LGFLOW: A NUMERICAL WATER-TABLE FOR FLUID FLOW VISUALIZATION BASED ON LATTICE-GAS AUTOMATA.

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Abstract. The present paper describes LGFlow, a two-dimensional interactive numerical *water table* for fluid flow visualization, developed for educational purposes and based on lattice gas models. Lattice gas models are relatively recent and were developed to perform hydrodynamic calculations, being object of considerably interest in the last years. Two models are used, the Boolean model and the Boltzmann model. In its simplest form, Boolean model consists of a regular lattice populated with particles that hop from site to site in discrete time steps in a process, often, called *propagation*. After propagation, particles in each site interact with each other in a process called *collision*, in which the number of particles and momentum are preserved. An exclusion principle is imposed in order to achieve better computational efficiency and a Boolean variable n_i (r, t) is assigned to each direction in a site to indicate the presence (n_i=1) or absence (n_i=0) of a particle in that direction. Boltzmann model has the same principles but works with real variables related to the ensemble average values of $<n_i$ (r, t)>. Despite its simplicity, these models reproduce Navier-Stokes equation behavior for low Mach numbers. The present work deals with two-dimensional models based on a hexagonal lattice. Intended to be a *self-learning* tool in fluid-mechanics education, LGFlow received an attractive and *user-friendly* graphics interface based on Coi-lib© with an on-line visualization window for velocity and pressure fields and boundary conditions are easily managed from *form* windows. This work, some visualization examples are given of fluid flow around obstacles and inside constrictions and compared with available data found in fluid mechanics literature.

Keywords: fluid flow, numerical water table, lattice-gas

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1. INTRODUCTION

This paper presents LGFlow, a numerical *interactive* water table developed for education purposes in the learning of fluid mechanics and related disciplines.

LGFlow simulation algorithms are based on Lattice Gas Automata models (LGA).

In lattice gas automata models (LGA), fluid is supposed to be represented by a finite set of particles. Each of these particles has a finite number of degrees of freedom and can move following, only, the directions of a regular lattice, jumping from one lattice node (sites) to another in unitary time steps. Each lattice node is the site of a collision process between particles. In this way, their dynamical evolution is described following a sequence of unitary time steps. Each time step evolution is performed, in accordance with a collision step followed by a propagation step.

Description of fluid flow by following the dynamical evolution of a finite set of material points in random motion, considering elastic collisions between these points, was achieved in the late XIX by Maxwell and Boltzmann, founding the Kinetic Theory of Gases.

In kinetic theory, continuous variables are used for describing space, time and velocities. Broadwell (1964) was the first to use discrete variables, proposing a three-dimensional model with six directions following the orthogonal directions of a Cartesian frame, establishing the Discrete Kinetic Theory.

The first LGA model was introduced in the early seventies by Hardy, Pazzis e Pomeau (1973, 1976). In the first half of the eighties, several papers from Wolfram (1983, 1984) on cellular automata had a great influence on LGA development. A critical step was given by Frisch, Hasslacher e Pomeau (1986). They suggested a hexagonal LGA model, further called FHP model.

LGA theoretical development was achieved by introducing *ensemble* averages over a set of LGA realizations. Chaos molecular hypothesis gives Boltzmann equation in discrete form, which has an H-theorem and a Fermi-Dirac distribution as equilibrium solution. Further, use of Chapman-Enskog method shows that FHP and several other LGA models are capable of retrieving hydrodynamic equations in the limit of low Reynolds and Mach numbers.

Boltzmann's equation describes *what is expected* to be the dynamical evolution of the particles distribution function N_i (**X**, T), related to direction i, lattice site **X** and time T, when a *great* number of LGA realizations are considered.

Boltzmann's equation gave rise to another kind of lattice gas models, presently called Lattice Boltzmann Models (LB) which are based on the relaxation of N_i to an *equilibrium* distribution N_i^o, written in the manner to retrieve hydrodynamics, without the intrinsic limitations of Fermi-Dirac based LGA older models.

An LB model based on a hexagonal plane lattice is used in LGFlow, for describing intermediate Reynolds number flows. Sample studies showed that LGFlow module based on LB model can be used up to Re=1000 in a Pentium-II, 124 Mb resident memory PC.

In the next, the basic fundamentals of lattice gas models are presented, followed by a brief presentation of LGFlow software and machine requirements. Finally, visualization results of using LGFlow as a numerical water table are presented and discussed.

2. LATTICE GAS FUNDAMENTALS

2.1 Kinetic Theory

Although kinetic theory dates from Bernoulli (1738), who tried to explain *elasticity* of gases considered them as a set of particles in random motion, its main development occurred in the second half of XIX century by Maxwell and Boltzmann. This was achieved by

introducing *probability theory* in the study of N-body problem in classical Lagrangian mechanics.

In fact, no *general* solution exists for the N-body problem when N is larger than 2.

Considering a gas as a set of a *very large* number N of material points, with translational degrees of freedom, it is possible to use probability laws when considering

$$f(\mathbf{r}, \mathbf{c}, t)$$

as a probability density function for the number of particles with velocities between **c** and **c** + d**c** found, at time t, inside an elementary volume d**r** of the physical space.

Considered as a continuous function, the velocity distribution function f(**r**, **c**, t) is modified in the absence of external forces by the streaming of particles and by collisions in **r, c** space. Its evolution is given by Boltzmann's equation:

$$\partial_t f + c_\alpha \partial_\alpha f = (\partial_t f)_{coll} \tag{1}$$

where ∂_t is a time derivative and ∂_α means a spatial derivative.

Boltzmann's equation has an H-theorem and an equilibrium solution, explaining irreversibility of macroscopic behavior as due to inter-particle collisions. In this way, collisions are considered to be the main mechanism responsible for dissipation phenomena in fluids.

In the early XX century, Chapman and Enskog, simultaneously, formally retrieved hydrodynamic transport equations from Boltzmann's equation, by considering the first statistical moments of the velocities distribution function (Chapman and Cowling, 1970):

$$\partial_t(\rho) + \partial_\beta(\rho v_\beta) = 0 \tag{2}$$

$$\partial_t(\rho v_\alpha) + \partial_\beta[\rho v_\alpha v_\beta] = -\partial_\alpha(p) + \partial_\beta\{\mu[\partial_\beta(v_\alpha) + \partial_\alpha(v_\beta)]\} + \partial_\alpha\{\kappa[\partial_\beta(v_\beta)]\} \tag{3}$$

where **v** designates fluid velocity.

In the above equations:

i) pressure p is directly related to mass density ρ by ideal gas law,

ii) first, μ, and second, κ, viscosity coefficients are given in terms of the collision term in the Boltzmann's equation and related to ideal gas behavior.

These two above remarks are very important in the context of lattice gas development. In fact, this means that: a) a set of particles follow ideal gas law, when *long-range* interaction are not considered; b) hydrodynamic equations are *insensible* to the details of collision processes, which appear related, only, to the transport coefficients themselves μ and κ.

The first observation is of no consequence in the low Mach number approximation for incompressible flow.

The last observation was the basis for the development of LGA models.

2.2 Lattice Gas Automata Models: Microscopic dynamics

In LGA models (Fig. 1), particles are restricted to move along the directions of a *regular* lattice, jumping from one lattice site to another after unitary time steps. Lattice particles are *not to be considered* as gas molecules, but just as *model particles*, with the same *overall* statistical behavior of a large set of gas molecules. In this way lattice particles follow *mass* and *momentum* conservation in collisions at lattice sites. For each time step, the dynamic evolution of the model is, then, given in two steps. In the first step, designated as *collision step*, the state of site X is changed following collision rules conceived so as to preserve total mass and momentum of the site. In the second step, called *propagation step*, particles are propagated to the neighbor sites, in accordance with their direction at site X after collision step. In addition, an *exclusion* principle is used, avoiding two particles to be, simultaneously, at the same link between two sites, at the same time step. Due to the nature of LGA models, this restriction is not to be considered as a *physical* restriction, but a way for reducing computational requirements, enabling to work with Boolean variables.

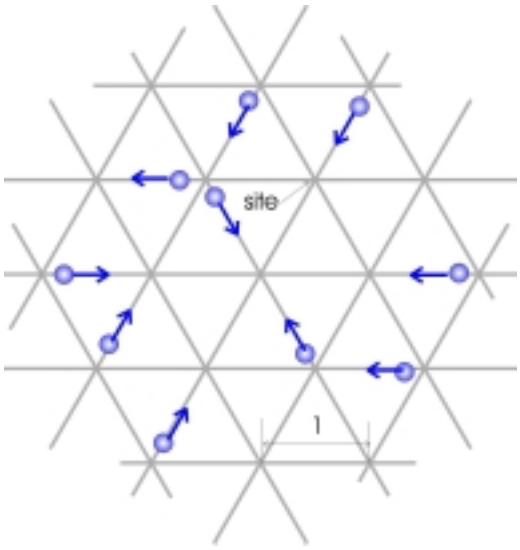

Figure 1. A hexagonal, two-dimensional lattice gas model.

Consider a regular lattice where each site **X** has b_m neighbors. A Boolean variable n_i (**X**, T) is assigned to site **X** to indicate the presence (n_i=1) or absence (n_i=0) of a particle in direction i at time T. Vector $\mathbf{c}_i$ indicates the unitary velocity vector pointing in direction i. A finite, at most b_r, number of rest particles is allowed to populate site X. Let $b= b_m + b_r$. Let S be the set of all possible states of a given lattice site. Obviously S has 2^b elements.

A given state s of S can be represented by the array:

$$s=(s_{o1},.. ,s_{obr}, s_1, ...,s_{bm}) \quad (4)$$

where the first b_r bits indicate rest particles and the following b_m bits indicate moving particles.

Microscopic evolution is described by the following equation:

$$n_i(\mathbf{X}+\mathbf{c}_i, T+1)=n_i(\mathbf{X},T) + \omega_i(n_{o1},.. n_{obr}, n_1, ..,n_{bm}) \quad (5)$$

where ω_i: $(n_{o1},.. n_{obr}, n_1, ..,n_{bm})\rightarrow\{-1,0,1\}$ represents the collision operator which can take the values –1, 1 or 0, depending on the state $(n_{o1},.. n_{obr}, n_1, ..,n_{bm})$ of site X, before the collision.

Considering α: SXS $\rightarrow$ [0,1] to be the transition matrix (with 2^b X2^b elements), the collision term can be written as

$$\omega_i(n_{o1},.. n_{obr}, n_1, .., n_{bm}) = \sum_s \left[\sum_{s'} \alpha(s,s')(s'_i - s_i) \prod_{j=1}^{b} \delta(n_{j+i}, s_{j+i}) \right] \quad (6)$$

where s' designates post-collision states.

2.3 Ensemble averages. Macroscopic behavior of a LGA model.

Lattice-gas models have three description levels. In the more detailed level, n_i(**X**,T) are described for every X and T. In general, this is too refined in the description of macroscopic phenomena. A less detailed description is given by furnishing the expected values $N_i=<n_i(\mathbf{X},T)>$, obtained as *ensemble* averages over a large number of realizations. In the third level, only the first moments of N_i are furnished for each X and T. In fact, in the continuum limit, when Knudsen number is very small, it can be show that the first moments of N_i are related between themselves through a closed system of equations, i.e., the hydrodynamic equations.

Classically, in the framework of *Fluid Mechanics*, we try to solve this closed system of equations and obtain numerical values for pressure and velocity fields. In LGA conception, expected values N_i (X, T) result from several Boolean realizations. Macroscopic equations are, then, obtained from the first moments of N_i. What we are going to show, in the following, is that, under certain restrictions, these moments satisfy classical hydrodynamic equations.

$N_i(\mathbf{X},T)$ is defined as the expected value of $n_i(\mathbf{X},T)$, over an *ensemble* of realizations, run using randomly chosen initial conditions and satisfies.

$$N_i(X+c_i, T+1)=N_i(X,T) + \Omega_i(N_{o1},.. N_{obr}, N_1, ..,N_{bm}) \quad (7)$$

which is the Boltzmann's equation for the lattice, in discrete form. Taking molecular chaos hypothesis into account, the collision term can be written as:

$$\Omega_i(N_{o1},.. N_{obr}, N_1, ..,N_{bm})=$$

$$< \omega_i (n_{o1},.. n_{obr}, n_1, .., n_{bm}) >= \sum_s \left[\sum_{s'} A(s,s')(s'_i - s_i) \prod_{j=1}^{b} N_j^{s_j} (1-N_j)^{1-s_j} \right] \quad (8)$$

It may be show that, as a consequence of *exclusion principle*, this equation has a Fermi-Dirac distribution as equilibrium solution.

2.4 LGA Hydrodynamic Equations.

The first two moments of distribution function N_i are:

$$\sum_i N_i = \rho \quad (9)$$

$$\frac{1}{\rho}\sum_i N_i c_i = \mathbf{u} \quad (10)$$

where $\rho=\rho(\mathbf{X}, T)$ is the total number of particles and $\mathbf{u}= \mathbf{u}(\mathbf{X}, T)$ is the macroscopic velocity in site X, at time T, in *lattice units*.

Using Chapman-Enskog method, a closed system of equations is obtained relating these two first moments, in the limit of low Reynolds number and Mach number M<<1

$$\nabla.\mathbf{v} = 0 \quad (11)$$

$$\rho\partial_t(v_\alpha) = -\partial_\alpha(p) + \rho\nu\partial_\beta\partial_\beta v_\alpha \quad (12)$$

where $\mathbf{v}=(h/\delta)\mathbf{u}$, h is a space scale and δ is a time scale, converting lattice to physical variables

For high Reynolds number, *non-physical* lattice effects are present in the hydrodynamic equations. These effects are to be attributed to the nature of Fermi-Dirac equilibrium distribution, associated with exclusion principle.

2.5 Lattice Boltzmann Model.

Lattice Boltzmann models are based on relaxation equations for the velocities distribution function. The most common are written as:

$$N_i(\mathbf{X}+\mathbf{c}_i, T+1)-N_i(\mathbf{X},T) = \frac{N_i(\mathbf{X},T) - N_i^o(\mathbf{X},T)}{\tau} \quad (13)$$

where τ is a relaxation time, in lattice units.

Equilibrium distribution, N_i^o, is written in the manner so as to retrieve hydrodynamic equations in the form

$$\nabla.\mathbf{v} = 0 \quad (14)$$

$$\partial_t(v_\alpha) + \partial_\beta\left[v_\alpha v_\beta\right] = -\frac{1}{\rho}\partial_\alpha(p) + \nu\partial_\beta\left[\partial_\beta(u_\alpha)\right] \quad (15)$$

describing incompressible flow, without the limitations of Boolean models and able to describe high Reynolds number flows.

3. FLOW SIMULATION IN LGFlow

3.1 Simulation Grid

LGFlow has a small grid editor (Fig. 2) and is able to open black and white bitmaps, where velocity is to be calculated at the grid points in the flow region.

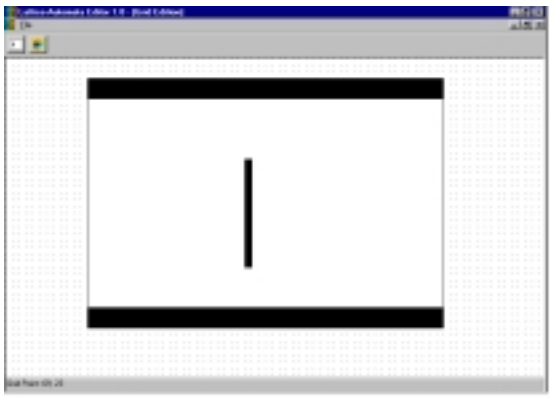

Figure 2. LGFlow grid editor.

B&W bitmaps are usually codified as rectangular arrays of black and white pixels. LGFlow uses a hexagonal plane lattice, where each site has 6 neighbors. This is performed in accordance with Fig. 3 showing how LGFlow establish a 6-neighboring relation on a rectangular grid.

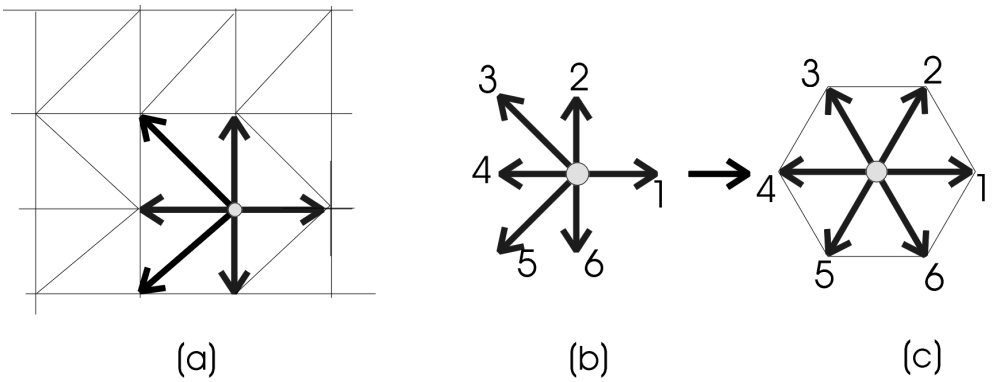

Figure 3 (a) Establishing a 6-neighboring relation on a rectangular grid. (b) Sites 1-6 are considered to be the 6 next neighbors of the central site 0. (c) Macroscopic velocity is calculated at central site by using the hexagonal configuration.

3.2 Boolean Model.

Evolution equation, Eq. (5), is the basic algorithm used by LGFlow for simulating flow. At time t=0, lattice particles are randomly distributed on the lattice sites. For each pre-collision configuration s, post-collision configuration s' is randomly chosen between those states s' with the same mass and momentum. This is performed by using a transition table located in computer resident memory and constructed, previously to simulation, following the particular LGA model used. LGFlow is based on a hexagonal lattice with b_m=6 and b_r=1; collisions exclude pre-collision state when transition is possible. This model is called FHP collision full-saturated model due to Frisch, Hasslacher e Pomeau (1986). In propagation step, each particle at direction i is propagated to the neighbor site $\mathbf{X}+\mathbf{c}_i$.

At solid boundaries, particles that reached boundary sites are bounced back in the same direction, at the next time step. This is the, frequently used, *bouncing-back* condition, avoiding flow slipping at the boundary, and assuring the limiting condition $\mathbf{u}=\mathbf{0}$.

In simulating incompressible flows, considering the state equation relating pressure to mass density, pressure gradients can, only, be promoted, associated to density gradients, which must, in turn, remain small. This problem is eschewed in conventional simulation by using Navier-Stokes *low Mach number approximation*. Nevertheless, in LGA simulation, flow is the result of billiard balls collisions and incompressibility can only be assured by

working with small $|\mathbf{u}|$ meaning small M=u/c_s, where c_s is the speed of sound in *lattice units*. It can be show that c_s=0.65, in present Boolean model. In this way, in LGA simulation a pressure gradient can only be created associated to a density gradient, which must be small, assuring M<<1 and avoiding compressibility effects.

For simulating flow, LGFlow Boolean module uses periodic conditions and a *pumping zone* at the beginning of the water-table. Periodic conditions assure that particles that escape from the end of the *water-table* are re-introduced at its beginning. In *pumping zone*, momentum is added to the particles, forcing them to the flow domain. In this way, LGFlow tries to mimic the real conditions related to a *real* hydraulic closed looping.

3.3 Boltzmann Model

LB model simulation is very easy to carry out. Initial conditions are source data and given in terms of ρ and components x and y of velocity **u** for each site **X**. Equilibrium distribution $N_i^o(\mathbf{X},T)$ is, then, calculated, for each site **X**. Boundary sites are considered to have an equilibrium distribution $N_i^o(\rho,\mathbf{u})$, given in terms of the specified velocity **u** at the boundaries. In the following steps, relaxation equation, Eq. (13), is, successively, used to calculate N_i. At each step, velocity is calculated using Eq.(10), giving the flow field and enabling visualization at LGFlow simulation window.

4. RESULTS

4.1 Boolean Model. Fig. 4 presents a partial view of the main flow visualization window of LGFlow, showing the simulation results of a plane Poiseuille flow, using a *Boolean model*. Physical domain had 20X80 points and simulation took about 5 minutes in a Pentium II, 400 MHz computer, after 10^5 steps. Although representing a very simple flow problem, Poiseuille flow has been used for validation purposes. Simulation was performed with Re=5 and M=0.09.

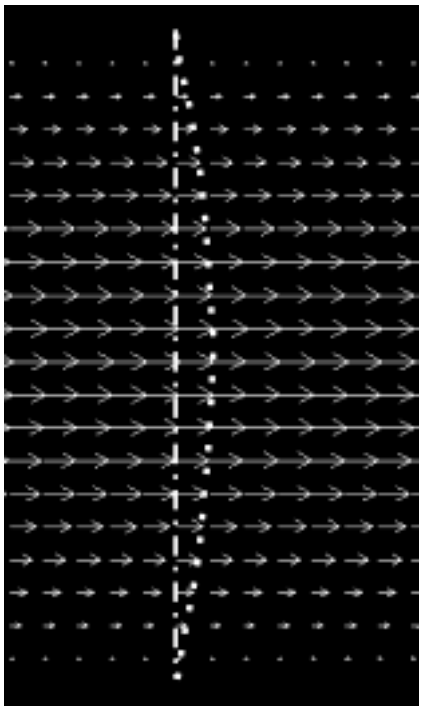

Figure 4 Partial view of LGFlow visualization window, showing a plane Poiseuille flow

Boolean models are most appropriate to simulate *low Reynolds number flows* and were successfully used by present authors to simulate fluid flow through porous structures, in the prediction of intrinsic permeability of petroleum reservoir rocks. In these cases Re ~1 (Santos *et al.*, 2000a,b). Results confirmed the reliability of Boolean method for calculating intrinsic permeability, for five different Brazilian sandstones. Fig. 5 presents a sample visualization of velocity field inside a two-dimensional porous structure, obtained by LGFlow. Pumping zone is 10 lattice units large, where a particle going to the left has a probability p=0.08 to be turned back to the right. Probability p corresponds to *pump strength* and will be responsible for accelerating the fluid toward the porous structure. Figure also shows two free flow zones, assuring flow uniformity, at the entry and rear faces of the porous structure.

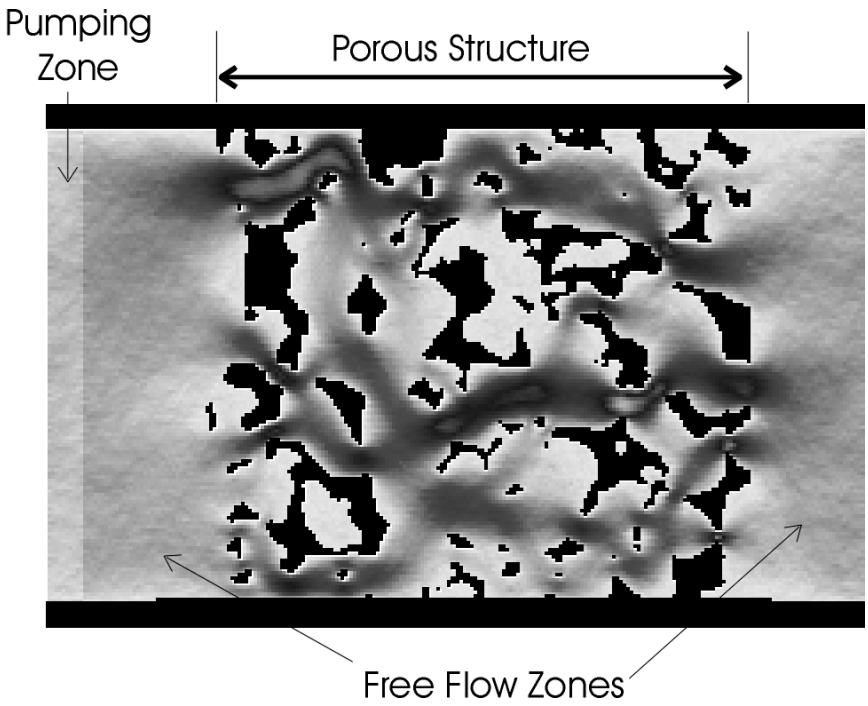

Figure 5. LGFlow simulation through a porous structure using Boolean model.

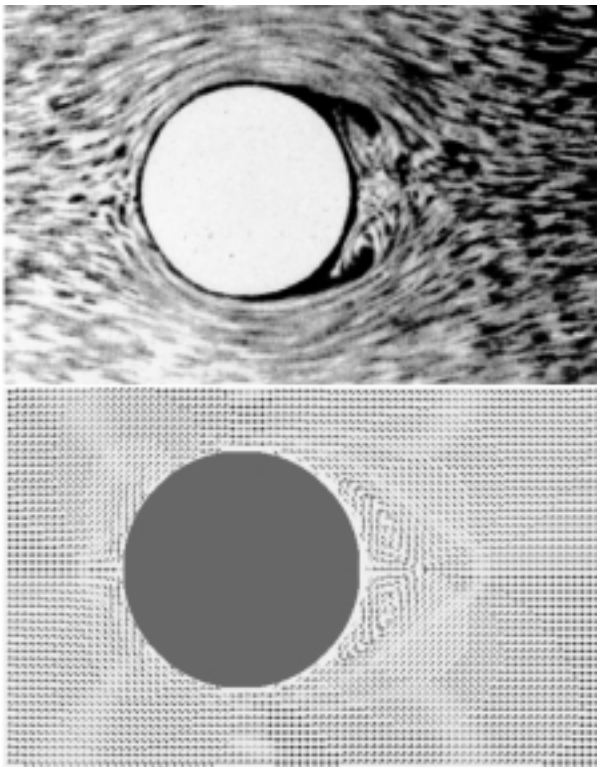

Figure 6. Flow past a circular cylinder. Re=70. Comparison with a flow visualization taken from Batchelor (1970)

4.2 Boltzmann Model. Fig. 6 shows simulation results using LB model for the flow past a circular cylinder at Re=70. Simulation starts by supposing fluid at rest at t=0 and by imposing a constant velocity to the right at all four boundaries. Results are related to the first 1000 simulation steps and simulation is compared to a flow visualization taken from Batchelor (1970). Both simulation and visualization show two vortices with opposed rotations, behind the cylinder, created as a result of boundary layer separation. These two vortices grow, moving downstream and asymmetry-generated instability degenerates the flow field to periodic waves, behind the cylinder (von Karman vortices).

This is shown in Fig. 7 for flow past a rectangular plate.

Considering flow against obstacles and inside constrictions LGFlow simulation results have been *qualitatively* compared with experimental visualization and numerical results, for several Reynolds number.

In addition, although partially, LGFlow has been validated against analytical and finite volume methods and by comparison with experimental data for several problems, including flow inside lit-driven cavities. In this sense, Fig. 8 shows the *real* transition when fluid starts

from rest attaining stationary state, when the plate closing a fluid cavity starts moving to the right at constant speed (Ghia, 1982). Simulation was performed for Re between 100 and 3200, giving excellent agreement with numerical results obtained by using finite volume methods. Figure 9 shows a comparison between simulation and Ghia's results for Re=1000.

5. CONCLUSIONS

Present paper describes the main models and algorithms used in LGFlow, conceived to be an interactive numerical water table for educational purposes.

In this way, LGFlow received an attractive and *user-friendly* graphics interface with on-line visualization windows for velocity and pressure fields. Boundary conditions are easily managed from *form* windows. LGFlow is, thus, easily managed by undergraduate and graduate students in the learning of fluid mechanics and related disciplines.

In addition, although based on a very simple hexagonal lattice, validation results, apparently, confirm the reliability of LGFlow to be used in simulating two dimensional flows.

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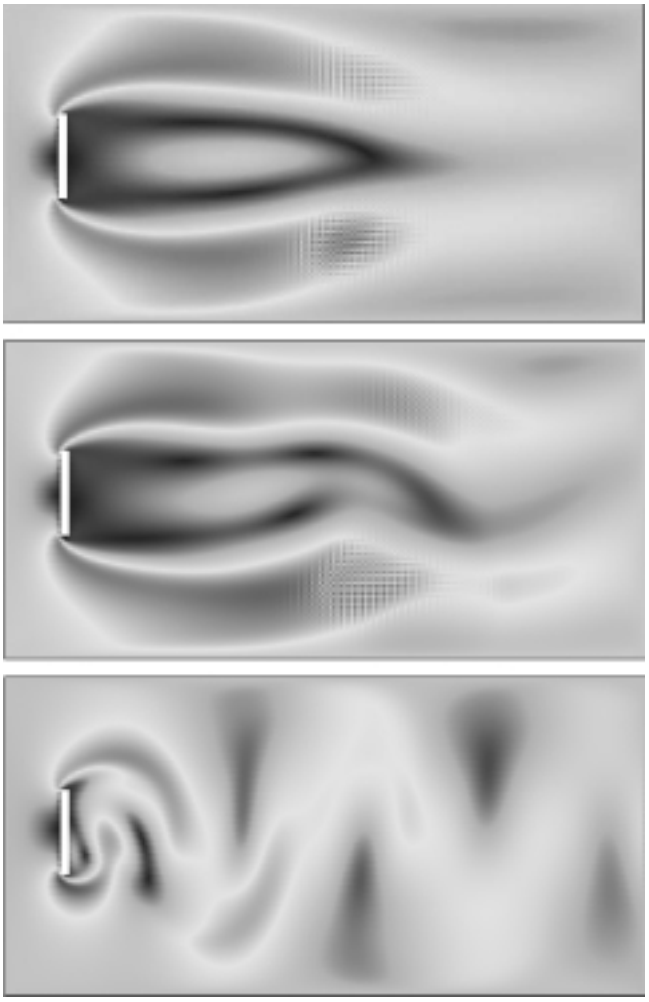

Figure 7. von Karman vortices: speed fields for 2000, 4000 and 15000 time steps (Re=467)

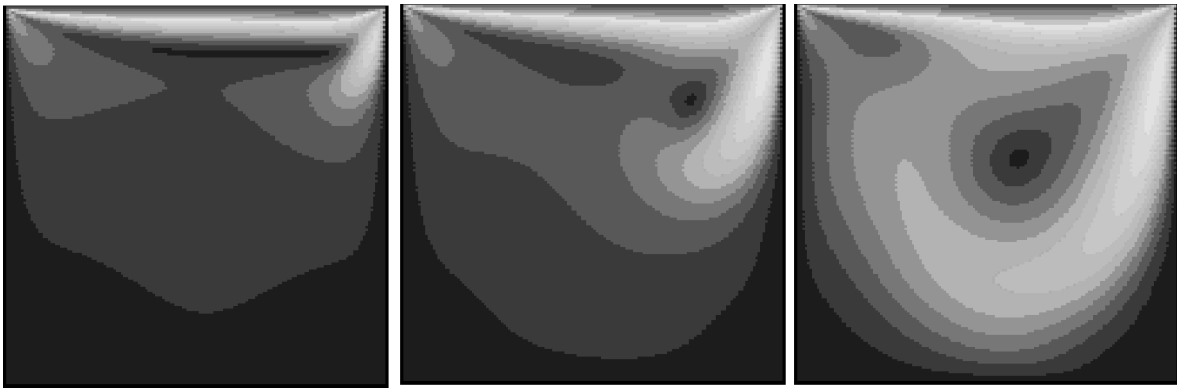

Figure 8. Lid -driven cavity: LB simulation starts from the rest to stationary state. Flow domain: 155X155. Figure shows speed fields for 2000, 6000 and 25000 time steps (Re=400, M=0.09).

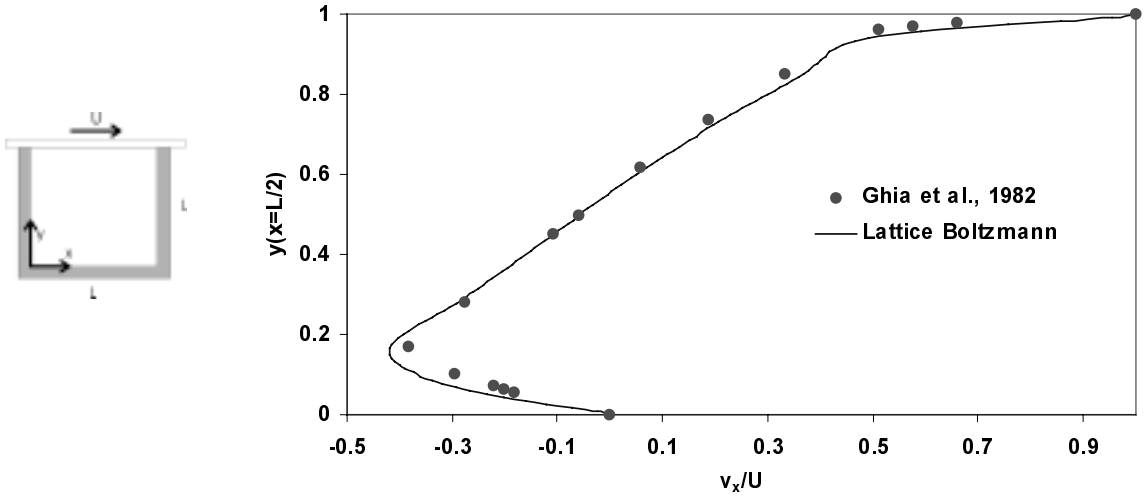

Figure 9 Velocity v_x (y) at x=L/2 for Re=1000, after flow attains stationary state.

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