords: lattice Boltzmann model, hydrodynamics.

Fig.: 4. Bibl.: 9.

Target setting. 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, the development of a mathematical model of fluid flow in the closed surface has become crucial in recent years.

Actual scientific research and issues analysis. The first series of in vitro systems have been developed to analyze human digestion [1, 2] at the beginning of the 1990s. Despite the large existing amount of data on the human and animal digestive tract, 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, it is very difficult to develop an *in vitro* system capable of accurately reproducing the fluid mechanical forces that promote digestion.

Singh et. al presented an advanced fluid dynamics program that offers a promising technique to characterize the mechanisms promoting digestion [4]. Computational fluid dynamics can be used to numerically model 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 conducted some initial attempts to simulate the gastric flow during digestion [5, 6], but the computational effort required to reproduce the geometry and motility of the stomach prevented a good characterization of the system.

Our work is devoted to the application of the lattice Boltzmann model (LBM) for modeling the processes of fluid flow on closed surfaces. This is a novel approach to obtaining acceptable results in reasonable computation time.

Uninvestigated parts of general matters defining.

The usage of the lattice Boltzmann model for simulation of fluid flow in closed surfaces like the human digestive tract has not been fully studied yet. Therefore, in this article, we attempted to investigate the possibility of using LBM in fluid flow simulation inside biological objects.

The research objective. The purpose of this paper is a study hydrodynamic processes in closed surfaces using the Boltzmann lattice model.

The statement of basic materials.

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

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

where F – an external body force, ∇_x, ∇_p, is the gradient in position and momentum space, and $\Omega^{\wedge}(f)$ 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:

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

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

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

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]:

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

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:

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

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:

$$\frac{f_k\left(x_k+v_k\Delta t, t+\Delta t\right)-f_k\left(x_k+v_k\Delta t, t\right)}{\Delta t} + \frac{f_k\left(x_k+v_k\Delta t, t\right)-f_k\left(x_{k'}, t\right)}{\Delta x_k} = \frac{-f_k\left(x_{k'}, t\right)-f_k^{(eq)}\left(x_{k'}, t\right)}{\tau}.$$

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

$$f_k\left(x_k + v_k\Delta t, t + \Delta t\right) - f_k\left(x_{k'}, t\right) = \frac{-1}{\tau}\left(f_k\left(x_{k'}, t\right) - f_k^{(eq)}\left(x_{k'}, t\right)\right), \tag{6}$$

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:

$$f\!\sim_k\left(x_{k'}, t + \Delta t\right) = f_k\left(x_{k'}, t\right) - \frac{1}{\tau}\left(f_k\left(x_{k'}, t\right) - f_k^{(eq)}\left(x_{k'}, t\right)\right). \tag{7}$$

2. Flow-related step: $f_k\left(x_k + v_k\Delta t, t + \Delta t\right) = f\!\sim_k\left(x_{k'}, t + \Delta t\right).$
(8)

In (7) and (8), the distribution function $f\!\sim_k$ 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:

$$\rho = \int_{-\infty}^{\infty} f(x, v, t)dv = \sum_{k=0}^{8} f_i = \sum_{k=0}^{8} f_k^{(eq)}, \tag{9}$$

$$u = \frac{1}{\rho}\int_{-\infty}^{\infty} v \cdot f(x, v, t)dv = \frac{1}{\rho}\sum_{k=0}^{8} v_k f_k = \frac{1}{\rho}\sum_{k=0}^{8} v_k f_k^{(eq)}, \tag{10}$$

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.

The described method is used in modeling the distribution of pressure in the human stomach. We modeled the stomach in 2 states – a normal state and an anastomosis state. They displayed on Fig.1 – black region denotes cavity, white region – obstacle.

To apply LBM we discretized each model into a square mesh with the size of 256×256, with both width and height equal to 0.45. Parameters of LBM itself are the following: $R = 1000, \rho = 1000$. We introduced boundary value in the top as a constant flow directed to the bottom, with a velocity equal to 0.05 m/s.

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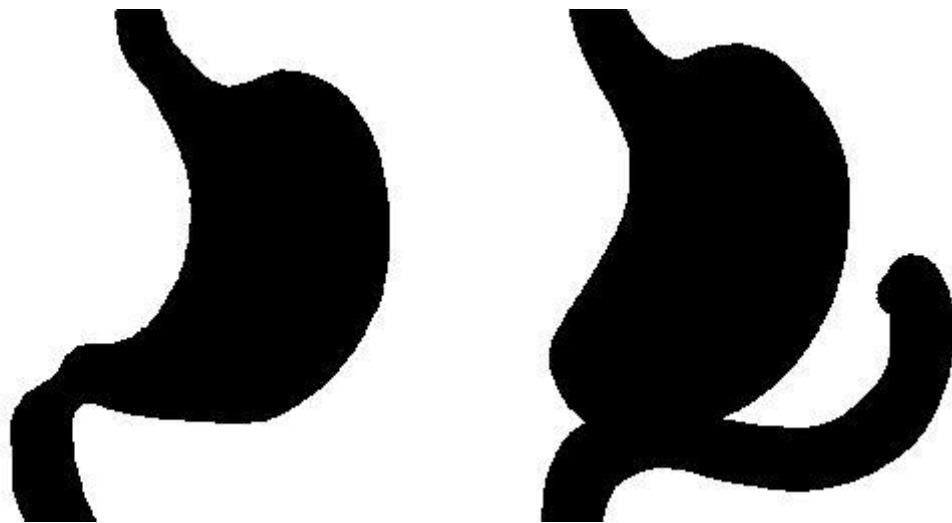

Fig. 1. Left –normal stomach, right – anastomosis

We measured pressure field distribution at modelling times t = 2.46 sec and t = 5 sec. Fig. 2 shows distribution in the case of anastomosis, fig. 3 shows normal state of human stomach.
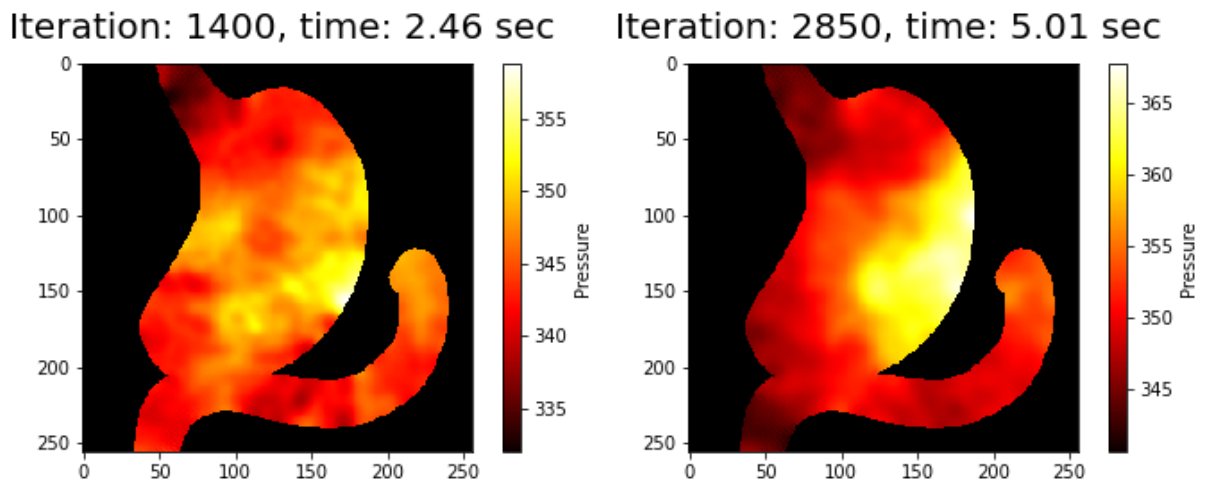

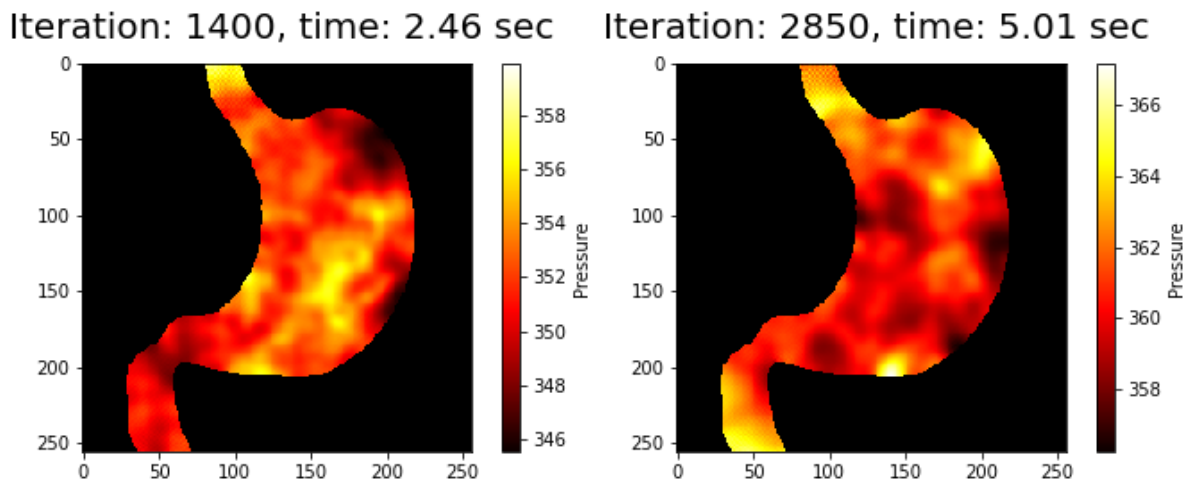Fig 2. Pressure field distribution in anastomosis model

Fig 3. Pressure field distribution in normal state

Results demonstrated higher density near the right wall of the stomach, in case of anastomosis than in the normal state. Also, anastomosis model shows high pressure in "blind bag" under stomach. In real situations it can cause development of negative consequences.

Another point is range of pressure values in both states are also different. At the modelling time 2.46 sec, in anastomosis state pressure field values fall in range from 330 to 360, in normal state – from 346 to 359. At the modelling time 5.01 sec, in anastomosis state pressure field values fall in range from 341 to 366, in normal state – from 357 to 366. We investigated relationship between average pressure inside stomach area and modelling time in aforementioned states. Fig.4 shows this relationship. During all period of modelling, average pressure in normal state is higher, than in anastomosis. Due to this outcome and previously mentioned results, we can conclude that pressure field in anastomosis state irregular in comparison to normal state of stomach.

Conclusions.

This paper investigates the application of the lattice Boltzmann model in the simulation of fluid motion 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. Conducted experiments show the clear distinction of modeled behavior between the normal state of the stomach and the anastomosis state. This result indicates the practical significance of our work.

Our paper clearly has some limitations. We investigated only the 2D domain, which cannot provide perfect accuracy. Despite this, we believe our work could be the basis for other improvements – handling the 3D domain and more sophisticated boundary conditions, combined with machine learning approaches.
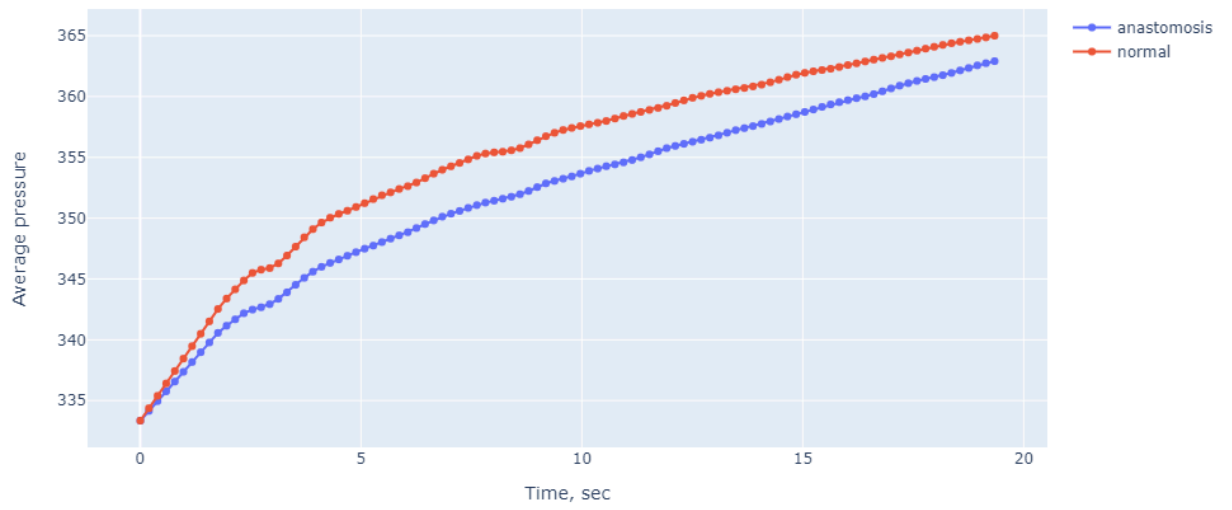
Fig.4 Average pressure during modelling

References

1. Aoki S. *Evaluation of the correlation between in vivo and in vitro release of phenylpropanolamine HCl from controlled-release tablets* /. Aoki S, Uesugi K, Ozawa H, Kayano M. // Int J Pharm, 1992 – Vol 85 – P. 65–73
2. Molly K. *Development of a 5-step multi-chamber reactor as a simulation of the human intestinal microbial ecosystem* / Molly K, Vandewoestyjne M, Verstraete W. // Appl Microbiol Biotechnol, 1993
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

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