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The Lattice Gas Cellular Automata approach for fluid flow in porous media

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1. Předmět a cíl práce / Object and purpose of work

In this work, fluid flow mechanism and its modelling is an object of study. With the development of nanoporous textile structures the following question suggests itself: Which theoretical approach is suitable for modelling of fluid flow in such structures? Since the fully discrete model of hydrodynamics, Lattice Gas Cellular Automata (LGCA), based on cellular automata conception was developed and verified for fluid flow, more and more researchers become to use this approach in fluid flow modelling and simulation. Lattice Gas Cellular Automata provide the more number of options for modelling of fluid flow in contrast to Nevier-Stokes equations. Because of its discrete nature it doesn't have limitations in continuity of the flow. It is valid in all regimes of flow – from the molecular flow to the continuum one.

Therefore, in a frame of this work following purposes were defined:

1. To study basic principles of Cellular Automata and Lattice Gas Cellular Automata.
2. Based on principles of LGCA to develop an algorithm for two-dimensional fluid flow computer simulation.
3. To verify created LGCA algorithm.
4. To demonstrate the suitability of Lattice Gas Cellular Automata approach for fluid flow in porous structure modelling.

2. Přehled současného stavu problematiky / Overview of current state issues

The subject of this work is a fluid transport through the porous media. The fluid flow through fibrous materials is a phenomenon which occurs in a range of technological processes and it is a subject of a wide interest in textile industry for all the time. The textile industry encounters with this phenomenon during a lot of production and finishing processes. Examples range from dyeing processes, over filtration to high performance textiles with improved wearing comfort. If we evaluate current scientific trends in global, and textile engineering especially, the new type of fibre materials becomes to be popular – i.e. textiles containing nanofibers and nanosize objects.

It was mentioned in [1], that a common requirement for understanding the transport properties of textiles is a detailed understanding regarding the transport of momentum through textile structures. This information is difficult to obtain experimentally and often the researches rely on "try and error" methods. During last several years, the study of fluid and heart transfer in porous structures was facilitated thanks to the range of software and modelling approaches. The commercial software Fluent is one of examples. It is based on a computation fluid dynamics (CDF) code that has been in use since 1983 and has been applied to a broad range of disciplines (e.g., aerospace, chemical, environmental, textile engineering, etc.). The solution of Navier-Stokes equations for fluid flow coupled with the energy and diffusion equations is the principle of Fluent software and others. The Finite Element Method (FEM) is usually used for a solution of nonlinear partial differential equation as Navier-Stokes equations are. Fluent is also considered as a powerful approach to obtain insights into momentum transport within textiles. The few skilled works [1, 2], which have used the Fluent software for simulation of transport phenomena in textile structures, were founded.

According to [3] traditional numerical simulations, represented by the Navier-Stokes equations, rely on the continuum approach. But the approach would break down, when the

length scale of the physical system decreases, concretely, when the Knudsen number became greater. *Knudsen number* (Kn) is defined here as a dimensionless parameter that determines the degree of appropriateness of the continuum model – the degree of rarefaction of gases encountered in a small flows through narrow channels and for an ideal gas it is:

$$Kn = \frac{\lambda}{L} = \frac{k_B T}{\sqrt{2}\pi {d_p}^2 pL}, \tag{1}$$

where λ is a mean free path of molecules $[m]$; L is a length characterizing the geometry of flow, such as the diameter for a circular capillary, or the width of a pore, i.e. any microscopic dimension of interest $[m]$, k_B is a Boltzmann's constant (approximately 1.38×10^{-23} [J/K]); T – temperature $[K]$; d – particle diameter $[m]$; p is a total pressure $[Pa]$.

From the Equation (1) it is evident: if the Kn is near or greater than one, the mean free path of a molecule is comparable to a length scale of the system or it is greater. If we take into account the structural characteristics of the nanofibre materials, the $Kn \approx 1$ is expected. The continuum assumption of fluid mechanics is no longer a good approximation. In this case discrete particle methods must be used instead of continuum approach.

As is shown in the Figure 1, only Boltzmann equation, which is based on the discrete kinetic theory, is valid for the whole range of Knudsen number. As it was mentioned in [3], an alternative to continuum model is the molecular one, which recognizes the fluid as a swarm of discrete particles. Position, inertia and state of all individual particles are calculated here either deterministically or probabilistically at all times. During last few decades a large number of molecular models/methods, which consider individual particle dynamics based on a Boltzmann distribution at the temperature of interest, have emerged. Those methods include: molecular dynamic (MD), direct simulation Monte Carlo (DSMC), dissipative particle dynamics (DPD), smooth-particle hydrodynamics (SPH), Lattice Boltzmann model (LBM) and Lattice gas cellular automata (LGCA). Those methods aren't based upon Nevier-Stokes equations, but closely related to kinetic theory and Boltzmann equation. Those methods are mentioned in literature as promising candidates effectively connecting microscopic and macroscopic scales and enabling to study transport phenomena in nanopores structures.

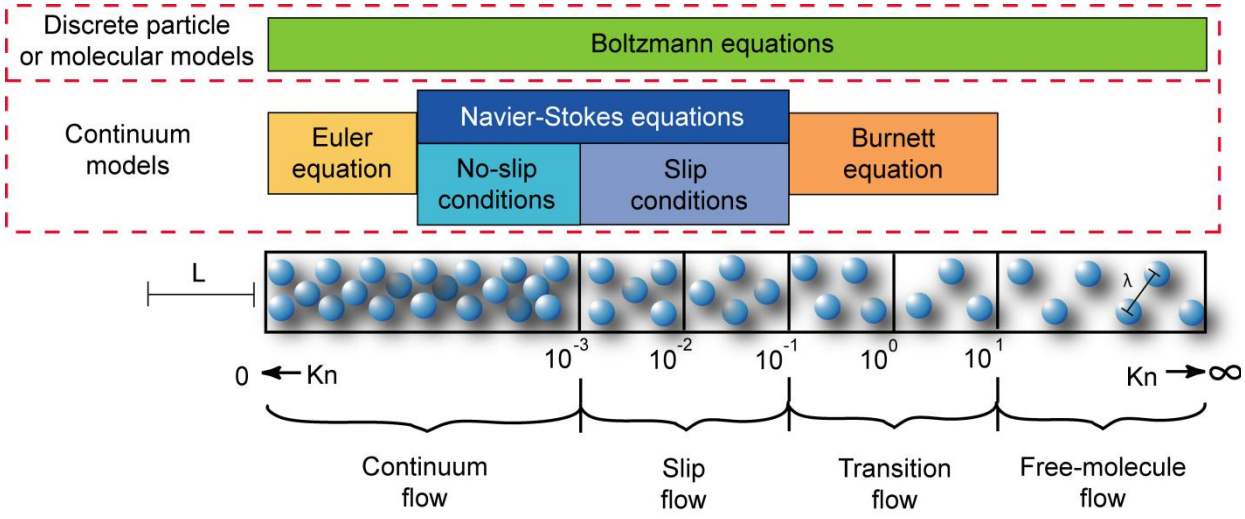


Figure 1: *Different regimes of fluid flow and methods for their description depending on Knudsen number*

3. Použité metody / Methods used

Lattice Gas Cellular Automaton model based on cellular automata conception is one of the fully discrete model of hydrodynamics and one of those, which reflects Boltzmann approach. This model was used in the frame of the work for fluid flow modelling. Nowadays, there is a number of LGCA models determined for various types of flow. The first LGCA model was introduced by Hardy, de Pazziz and Pomeau in seventies of the last century [4]. This model nowadays is known as a HPP model. It led to a lot of interesting results, but due to using the square geometry of the lattice it had limited applications because of its anisotropic behaviour. It was not refined until 1986, when Frisch, Hasslacher and Pomeau designed their own model, based on a hexagonal lattice. This model was called as the first FHP model (FHP-1 LGCA model). Then FHP-2 and FHP-3 models follow the basic FHP-1 LGCA model.

Lattice gas models based on cellular automata are representatives of fully discrete models. Based on the detailed information about individual particles, such as their positions, masses, and velocities, they enable to describe the behaviour of fluid systems at a molecular level under various conditions. Thus, lattice gas models entered into the history as an alternative for fluid system's modelling. Detailed description of Lattice Gas Cellular Automata is accessible for example in [5-7].

According to *Reviet* [6] lattice gas models are based on cellular automata rules and must also satisfy following conditions:

1. Lattice Gas Cellular Automata are presented by a set of individual automata, which are tied geometrically to the nodes of a regular Bravais lattice of dimension D. Individual automata in fact can also be called as a "node" (see *Figure 2, 1)*. Nodes are labelled by their position vector $\boldsymbol{r}$, which takes only discrete values. All individual automata are taken to be identical.
2. Any individual automaton has 2^bpossible internal states, where b is a Boolean variable, it is integer and it represents the number of channels (or communication channels) between nodes (see *Figure 2, 2*). Channels are also tied geometrically to the Bravais lattice – in fact, they are links between neighbour nodes of the lattice.
3. Similarly to cellular automata, the elementary evolution process of LGCA is repeated at discrete time steps and it is separated by a time increment Δt. In lattice gas models Δt is equal to the unity (time unit – $t.u.$), when the information presented in channel i at the node $\boldsymbol{r}$ goes to the node $\boldsymbol{r} + \boldsymbol{v}_i$, where $\boldsymbol{v}_i$ is the velocity vector (see *Figure 2, 4*). In contrast to cellular automata, in LGCA the information is presented by fictitious particles occupying channels i. The maximal number of particles in a node is done by b. In the most part of the lattice gas models (in the non-thermal LGCA: HPP, FHP-1) particles (*Figure 2, 3*) of the same mass m (in $m.u.$ – mass unit) and velocity v are moving on an underlying regular Bravais lattice, which has the unitary distance Δl (in $l.u.$ – length unit) between neighbouring nodes. But there are also multi-speed lattice gas models: FHP-2 and FHP-3 LGCA models that contain extra particles with zero velocity; particles in a GBL model, named after *Grosfils*, *Boon* and *Lallemand*, has three different velocities.
4. The elementary evolution process of LGCA is a sequence of two phases: the collision and the propagation one.

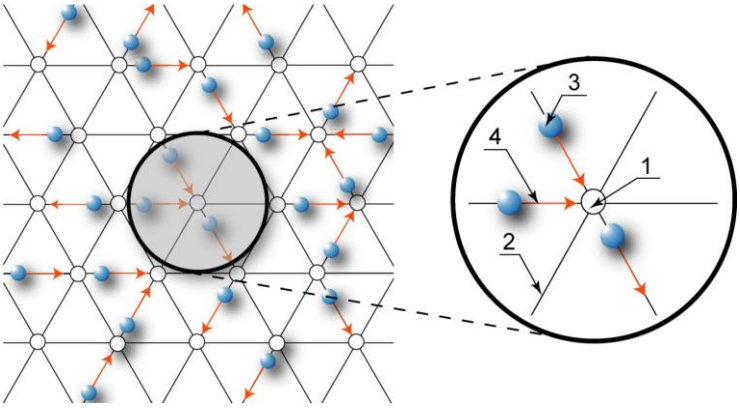


Figure 2: *Representation of the LGCA model underlaid by the hexagonal Bravais lattice:* ***1*** *– the node, i.e. the individual automaton,* ***2*** *– the channel,* ***3*** *– the moving particle,* ***4*** *– the direction of moving [11]*

From the information presented below it is obvious that the main characteristic of the LGCA models is a fully discreetness, since main parameters (time, distance and mass) are discrete. Basically LGCA models differ by collision rules; however, principles of the collision phase implementation are identical.

Collision phase in LGCA models

In Lattice Gas Cellular Automata the collision phase occurs in each time step. It proceeds in accordance with collision rule, which is chosen to conserve a number of particles, a mass and a momentum at each site of the lattice (i.e. in every individual automaton). According to the [6] conservation of the local particle number n and the mass m at the node $\boldsymbol{r}$ is described as follows:

$$\sum_{i=1}^{b} {}^{n}n_i(\boldsymbol{r}) = \sum_{i=1}^{b} n_i(\boldsymbol{r}) \tag{2}$$

$$\sum_{i=1}^{b} {}^{n}m_i(\boldsymbol{r})\, {}^{n}n_i(\boldsymbol{r}) = \sum_{i=1}^{b} m_i(\boldsymbol{r})\, n_i(\boldsymbol{r}) \tag{3}$$

In Equations (2) and (3) the initial distribution of the colliding particles in the node $\boldsymbol{r}$ at individual channels i's is represented by $n_i(\boldsymbol{r})$, while the post-collision state in the same node and channel is given by the "new" ${}^{n}n_i(\boldsymbol{r})$ values. It is evident, if the individual masses of all particles in the node $\boldsymbol{r}$ are equal to 1, then the total mass in the node $\boldsymbol{r}$ is equal to the total number of particles.

The local momentum conservation during the collision phase may be expressed using its components ${}^{n}p_a(\boldsymbol{r})$ and $p_a(\boldsymbol{r})$ as:

$$\sum_{i=1}^{b} {}^{n}p_i(\boldsymbol{r}) = \sum_{i=1}^{b} {}^{n}m_i(\boldsymbol{r})\, {}^{n}n_i(\boldsymbol{r})\, v_{ia}(\boldsymbol{r}) = \sum_{i=1}^{b} m_i(\boldsymbol{r})\, n_i(\boldsymbol{r})\, v_{ia}(\boldsymbol{r}) = \sum_{i=1}^{b} p_i(\boldsymbol{r}) \tag{4}$$

where $a = 1, \ldots b$ denotes the components of velocity vector (the number of velocity components is given by the connection number b).

Typical two and three-particle collisions in the FHP-1 LGCA are presented in *Figure 3a*. Among all collisions some of them are considered to be effective, when the rotation of the

velocity vectors by 60° has a place. All effective collisions of the FHP-1 LGCA model are presented in *Figure 3b.*

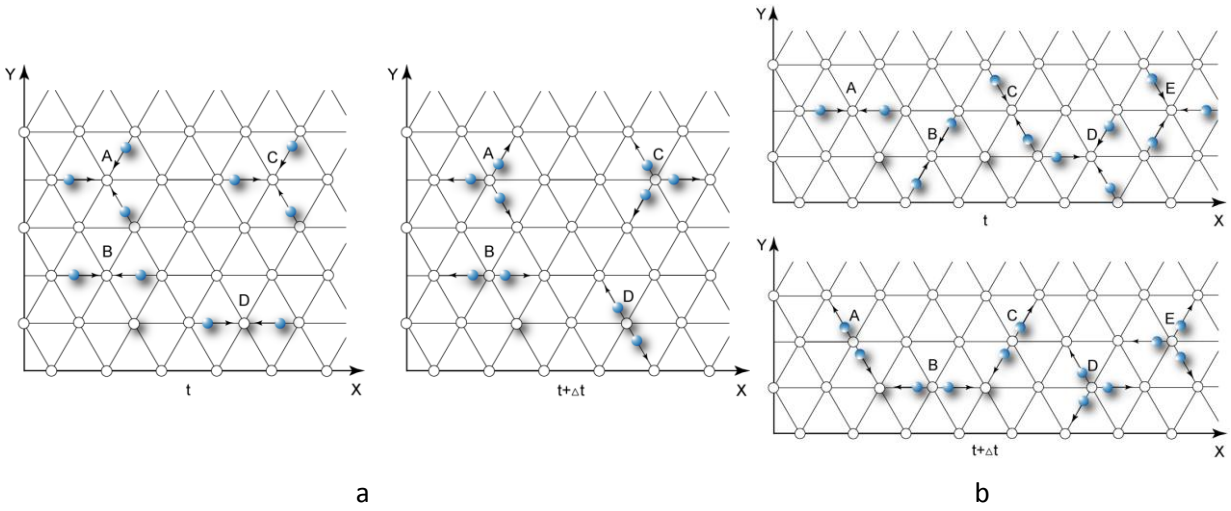


Figure 3: *Typical two- and three-particle collisions (a) and effective collisions (b) in the FHP-1 LGCA model [11]*

Propagation phase in LGCA models

During the propagation phase, every particle is shifted from the node $\boldsymbol{r}$ to the node $\boldsymbol{r} + \boldsymbol{v}_i \Delta t$, i.e. if a particle is present at a moment t in a node $\boldsymbol{r}$, it is shifted to the neighbouring node at time $t + \Delta t$ according to the direction i of velocity vector. This type of propagation phase takes a place inside the whole Bravais lattice. At the boundaries of the lattice there are various methods how to realize the propagation of particles.

One of the methods is so-called "periodic boundary condition" [6]. In that case the boundary parts of the lattice, on which the propagation phase is implemented, has to be connected to the form of a loop (see *Figure 4*). This wrapping of opposite sides of a finite lattice leads to a periodic motion of the individual particles. The escaping particles return to the finite lattice on the opposite sides of its boundaries.

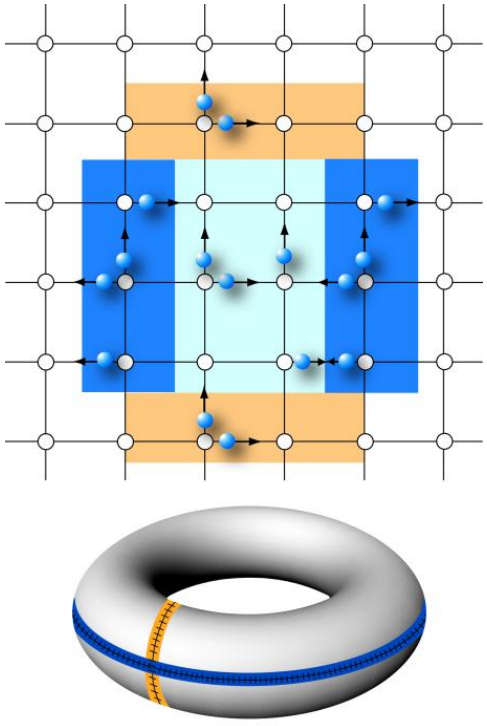


Figure 4: *The principle of periodic boundary conditions for two-dimensional square LGCA (HPP model [11]*

Another method is in conflict between the theoretically infinite lattices used in LGCA models and limited memories of computers. This method is called as a reflective boundary condition. This type of boundary conditions is based on various types of particle collision with solid walls (see *Figure 5*). According to *Rivet* [46] the following types of reflections are:

1. Bounce-back reflection – also known as a no-slip boundary condition (see *Figure 5*, node A).
2. Specular reflection – is also known as a free-slip boundary condition (see *Figure 5*,

node B).

3. Diffusive reflection – is a combination of the bounce-back and specular reflections, it is occurring with chosen probabilities *P* (see *Figure 5*, node C).

Red nodes in the *Figure 5* represent moveless particles of the solid surface (for example, solid walls or surface of any obstacle). Black arrows illustrate the momentum vector of particles. Blue arrows show the possible directions of the momentum vector as a result of diffusive type of reflective boundary condition.

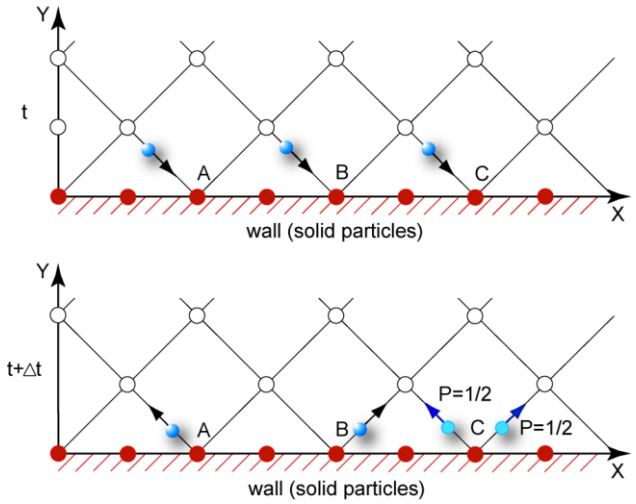


Figure 5: *Various reflective boundary conditions:* ***A*** *- bounce-back reflection,* ***B*** *- specular reflection,* ***C*** *- diffusive reflection [11]*

4. Přehled dosažených výsledků / Scoreboard

4.1.Creation of the FHP-1 Lattice Gas Cellular Automata algorithm

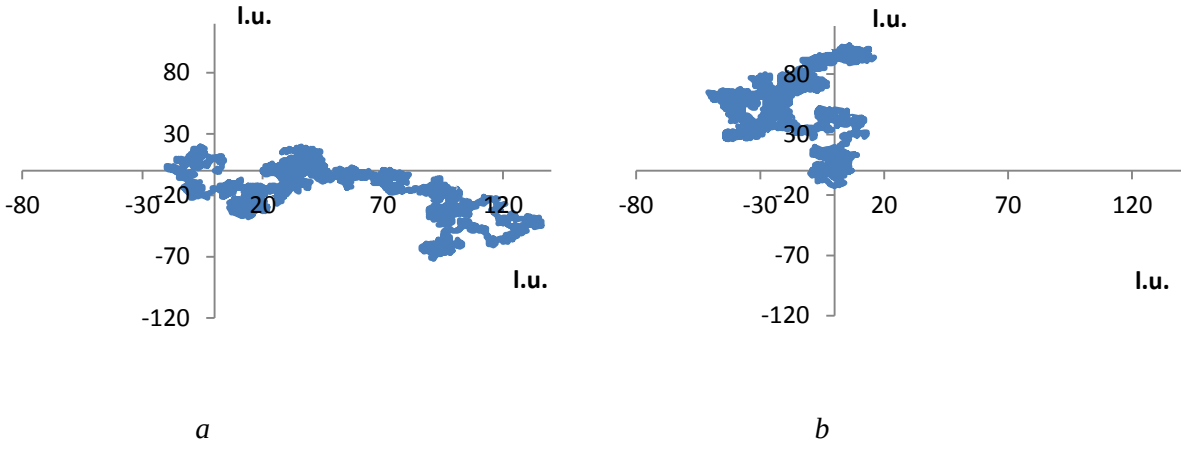
In a frame of this work a two-dimensional non-deterministic Lattice Gas Cellular Automata algorithm based on the FHP-1 LGCA model was developed and described in detail. The algorithm allows fluid flow simulation under various conditions (i.e. fluid flow inside the channel, trough porous media and under various boundary conditions). Algorithm was created in a C++ programming language, Borland version 4.0. Basic skeleton of the algorithm and function of its particular code fragments were minutely described in the thesis. The basic Lattice Gas Cellular Automata algorithm has an universal structure and was three times modified for various simulation studies. Phases of the LGCA evolution process (collision and propagation) take place in subroutines of the algorithm. If boundary conditions are changed, it does not interfere into the main part of the algorithm. Due to adaptation of the hexagonal lattice to the square one and using different arrangement of neighbourhood in add and even rows of the lattice calculations inside the algorithm are more complicated. On the other hand, this approach allows productively utilizing all points of the simulation domain. The main feature of the created LGCA model is its non-deterministic evolution in time. During the collision phase new state of a finite automaton is always generated randomly according to the conservation of mass and momentum in the individual automaton (i.e. lattice node). No predefined matrix of states was used. This property allows the fluid flow modelling in more realistic way.

4.2. Verification of the created FHP-1 LGCA algorithm for Brownian motion

The created LGCA algorithm was verified using two independent tests. First of them, Brownian motion, simulates molecules motion and was aimed on a monitoring of the one moving particle among many other fluid particles.

The modified LGCA algorithm was applied for a two-dimensional Brownian motion simulation. Brownian motion was simulated inside the simulation domain of the fixed size for

the period of time $t = 4000\ time\ units$. By mean of this test the set of random Brownian particle's paths was obtained. It was noted that paths walked by the Brownian particle are far from linear. The straight type of the pass is evident in *Figure 6a*. Many movements round and round or returning back to the starting point were monitored also (see *Figure 6b*).



a *b*

Figure 6: *Examples of the Brownian particle paths after 4000 time units:* ***a*** *– the straight type of the path;* ***b*** *– the "bonsai tree" shape of the path*

According to the theoretical assumption the linear relationship between the mean square displacement R^2 of the Brownian particle and time is expected. Based on two computer simulation experiments, varied in density of the lattice gas, the theoretical assumption was proved (see *Figure 7*). It can be argued that algorithm is working in a right way according to the results obtained in that test. Simulated system exhibits behaviour close to the real one. To limit the degree of data fluctuation around the linear regression the usage of biggest size of the simulation domain and extension of the simulation period were suggested.

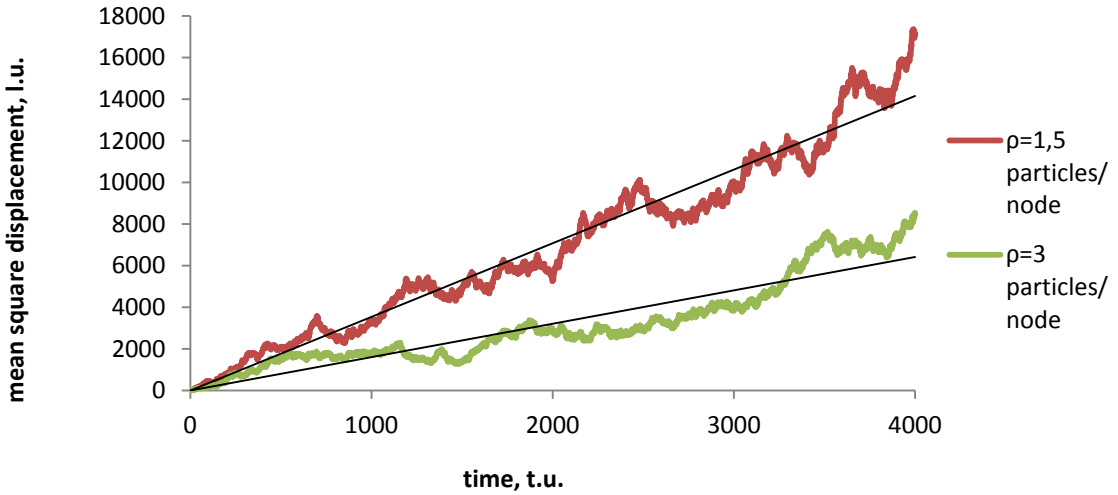


Figure 7: *The main square displacement of the Brownian particle as a function of time, for lattice gas densities ρ=1,5 particles/node and 3 particles/node*

It should be noted that this simulation can be used not only for the verification of a newly developed algorithm. Modified LGCA algorithm allows the study of diffusion phenomena including calculation of the diffusion coefficient. Another possible usage of the algorithm is modelling of polymer molecule shapes.

4.3. Verification of the created LGCA algorithm for Poiseuille flow

Because Lattice Gas Cellular Automata algorithms, developed for fluid flow modelling, are predominantly verified by means of Poiseuille flow simulation, the aim of the second benchmark test was:

- simulation of an incompressible fluid flow between two stationary parallel plates driven by constant body force;
- verification of the parabolic velocity profile;
- verification of the Darcy's law.

The special Lattice Gas Cellular Automata algorithm based on the created basic LGCA algorithm was designed for that reason. The bounce-back type of reflective boundary conditions was used along the walls of a channel and periodic boundary conditions were applied at the both vertical boundaries of the channel (see *Figure 8*). Behaviour of the simulated system was studied under various simulation setups varied due to the channel width d (it was $25\sqrt{3}/2$, $50\sqrt{3}/2$, $75\sqrt{3}/2$ and $100\sqrt{3}/2$ $l.u.$) and pressure gradient. The pressure gradient was created in terms of reversing particle momentum vectors in a position of an imaginary ventilator with certain probability. This flipping mechanism was impressed merely on particles with negative x components of velocity. The average change of the x component of the particle momentum at a particular node during one time step (i.e. 1 $t.u.$) was expressed as f_x. Five values of the f_x were simulated ($f_x = 2$, 1.4, 0.4, 0.2 and 0.03). The higher the value of f_x was, the higher pressure gradient was created and the faster flow was simulated.

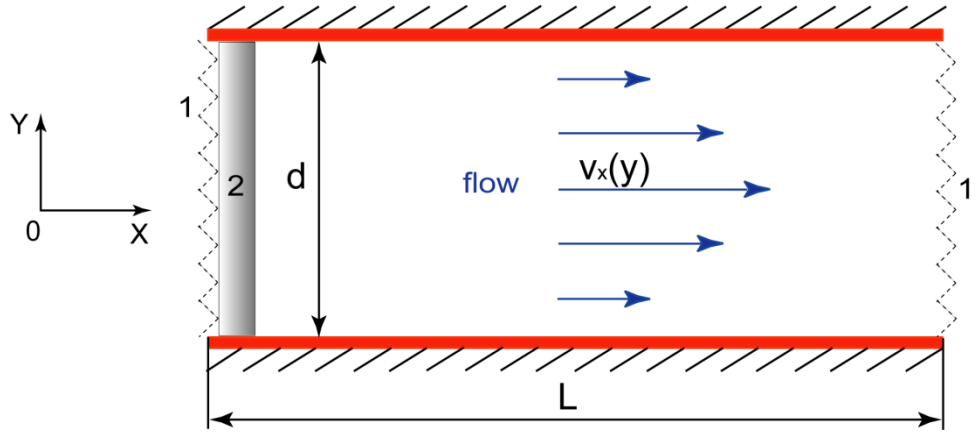


Figure 8: *The geometry of two-dimensional channel for Poiseuille flow simulation:* ***1*** *– periodic boundary conditions,* ***2*** *– the imaginary ventilator,* ***L*** *is the length and* ***d*** *is the width of the channel*

Twenty simulation experiments were realized. First, the x component of flow velocity was averaged over the whole channel length L for each horizontal row of the lattice nodes over 5 000 $t.u.$ in the steady state region of the flow in order to obtain velocity profile. Thus twenty different parabolic profiles of flow velocity were obtained. As an example, parabolic velocity profiles for channel width $d = 75\sqrt{3}/2$ $l.u.$ according to the values of f_x are presented in *Figure 9*.From the simulation results the faster fluid flow was simulated, the smoother velocity profile was obtained. The channel width had a little effect on a shape of the velocity profile. The smaller the channel width was simulated, the more peaked velocity profile was obtained.

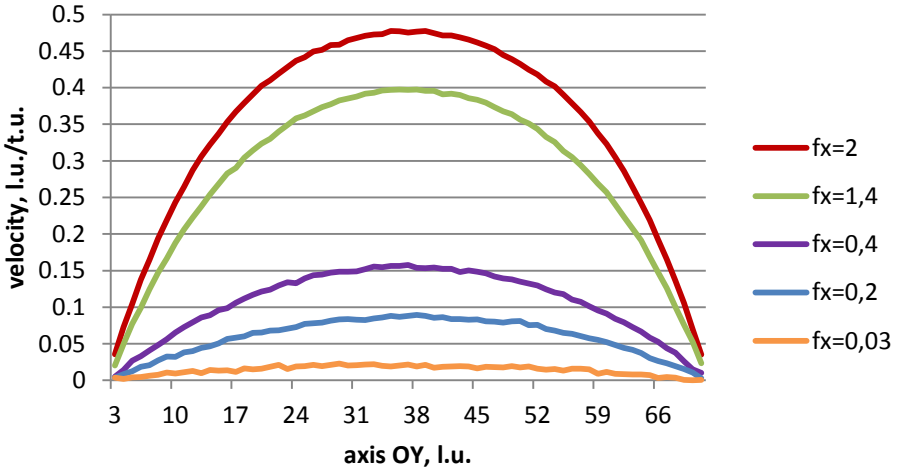


***Figure 9**: Parabolic velocity profiles for the channel of the size $L = 550\ l.u.$, $d = 75\sqrt{3}/2\ l.u.$ and various f_x*

The relationship between flow rate and channel width was also studied. Predicted and simulated results were obtained and compared. Good agreement between both types of results was here observed for a range of channel width $25 \div 100\sqrt{3}/2\ lattice\ units$, and flows created by the pressure gradient as a result of $f_x = 0{,}4 \div 0{,}03$. These results provided information about the appropriate settings for future simulations.

Furthermore, based on a computer simulation outputs the Darcy's law was verified. The linear dependence between flow rate in a steady state and pressure gradient was proved for all simulated channel width. As an example, flow rate as a function of the pressure gradient for channel width $d = 75\sqrt{3}/2\ l.u.$ is presented in *Figure 10*.

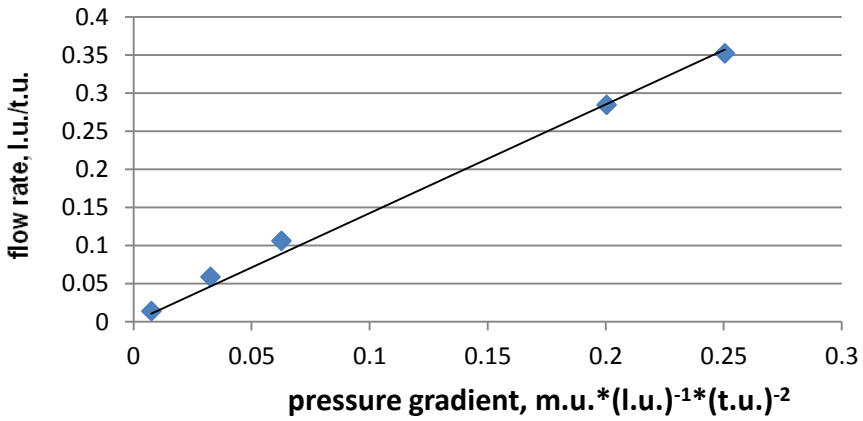


***Figure 10**: Varification of the Darcy's law. The flow rate as a function of pressure gradient for channel width $d = 75\sqrt{3}/2\ l.u.$ and various f_x*

Pressure gradient was here obtained as a "total force" nf_x divided by the product of the channel length and the channel width $L \times d$, where n represents the number of lattice nodes occupied by the imaginary ventilator.

All outputs of the presented Poiseuille flow simulation are in a good agreement with similar simulation experiment realized by *Rothman* in [8].

4.4.Computer simulation of the two-dimensional fluid flow through porous structure

The developed LGCA algorithm was applied to the simulation of a fluid flow through porous structure and used for the study of a physical phenomenon, the existence of which has not been demonstrated experimentally using accessible visualization techniques. The phenomenon concerned to the fluid flow through assembled filters. The theoretical assumption that special orientation of the fluid inside those filters leads to the good filtration characteristics of them was founded in literature [9]. Relationship between filtration characteristics and geometry of the internal structure of the filter was empirically obtained [10]. But hypothesis concerning to convolution of the flow direction at the boundary with porous media was not proved.

Developed LGCA algorithm was modified for that study. Based on twelve computer simulations the reorganization of the fluid flow inside declined porous structure was obtained for different simulation setups. The design of the assembled filter was slightly simplified: fluid has flown only trough the one part of a filter pleat. For that reason, porous medium was placed in the middle part of the channel at the defined inclination angle α (see *Figure 11*). Influence of the inclination angle (i.e. 15^o, 35^o and 55^o) and porosity of the porous medium (0.95, 0.9, 0.85 and 0.7) was studied.

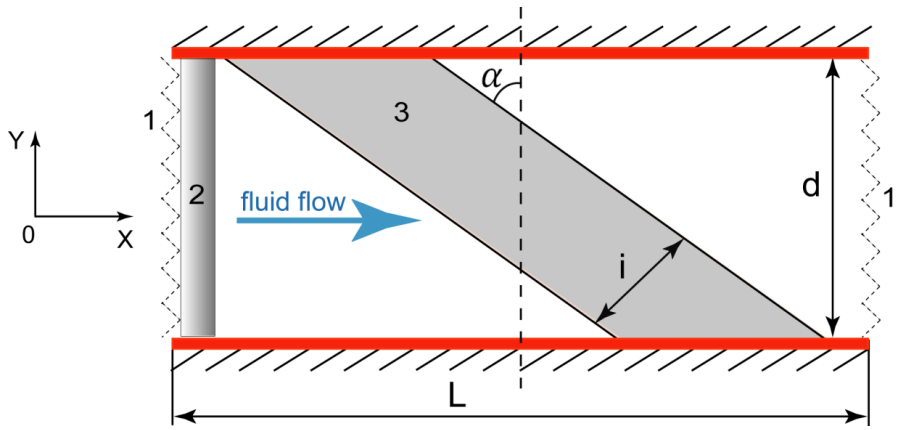
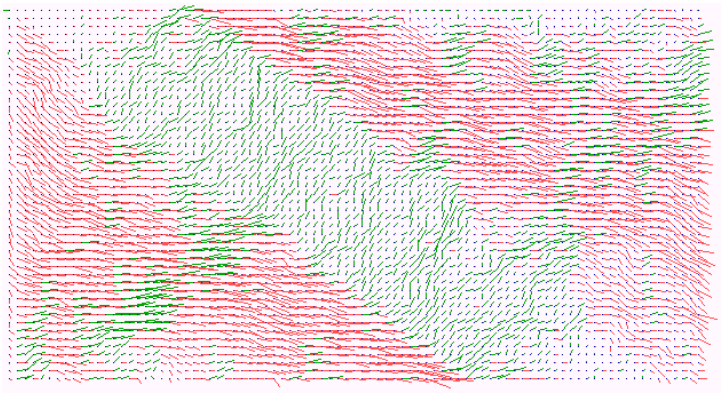


Figure 11: *The geometry of two-dimensional channel for fluid flow through porous medium simulation:* ***L*** *is the length and* ***d*** *is the width of the channel,* ***α*** *is an inclination angle of the porous medium,* ***i*** *corresponds to the thickness of the porous medium, 1 – periodic boundary conditions, 2 – the imaginary ventilator created the flow.*

For that reason velocity fields were monitored and expressed by graphical manner for all setups of the simulated system. Velocity vectors were obtained by averaging over $5\ l.u.\times 5\ l.u.$ squares on the lattice and over a period of time when the steady flow state was achieved.

From the *Figure 12a* it is evident that on the interface between the free channel area and the porous structure appears a reorganization of fluid velocity directions. For better realization of the velocity vectors two colours were used. If the velocity vector pointed in a first or second quadrants (i.e. it is from the interval $(0, \pi]$), then it got green colour, other way, it turned into red one. Here it is possible to see that the fluid enters into the porous material perpendicularly. The same results were obtained when the inclination angle α of porous medium was 15^o, and 55^o and the porosity was 0,9 and 0,85. Some regions of the porous medium were relatively stagnant. The local fluid flow in "blind pores" close to channels walls was zero.

a



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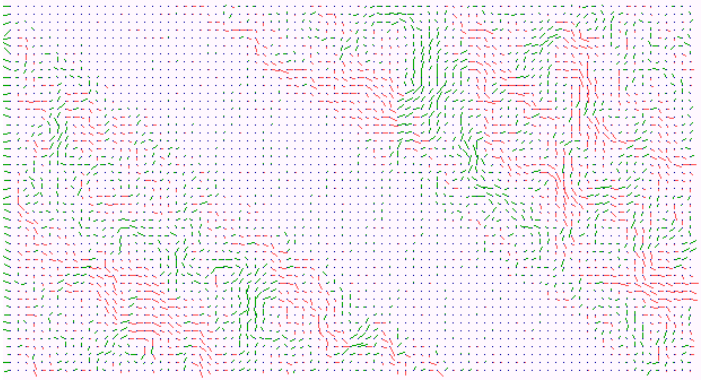

Figure 12: *Directions of the fluid velocity vectors inside the declined porous material with random structure for porosity 0,95 (a) and 0,7 (b). The inclination angle is α=35°.*

In a case of very dense structure of the porous medium (i.e. porosity 0,7 – see *Figure 12b*) stagnant area was obtained over the whole space of the porous medium. The geometry of this porous medium corresponds to the structure of nanofibre materials suitable for filtration. The local fluid flow in such a dense porous structure was close to zero. Winding paths monitored in front of, and behind the porous medium. Circulating eddies were monitored in those parts of the channel.

The results obtained from the computer simulation have shown that proposed LGCA algorithm is suitable for a theoretical prediction of a fluid flow through porous structures and also it can be used as a visualization tool.

5. Zhodnocení výsledků a nových poznatků / Evaluation of results and insights

Based on a study that was done in a frame of this work, the suitability of Lattice Gas Cellular Automata approach for fluid flow in porous structures modelling was demonstrated. Contributions of this work can be formulated as following:

- It was pointed that the theoretical approach, Nevier-Stokes equation, that being used as a theoretical description of the fluid flow phenomenon for many years, is not suitable for a study of fluid flow in all range of modern textile structure. It has limitations in continuity of the flow and it is not valid when fluid flows through the nanoporous structure. It was found, that Bolzmann approach is valid in all regimes of the flow because of its discrete nature. Therefore models/methods, which consider individual particle dynamics and reflect Boltzmann equation, are suitable for study the transport properties of nanomaterials and multilayer textiles.
- According to the principles of the Lattice Gas Cellular Automata my own FHP-1 LGCA algorithm was created. It is proposed for two-dimensional non-deterministic fluid flow simulation. Main blocks of the basic algorithm are developed for general-purpose computers, their specification and functions are analysed in detail.
- Tree modifications of the created algorithm are presented. Two of them are used for verification of the algorithm. Simulations of the Brownian motion and Poiseuille flow are here presented as benchmark tests. Both tests were successful and proved a good agreement between theory and results obtained from these simulations. Algorithm

created for the Brownian motion simulation additionally allows the study of diffusion phenomena and modelling of polymer molecules shapes.

- Modified LGCA algorithm, was used in a study of a special type of filters – i.e. assembled filters. Fluid flow through inclined porous structures of different porosity was studied. One of the simulated porous media had a similarity with the random nanofibre structure. The theoretical assumption that fluid flows perpendicularly to the surface of filter pleats was proved by a set of computer simulations. Thus, it was concluded that LGCA approach is suitable for a theoretical prediction of the fluid flow inside porous structures and also it can be used as a visualization tool.

6. Práce autora se vztahem ke studované problematice / Publications related to the author studied the issue

Chapter in a book:

- **Lukas, D. and Ocheretna, L.** The cellular automata lattice gas approach for fluid flows in porous media. [ed.] N. Pan and P. Gibson. Thermal and moisture transport in fibrous materials. Cambridge: Woohnead Publishing Limited, 2006, pp. 357-401.

IF publication

- **Lukas ,D., Pan, N., Sarkar, A., Weng, M., Chaloupek, J., Kostakova, E., Ocheretna, L., Mikes, P., Pociute, M., Amler, E.** Auto-model based computer simulation of Plateau–Rayleigh instability of mixtures of immiscible liquids. Physica A: Statistical Mechanics and its Applications, Volume 389, Issue 11, 1 June 2010, pp. 2164-2176.

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- **Očeretna, L.** Teorie buněčných automatů. Klas modelu FHP. Písemná práce ke zkoušce „Vybrané partie z teorie oboru", FT TUL, Liberec 2003.
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8. Summary

The thesis is focused on the modelling of fluid flow in porous media. The aim of the work was to develop an appropriate model for simulation of fluid transport regardless of the flow regime.

The model, developed in the frames of the work, is based on Lattice Gas Cellular Automata. The model is non-deterministic and fully discrete. It is presented by means of algorithm created in a C++ programming language. The algorithm allows computer simulation of the fluid flow through different porous structures, including nanofibre materials, where the pore size is on the order of free path of molecules and flow thus loses its continuous properties.

The model is verified for two phenomena as the Brownian motion and Poiseuille flow are. The presented model is used to the study of fluid flow inside assembled filters with different density of porous media. Simulation results proved the hypothesis regarding to the reorganization of the flow inside the filter and its orientation perpendicularly to the pleat surface.

Předložená disertační práce je zaměřena na modelování proudění tekutiny porézním prostředím. Cílem práce bylo vytvoření vhodného modelu pro simulaci transportu tekutiny nezávisle na režimu jejího proudění.

Předložený model vychází z podstaty buněčných automatů a využívá rysy mřížového plynu. Model je nedeterministický a plně diskrétní. Pomocí programu vytvořeného v C++ programovacím prostředí umožňuje počítačovou simulaci a studium proudění tekutiny různými porézními strukturami, včetně nanomateriálů, kde velikosti pórů řádově se blíží délce volné dráhy molekuly a proudění tak ztrácí své kontinuální vlastnosti.

Funkce modelu jsou ověřeny pomocí dvou testů, tj. simulací Brownova pohybu a Poiseuillova proudění. Předložený model je použit na studium proudění tekutiny skládanými filtry s různou hustotou porézního prostředí. Výsledky simulací prokazují hypotézu týkající se orientace proudění kolmo k povrchu skladů filtru.

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