LATTICE GAS HYDRODYNAMICS SIMULATION OF FLUID FLOWS INSIDE A POROUS MEDIUM

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ABSTRACT

A lattice gas hydrodynamic model of fluid flow inside a porous medium was developed and benchmarked against analytical solution for a conduit flow case. The porous medium was modeled using a new method of generating the porous geometry using fractals. A fractal dimension was used to control the porosity of medium. As the fractal dimension increases, the porosity of the medium increases. The lattice gas hydrodynamic realistically tracks the micro-scale behavior of the fluid inside the porous medium. The complex flow structure (including back flow) is clearly predicted by the model.

INTRODUCTION

Simulation of fluid flows inside porous media is complicated by the complex flow geometry. Because of this complexity, classical methods such as finite difference, finite volume, and finite element are most incapable of predicting details of flow inside a porous medium. Such flows are important for researchers who are seeking to understand important phenomena such as oil and gas recovery in a reservoir or mechanics of radionuclide or contaminant transport. In this work we have developed a discrete method for modeling of transport phenomena in a porous medium based on lattice gas cellular automata (LGCA). Lattice gas methods were first explored by Ulam and Von Nuemann at Los Alamos during 1960s. The LGCA method consists primarily of a discrete-time discrete-space dynamical system that describes the real world problem. The physical problem may contain discontinuities (such as fractured rock). In LGCA, representative particles reside on a regular lattice. These particles experience local interactions among themselves governed by a set of collision and translation rules. In this work we will focus on application of LGCA in porous medium where a two-dimensional flow inside a porous medium is simulated by LGCA. A new contribution of this work is a unique method of generating the porous medium. The extension to three dimensions will also be discussed.

Background On Discrete Models

The derivation of Navier-Stokes Equations (NSEs) has its roots from the theory of elasticity where the fluid is assumed to behave as an elastic material. The continuum approach was impeded into this derivation. The NSEs experience difficulty when the medium contains discontinuities. An example of a discontinuity is flow inside porous medium containing fractures. Also, NSEs solution is extremely difficult to obtain in complex flow geometries present in a porous medium. Traditional methods for modeling of flow of homogeneous fluids in saturated porous media have been based on Darcy's law model. However, many limiting assumptions are normally imposed on

Darcy's model to allow for solution using finite element or finite difference methods. Hardy, Pazzis, and Pomeau introduced the first discrete space discrete time fluid dynamic system on a square lattice (Pomeau et. al. 1976). It was a simple binary model where particles resided on the vertices on a square lattice. These particles hopped from their site to neighbor sites without continuum limitation on their movement. After particles hopped to the nearest neighbors a collision step occured between particles. The collision step was governed by two rules. First, momentum was conserved, and second, mass (or the total number of particles) was conserved. This system was absolutely stable, however, it suffered from lack of isotropy. The model results did not agree with traditional NSE results. Consequently, the HPP model was not successful. In 1986, three French scientists Frich, Hasschler, and Pomeau presented a discrete space discrete time system on a hexagonal lattice (Frisch et. al., 1986). The hexagonal lattice satisfied isotropy and gave good results as compared with traditional NSE predictions. This model is known as the FHP.

Hexagonal Lattice Gas (FHP) Model

In this work, the hexagonal lattice gas (or the FHP) model was used. This model reproduces the behavior of the NSE on a two dimensional hexagonal lattice. It consists of a population of particles with unit mass and unit velocity that reside on a discrete space hexagonal lattice. The particles can hop in any six directions. Only one particle is allowed to travel in any direction in a cell. This step is called the translation step. Following the translation step is the collision step where particles, as in the HPP model, collide. The output of the collision is governed by conservation of mass and momentum. Because of the discrete nature of this model states and collision rules can be treated as Boolean operators where 1 means particle occupancy at a lattice location and 0 means absence of such a particle.

Macroscopic Quantities

Macroscopic quantities such as density, momentum, pressure, and temperature can be constructed from the FHP model using statistical averaging. Taking η_i as a Boolean variable that holds a value of 1 if a particle is present at a lattice site and a value of 0 if a particle is absent. Also, taking f_α to be the time average of n_α. Thus macroscopic density can be expressed as (Rothman, 1988)

$$\rho = \sum_{\alpha=1}^{\alpha=6} f_i \ . \qquad \text{(Eq. 1)}$$

Momentum can be expressed as

$$\rho u = \sum_{\alpha=1}^{\alpha=6} f_\alpha \cdot \mathbf{e}_\alpha \ . \qquad \text{(Eq. 2)}$$

These are the macroscopic relations on a discrete space discrete time dynamic system.

Porous Geometry Modeling Using Fractals

A new contribution of the worked described here is a unique method of generating the porous medium flow geometry using fractal mathematics. Fractal structure is important because it allows us to describe random structures with a mathematical model. Definitions of fractals are often dependent on the fields in which they are applied. However, all fractal structures have general characteristics: self-similarity, expression of a power-law relationship between two variables, and characterization of the fractal dimension.

One of the most useful mathematical models for random fractals in nature is the fractional Brownian motion (fBm) (Barnesly et. al., 1988). This model is created using white noise. White noise is generated using a pseudo random number generator. Taking the integral of the white noise over a specific frequency range will give the fBm motion. Most of the fractal computer graphics simulation nowadays depends on the fBm method. The fBm is only a function with one variable, usually time, which is characterized by the noise. The magnitude of the noise depends on the change of the fBm in successive time events. To provide insight into the ordering of the fBm a general statistical method called spectral synthesis method (SSM) is used. This method gives a measure of the fluctuation over a time scale. In this method we analyze the amplitude of the fBm rather than preserving the fBm motion. Because the amplitude of the fBm is a function of the frequency, the spectral density is a function of density. In general the spectral density is proportional to the frequency in the fBm model (Barnsely et. al., 1988).

$$S \propto \omega^{\beta}, \qquad \text{(Eq. 3)}$$

where the value of β is between -1 and -3 (Hardy et. al., 1994). The SSM depends on the Fast Fourier Transform to analyze the fBm motion. The discrete amplitude of spectral density is calculated from the equation

$$R_m = \sqrt{S(\omega_m)}. \qquad \text{(Eq. 4)}$$

The phase of the spectral density is assigned randomly between $-\pi$ and π. Thus the amplitude and phase arrays are converted into complex one using

$$G_m = R_m \cos(\theta_m) + iR_m \sin(\theta_m). \qquad \text{(Eq. 5)}$$

With the corresponding complex array G_m the inverse Fourier transform is taken to generate fBm sequences. Applying the same concept for two-dimensional case, the spectral density model is given by (Hardy et. al., 1994)

$$S(\omega_x, \omega_y) = A_{sd} \cdot \frac{B_{sd}}{\left(\omega_x^2 + \omega_y^2\right)^D}, \qquad \text{(Eq. 6)}$$

where ω_x, ω_y are the frequencies in x, and y directions. A_{sd} and B_{sd} are controlling parameters.

The corresponding discrete Fast Fourier transform (FFT) and Inverse Fast Fourier transform (IFFT) are given respectively by

$$A(x,y)=\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}a_{kl}e^{2\pi kix/N}e^{2\pi ily/N}\,, \qquad \text{(Eq. 7)}$$

$$X(x,y)=\frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}A(x,y)e^{2\pi kix/N}e^{2\pi ily/N}\,, \qquad \text{(Eq. 8)}$$

where, a_{kl} is the magnitude of the spectral density and N is the number of points in x or y directions.

As can be seen from equation 6, the parameters that control the spectral densities are spatial frequencies in x, and y directions, A_{sd}, and D. In general, D is often called the fractal dimension (Barnsely, et. al) that dedicates the fractal behavior of the final distortion. This parameter, which controls the magnitude of the fractal noise, distinguishes between different fractal geometries. If layering is present in the data, the spectral synthesis method produces data that takes the form of layering (Hardy et. al., 1994). This layering effect is impeded in B_{sd} . In the present work the value of B_{sd} is set to one so that completely noisy fractal geometry is generated. The fractal dimension will control the fractal geometry where it will be the only parameter that controls the fractal geometry. The range of D was changed from -3 to +5. Each value of D corresponds to a completely different geometry. For example, the values less than one correspond to a very noisy structure that looks like crushed rocks.

Computational Results

In this work we employ the FHP model to model and investigate micro-scale fluid mechanics in porous media. A benchmark problem with a known analytic solution was selected for the validation of our LGCA code. The problem consists of flow between two horizontal parallel plates driven by a uniform pressure gradient. The vertical distance between the plates is taken to be 512 vertical lattice gas sites. A periodic boundary condition is imposed on the system to guarantee conservation of mass. The initial density at each lattice site is 1.26. The total number of time iterations is 10000 plus an additional 2000 time steps for velocity averaging. The LGCA computational results were compared with the work of Kohring 1992. The results compare well between LGCA predictions and the analytical solution.

The LGCA code was modified to predict the flow between fractal obstacles and at the same time calculation of microscopic physical properties such as density, momentum, viscosity and permeability. Different fractal geometries with different degrees of randomness were used to simulate different porous media. Figure 2 shows different geometries that can be generated using fractals. Figure 2(a) shows fractal geometry that resembles sand where the value of D was set to –5. Figure 2(b) shows a fractal geometry that looks like crushed rocks (D = –1). Figures 2(c), and (d) show a very permeable fractal porous geometry. The value of D was set to 4, and 3 respectively. Figure 3 shows a sponge fractal geometry with constant depth generated for D = -5 and extruding the image in Z direction.

Figure 4 shows LGCA calculated flow inside a fractal porous geometry for D=3. The results are plausibly realistic. However, no other results were available to compare against the detailed LGCA calculations. The complexity of the fractal geometries prohibit use of traditional methods.

Model Extension to Three Dimensional Flows

The FHP model satisfies isotropy and resembles NSE on a two-dimensional lattice. However, the extension of the method to three-dimensional is not straightforward since there is no three-dimensional space-filling solid lattice that satisfies isotropy. Although, the icosohedron satisfies isotropy, it is not a space filling geometry. The first researchers (Frisch, Dumieres, and Lallemend) who worked in three dimensions, faced this problem (d'Humieres et. al., 1987). To overcome this problem, they made a detour to use a four-dimensional face centered hypercube (FCHC), that posses isometry in four dimension, then they took the projection of the 4-D model to a three dimensional space (Henon, 1987). The fourth dimension has a unit length with periodic boundary condition (Henon 1987). This detour resulted in greater number of particle states at a site (24 states) resulting in a dramatic increase in the overall memory and CPU time. Regardless of the problems in FCHC model, it is the only geometry that possesses isometry. The FCHC has 24 possible states. There are 24 neighbors at each site. The number of possible outcomes of these states is 2^{24} (16,777,216) excluding any rest particles in the model. In practice, the implementation of such a large number of possible outcomes is memory and CPU exhaustive. A special purpose supercomputer is needed to store the 2^{24} possible outcomes at each site in a look-up table.

Based on a review of the literature, no previous published work has incorporated all 2^{24} outcomes. Researchers (Henon, 1987, Somers et. al. 1989 & 1990), have suggested methods to reduce the size of this look-up table utilizing the isometries in the FHCH model. There are 1152 isomteries in this model. This will dramatically reduce the size of the look-up table to 18736 possible rules excluding rest particles (Somers et. al., 1990). Unfortunately, there are no known efficient algorithms to resolve the 1152 isomtries (Somers and Rem 1989). The best-known algorithm is the one developed by Somers and Rem that uses only 106496 possible outcomes. Although the look-up table size was reduced, the method's efficiency and accuracy was affected. Even the implementation of this look-up table requires a supercomputer.

The LGCA is not applicable to higher Reynolds number without some special modifications. One technique is to add rest particles to the model but this increases the look-up table dimension dramatically (Henon, 1988). For that reason no more than three rest particles have been attempted.

Because of the aforementioned problems with the LGCA, we have refocused our current efforts on Lattice-Boltzmann methods for micro-scale modeling of unsaturated flows in a fractured or discontinuous porous medium. That work will be reported in our future publications.

DISCUSSION OF RESULTS

The value of D was ranged from –5 to 4 to generate different porous fractal geometries. As the fractal dimension decreases, the porosity of the medium decreases (see Figures 2). The LGCA model realistically tracks the micro-scale fluid behavior in simulated porous medium (see Figure 4). The flow was imposed by a constant pressure gradient inside the duct that contains the porous media to ensure a driving force for the fluid. The upper and lower walls of the duct were assumed impermeable where no mass crosses the boundary. A periodic boundary condition at the duct inlet and exit was assumed to guarantee conservation of mass and momentum. Looking at Figure 4, some kind of small regions of circulations is shown also; convergent and divergent of fluid is shown on the same figure. This figure shows the power of the LGCA to model complex geometries. The resolution of Figure 4 was 256×256. This porous geometry was chosen to give details inside any kind of porous media whether it is crushed, sand or very permeable. The geometry that was taken to model flow inside it is Figure 2(c).

Future work could be extended to model flow inside unsaturated flow in porous media or flow inside fractured porous media using LGCA. This work could be extended to use Lattice Boltzmann method to model flow inside the same fractured porous media. Some thoughts to model flow inside three dimensional porous media is also under consideration.

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APPENDIX: GRAPHS AND IMAGES:

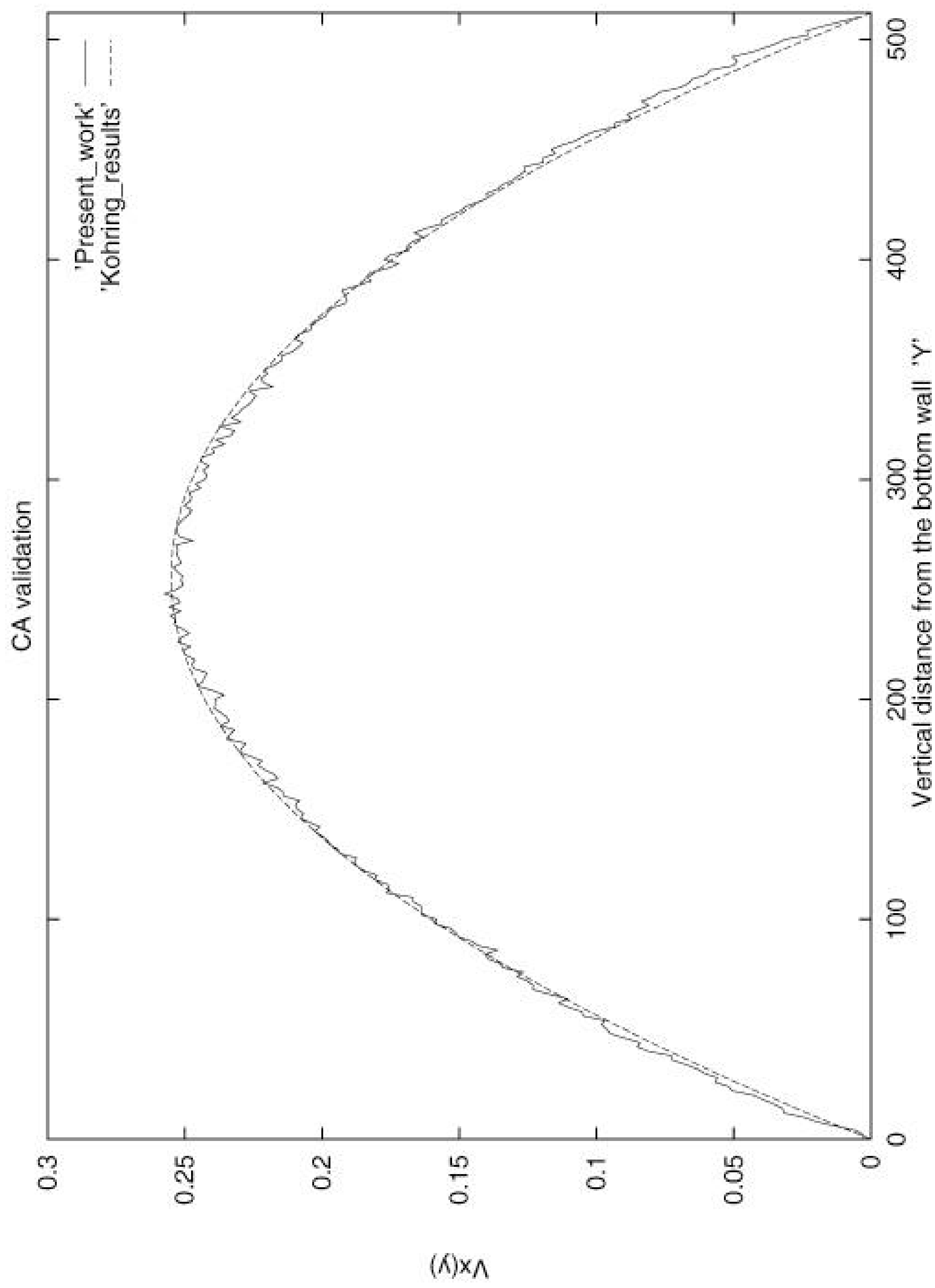
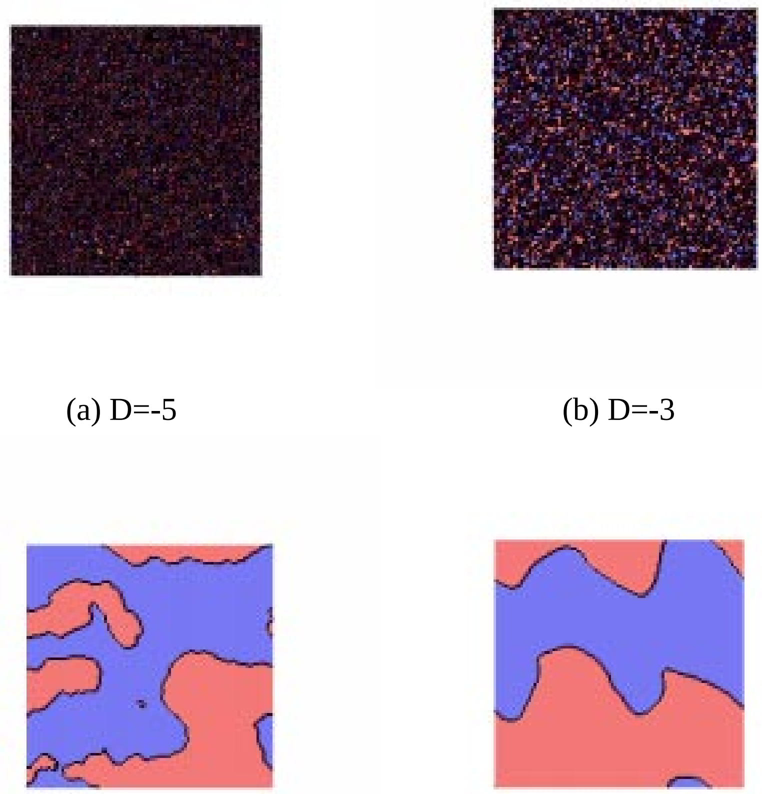


Figure 1: Model Validation of LGCA using a benchmark problem of flow inside a duct with the work of Kohring 1992



(a) D=-5

(b) D=-3

(c) D=1

(d) D=3

Figure 2: Different porous medium geomtries at different fractal dimension D

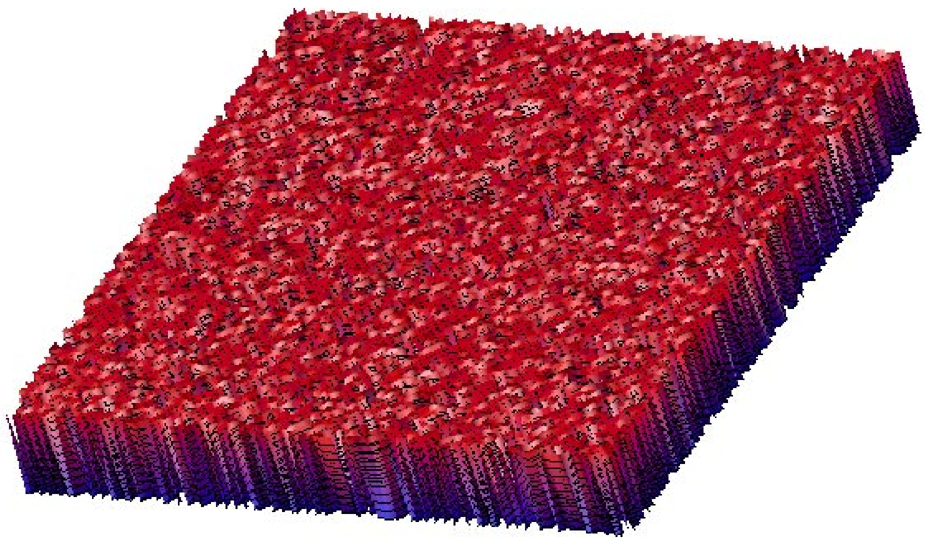


Figure 3: A porous medium the looks like a sponge generated by setting D to –5 and extruding the image in the Z-direction

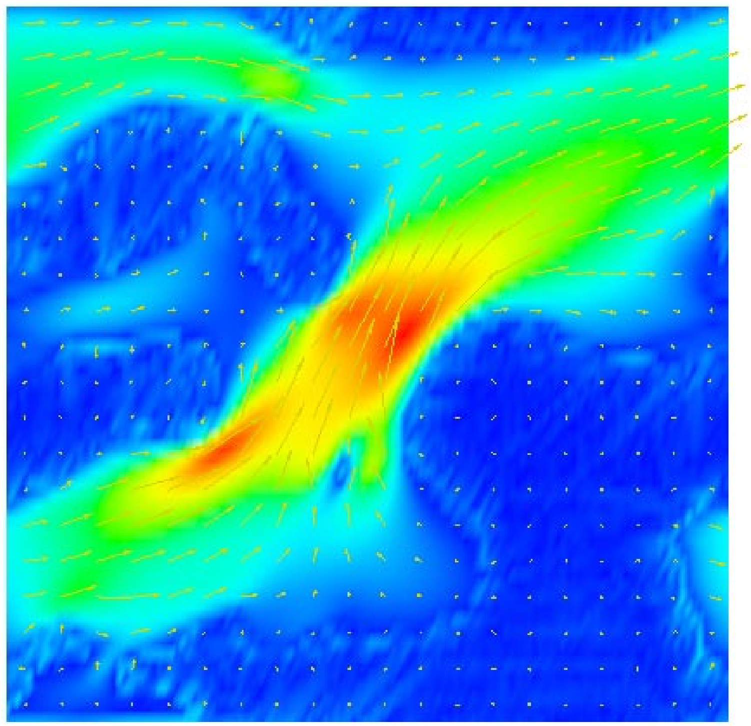


Figure 4: LGCA prediction of flow inside a porous medium generated for a fractal dimension D=3