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MODELING OF LIQUID VORTICITY USING CELLULAR AUTOMATON

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***Abstract*—*A method has been developed for constructing large-scale electrophysiological models using extended cellular automata and for running such models on a cluster of shared memory systems. A method is proposed, including the extension of the language cellular automaton for the implementation of quantitative calculations, the construction of the whole-heart model with the Visible Human Project data, the parallelization of the model on a cluster of computers with a general and a simulation algorithm that connects the activity of cells with an electrocardiogram. It is shown that electrical activity at the level of canals, cells and organs can be traced in the extended system of cellular automata. Examples of some signals of electrocardiograms simulated by a two-dimensional cut are given. Also, an evaluation of the performance of a three-dimensional model on a four-member cluster.*

Index Terms—Cellular automata; derivation of hydrodynamics; molecular dynamics; hexagonal grid; Navier–Stokes equations.

I. INTRODUCTION

This article concentrates on description of new algorithm of the liquid's dynamic based on cellular automaton. One of the well-known methods of modeling of liquids is Lattice gas automata model and its subspecies: FHP and HPP models [1], [2]. The model presented in the article has several common features with FHP model or rather cellular automata grid form which is used in both models. Still presented algorithm is a new approach which has own benefits.

Main idea of the modeling of continuous dynamic of liquid using the cellular automaton lays in fact that the synergy of big quantity of micro-particles leads to the emergent macroscopic phenomena. Cellular automaton is by nature discrete mathematical model which consists of array or, by other words, grid of cells that are essentially finite automatons and which interact with each other according to the set of predefined rules [3]. The state of the cell is basically any computable entity which is dictated by the need of the research. For example velocity and direction of liquid molecule. The matter of interest is behavior of the model "in large" which is relevant to the results obtained by analytical methods like Navier–Stokes equation [4]. From the perspective of computability cellular automats are natural representation of emergent phenomena [5].

II. ANALYSIS OF RESEARCHES

Frish-Hasslacher-Pomeu (FHP) model variations like FHP-I, FHP-II are commonly used for liquid and gas modeling, [6]. FHP model was introduced in 1986 by Uriel Frisch, Brosl Hasslacher and Yves Pomeau.

The model works on hexagonal grid whose sites are connected with nearest neighbors by the links (Fig. 1).

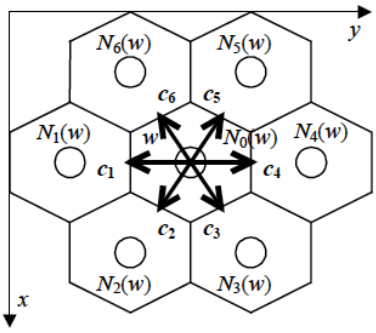

Fig. 1. FHP model hexagonal grid collision and propagation (or streaming)

Each site represents the fluid particle which moves along the links during the propagation step following an exclusion principle which states that only one particle is allowed to move along the link. Each particle is considered to be of constant mass and moves with unit velocity. After end of the propagation phase the collision phase begins. During this step particles that turn up to be in one site change their move directions according to preset rules.

The computation is representative in the sense of viscosity of moving fluid and velocity is derived from Reynolds law.

$$\mathrm{Re} = Vd / v.$$

III. PROBLEM STATEMENT. PURPOSE AND OBJECTIVES OF RESEARCH

The problem of determining the vorticity of a liquid flow in a tube (blood vessel) of finite

dimensions reduces to solving a boundary value problem for the Helmholtz equation

$$\frac{\partial \omega}{\partial t} - \nabla \times (v \times \omega) = \nu \nabla^2 \omega,$$

$$\omega = \nabla \times v,\ \nabla \cdot v = 0;\ \omega = (0, \zeta, 0);\ \zeta = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial r}.$$

$$u = \frac{1}{r}\frac{\partial \psi}{\partial z},\ w = -\frac{1}{r}\frac{\partial \psi}{\partial r}.$$

where is the current function, is the radius of the cylinder, l is the length.

$$0 \le r \le 1,\ 0 \le z \le z_0,\ z_0 = l / a.$$

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Vorticity is determined through the vorticity function

$$\Gamma = -r\zeta = r\left(\frac{\partial w}{\partial r} - \frac{\partial u}{\partial z}\right).$$

The Navier–Stokes equation for (in a cylindrical coordinate system):

$$\frac{\partial \Gamma}{\partial t} + u\frac{\partial \Gamma}{\partial r} + w\frac{\partial \Gamma}{\partial z} - \frac{2u\Gamma}{r} = \frac{1}{Re}\Delta\Gamma.$$

Boudary conditions:

$$\psi = u = \frac{\partial w}{\partial r} = \Gamma = 0,\ r = 0,\ 0 \le z \le z_o,$$

$$\psi = u = w = 0,\ \Gamma = \frac{\partial w}{\partial r},\ r = 1,\ 0 \le z \le z_o,$$

$$\psi = u = w = 0,\ \Gamma = \frac{\partial w}{\partial z},\ 0 \le r \le 1,\ z = 0, z_o.$$

The solution of this nonlinear boundary value problem will be sought using the approximating Boltzmann equation [7], whose solution is based on the use of cellular automata.

IV. Solution of the Problem

As a precondition we have next initial parameters of the experiment:

– size of the container with resting liquid

$$S := (rows \mid element \in N,\ columns \mid element \in N);$$

– width of the incoming stream

$$d := (startIndex \in N \mid 0 \le startIndex < endIndex,\ endIndex \in N \mid endIndex < columns);$$

– initial velocity of incoming particles

$$v_0 \in Q \quad \text{and} \quad v_0 > 0;$$

– number of waves of incoming particles

$$waves \in N \quad \text{and} \quad waves > 0.$$

Necessity of the parameter waves will be seen below during further analysis of algorithm. Describing cellular automaton we need to describe configuration of the grid, the state of the automaton cell, the neighborhood and the algorithm of evolution of the automaton.

As in the FHP model the grid of our model is hexagonal with pointy topped hexagons. The number of hexagons is *CellsQuantity* = *rows*·*columns*. Offset coordinate system, specifically "event-r" horizontal layout, is chosen for indexing the cell [7].

Each cell has it's own index:

$$CellIndex := (x \in N \mid 0 \le x < columns,\ y \in N \mid 0 \le y < rows).$$

One of the main differences between presented model and FHP is that grid cell represents the moving particle, not the site of the liquid's space with velocity channels, which interacts with neighbors (description of interaction see below) and the state of the cell is its velocity decomposed along the abscissa and ordinate:

$$State := (Xproj \in Q,\ Yproj \in Q \text{ and } Yproj \ge 0).$$

In current version of algorithm the particle is allowed to move only forward.

Neighborhood of the Current Cell Index, which is the Cell Index, includes 4 cells: and based on chosen layout the rules to define the addresses of the neighbors are:

$$\{LeftNeighbor,\ UpLeftNeighbor,\ UpRightNeighbor,\ RightNeighbor\},$$

and based on chosen layout the rules to define the addresses of the neighbors are:

1) $LeftNeighborIndex := CellIndex,$

where $x := CurrentCellIndex(1) - 1$

and $y := CurrentCellIndex(2).$

2) $UpLeftNeighborIndex := CellIndex,$

where $x := CurrentCellIndex(1) - 1,$

and $y := CurrentCellIndex(2) + 1,$

if $CurrentCellIndex(2)$ is Odd

or $x := CurrentCellIndex(1)$

and $y := CurrentCellIndex(2) + 1,$

if $CurrentCellIndex(2)$ is ***Even.***

3) $UpRightNeighborIndex := CellIndex,$

where $x := CurrentCellIndex(1)$,
and $y := CurrentCellIndex(2) + 1$,

if $CurrentCellIndex(2)$ is Odd

or $x := CurrentCellIndex(1) + 1$

and $y := CurrentCellIndex(2) + 1$,

if $CurrentCellIndex(2)$ is ***Even.***

4) $RightNeighborIndex := CellIndex$,

where $x := CurrentCellIndex(1) + 1$,
and $y := CurrentCellIndex(2)$.

Whole experiment is based on the hypothesis that during collision of three particles which are represented by hexagons of the grid their impulses are decomposed as the binary fractal tree (Fig. 2). Considering the unit mass of each particle it can be eliminated from the computations.

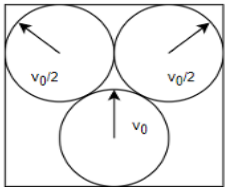

Fig. 2. Binary distribution of the forces

On the Fig. 3 below high-level program execution is described. Having all preconditions stated above we start with adding new wave to the cellular automata grid. Then we proceed to the computation of the grid on step t to the step $t + 1$. Adding the new wave means to set the Y_{proj} of the State of $Cell$ where $d(0) \le CellIndex \le d(1)$ equal to v_0.

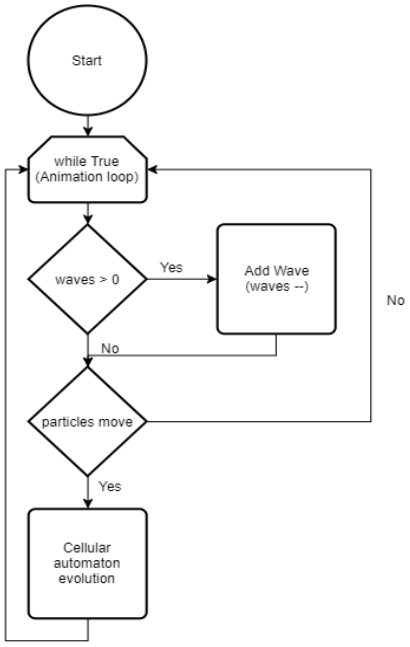

Fig. 3. High-level flow of the program

Describing computation of evolution of cellular automaton we need two variables:

$CurrentCtepGrid$, and $NextCtepGrid$.

$CurrentCtepGrid$ is defined in the global scope of the program and $NextCtepGrid$ is defined in the Cellular automaton evolution procedure. The flow diagram of the procedure is described on Fig. 4. From the flow-chart we can see that after transmitting impulse to the up left and up right neighbors the impulse of transmitter is set to 0 due to conservation law. Also there are traverse impulses in each row of the grid which eliminate each other leaving the edge effect. Transmission of the traverse impulse proceeds according to the general rules of cellular automaton Fig. 5.

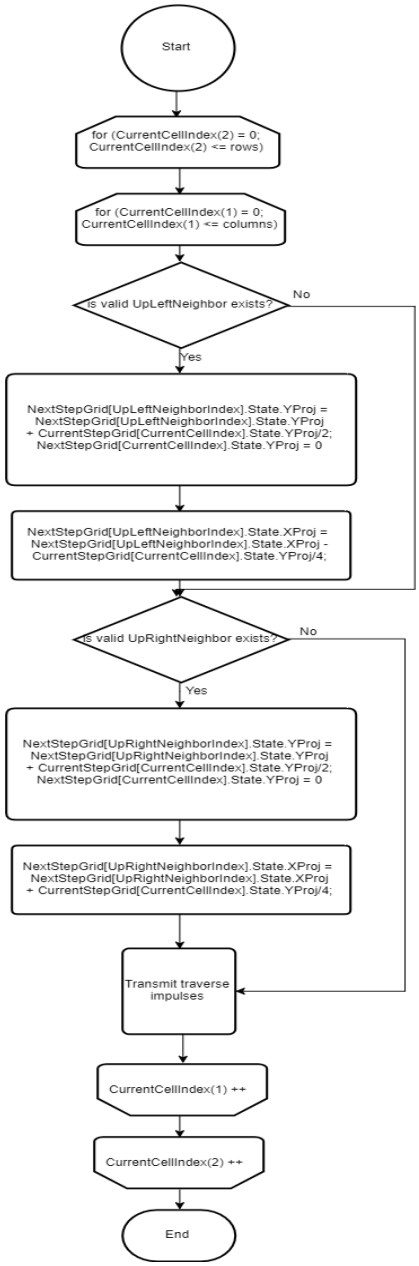

Fig. 4. Algorithm of binary decomposition of impulses

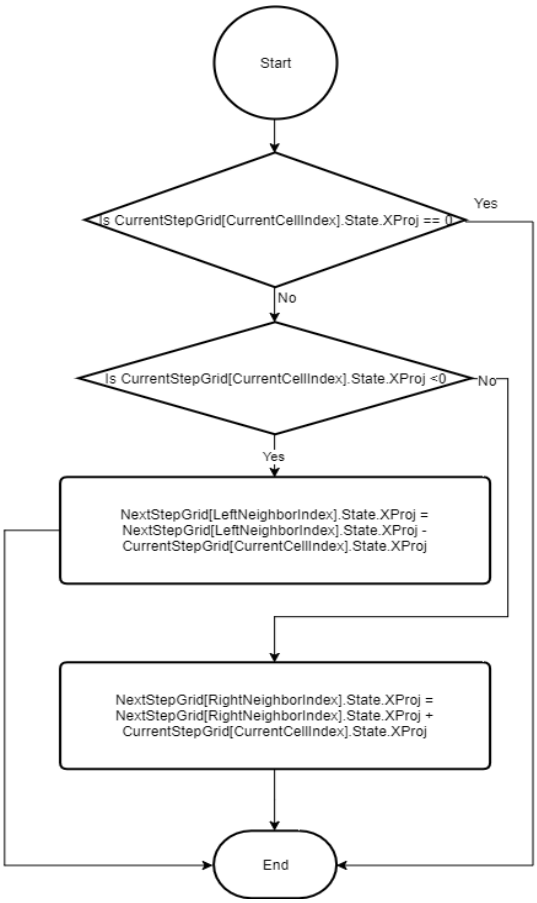

Fig. 5. Cross impulse transmission algorithm

The result of computational experiment is shown on Fig. 6.

Preconditions:

$$S = (100,100), \quad d = (40,60),$$
$$v_0 = 100, \quad waves = 10.$$

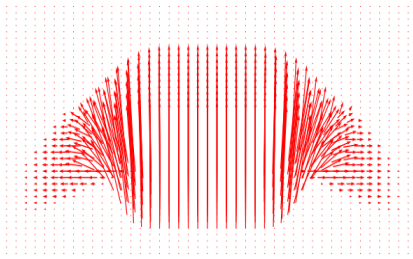

Fig. 6. Results of the computational experiment

From the Fig. 6 we can see that introduced hypothesis makes sense.

V. Conclusions

Animation of the presented cellular automaton evolution shows similarity with the shape of real ring vortex. Still it is just the beginning of the future researches either from physical and computational perspectives.

VI. References

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Є. А. Настенко, А. В. Радагуз. Моделювання вихорів у рідині за допомогою клітинних автоматів
Розроблено метод побудови великомасштабних електрофізіологічних моделей з використанням розширених клітинних автоматів і для запуску таких моделей на кластері поділюваних систем пам'яті. Запропоновано метод, включаючи розширення мовного клітинного автомата для реалізації кількісних обчислень, побудови моделі щирого серця з даними Visible Human Project, розпаралелювання моделі на кластері комп'ютерів із загальною і алгоритм моделювання, який пов'язує активність клітин з електрокардіограмою. Показано, що електричні активності на рівні каналів, клітин і органів можна простежити в розширеній системі клітинних автоматів. Наведені приклади деяких сигналів електрокардіограм, які імітуються двовимірним зрізом. Дано оцінку продуктивності тривимірної моделі на чотириланковому кластері.
Ключові слова: клітинний автомат; гексагональна сітка; дискретна модель; молекулярна динаміка; рівняння Нав'є–Стокса.

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Е. А. Настенко, А. В. Радагуз. Моделирование вихрей в жидкости с помощью клеточных автоматов
Разработан метод построения крупномасштабных электрофизиологических моделей с использованием расширенных клеточных автоматов и для запуска таких моделей на кластере разделяемых систем памяти. Предложен метод, включая расширение языкового клеточного автомата для реализации количественных вычислений, построения модели всего сердца с данными Visible Human Project, распараллеливание модели на кластере компьютеров с общей и алгоритм моделирования, который связывает активность клеток с электрокардиограммой. Показано, что электрические активности на уровне каналов, клеток и органов можно проследить в расширенной системе клеточных автоматов. Приведены примеры некоторых сигналов электрокардиограмм, имитируемых двумерным срезом. Дана оценка производительности трехмерной модели на четырехзвенном кластере.
Ключевые слова: гексагональная сетка; дискретная модель; клеточный автомат; молекулярная динамика; уравнения Навье—Стокса.

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