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Simulation of Flow Through a Two-Dimensional Random Porous Medium

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The cellular automata approximation of two-dimensional hydrodynamics is used to model flow between randomly placed, partially overlapping circles. The flow resistance is first roughly proportional to the number of circles and then increases more strongly for higher numbers of such obstacles.

KEY WORDS: Cellular automata; hydrodynamics; porous media.

Cellular automata[1] have been studied intensively in particular for two-dimensional hydrodynamics.[2] In these lattice gases, one lets particles move with unit velocity along the bonds of a triangular lattice, or they rest on one of the sites. Two particles moving toward the same site scatter there according to the usual conservation laws. Several detailed descriptions of the algorithm have been published.[3-5] Flow around obstacles[6,7] was simulated in agreement with experimental findings. The method seems to be particularly suitable for flow at low velocities around complicated boundaries, like porous membranes.[8]

Thus the flow of water or oil through a porous medium like sand has been mentioned[9] as an example where this lattice gas approximation is better than other methods; and various simulations were published or announced.[9-13] Since this triangular lattice is restricted to two dimensions, we prefer to work with a well-defined and reproducible model medium, and do not use pictures of cuts through three-dimensional natural porous media. Thus, following the simulations of a flow around a cylinder,[6,7] we now place many parallel cylinders (i.e., circles in two dimensions)

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randomly on the lattice. All circles have the same radius, and they are allowed to overlap.

The fluid flow is thought to happen within a channel. Thus the lattice is placed between two parallel horizontal lines, and the fluid flows from left to right, according to a parabolic Poiseuille velocity profile if no obstacles are present. Reflections on the solid boundaries, and the pressure exerted by the fluid on the cylindrical obstacles, are calculated as in ref. 6; our algorithm[5] reaches 30 sites updated per microsecond on one Cray-YMP processor. On the left (upstream) end of the sample, we took as a boundary condition a parabolic velocity profile. For every configuration of cylinders, eight lattice gases were simulated differing only in the random numbers used for the initial velocity distribution. We worked with unit density and with the same scattering rules as in ref. 5; thus the viscosity is about 1/2 in dimensionless units, as given in ref. 5 for typical system sizes.

The circles were allowed to overlap with and exceed the upper and lower boundaries, but were restricted to be in the center half of the horizontal extension of the lattice, in order to have the two ends of the channel free from obstacles. (Rothman[10] instead used square obstacles which were forced to be well separated.) We used lattice sizes $900 * 300$, $2000 * 666$, $3000 * 1000$, $4800 * 1600$, and made a test run of a few seconds only for $6900 * 2300$; for $300 * 100$ lattices the fluctuations were too large. All circles had a diameter of 2% of the horizontal lattice extension, i.e., 40 for $2000 * 666$ lattices.

In principle, the flow velocity should be as small as possible, since a maximum unit velocity is reached if all molecules in a region move in the same direction. Thus in a narrow neck between two circles the algorithm is inaccurate if the fluid flow velocity away from the neck is not much smaller than unity. Actually, we avoid here the critical phenomena near the percolative phase transition[14] and work under conditions where there is still lots of room for flow. Thus the systematic effects from a variation of the initial velocity amplitude were of the order of the statistical fluctuations. Forces and final velocities were roughly proportional to the initial velocity in agreement with Darcy's law.[10] Thus we took 1/4 as the initial maximum fluid velocity in the center of the "channel".

Boundary conditions were taken similar to ref. 6: The leftmost lattice layer was occupied with particles such that their *average* velocity points to the right and follows a Poiseuille profile. The rightmost layer was occupied with velocities taken from many layers further upstream. For intermediate porosities the average velocity far from the ends and obstacles thus decayed in time until it settled to a stationary value about which it fluctuated. The pressure behaved similarly. Thus we averaged over the latter half of the simulation in order to avoid the initial nonequilibrium phenomena.

The actual average flow velocity $\langle v \rangle$, which can be much smaller than initially, was determined by summing over the particle velocities at columns 61–120 of our lattices. The pressure was calculated as in ref. 6 through the total force f exerted by the momentum transfer from the particles to the obstacles. The flow resistivity is then proportional to $f/\langle v \rangle$, and the permeability to the reciprocal ratio $\langle v \rangle/f$. The porosity ($= 1 -$ filling factor) is the fraction of open area and is $\exp(-\pi R^2 N/\text{Area})$ because of the overlap of the circles. This porosity shrinks from 1 to 1/2 in the range of Fig. 1.

The forces and velocities in the model are dimensionless and could be translated into material-dependent units. To get material-independent results, we normalize the results through the data found for a single cylinder in the center of the lattice. For a small number of cylinders, the force at fixed velocity is proportional to the number of obstacles. Our scaled permeability P_s is thus defined as the ratio of the average stationary velocity $\langle v \rangle$ to the force f, multiplied by the number N of cylinders and normalized by the same ratio for the single cylinder in the lattice center:

$$P_s \propto N\langle v \rangle/f$$

For small N this scaled permeability should be a constant near unity, and for large N near the percolation threshold it should go to zero.

Usually we made 2400 time steps and averaged over the last 1200 of them, evaluating the configurations every 200 time steps. In some cases, also two and four times longer runs were made to see that P_s no longer depends on time for $2000 * 666$ lattices. For large N or for lattice sizes $3000 * 1000$, equilibrium has not yet settled after 2400 iterations, and 4800 steps were used. (One reason why these relatively[9] short times may suffice is that, as in ref. 6, initially the whole lattice was filled with a Poiseuille flow as was used later for the upstream boundary condition. Thus, viscous friction starts in the porous medium already at the beginning of the simulation, not when a shock wave from the upstream end has traveled through the medium. The latter effect takes more time.[19])

Our numerical results give a scaled permeability which remains of order unity even for a relatively large number of circles when overlaps and close-by circles occur. Figure 1 shows an example with 50 circles, as well as our main results. Only when 100 and more circles are spread over our $2000 * 666$ lattice is the scaled permeability reduced appreciably. The different data in Fig. 1 for the same lattice size and the same N correpond to different distributions of obstacles and give an impression of the statistical errors. For the smallest lattices our circle radius is only 9 and thus only of the order of the mean free path determined by Rothman[10]; for the two

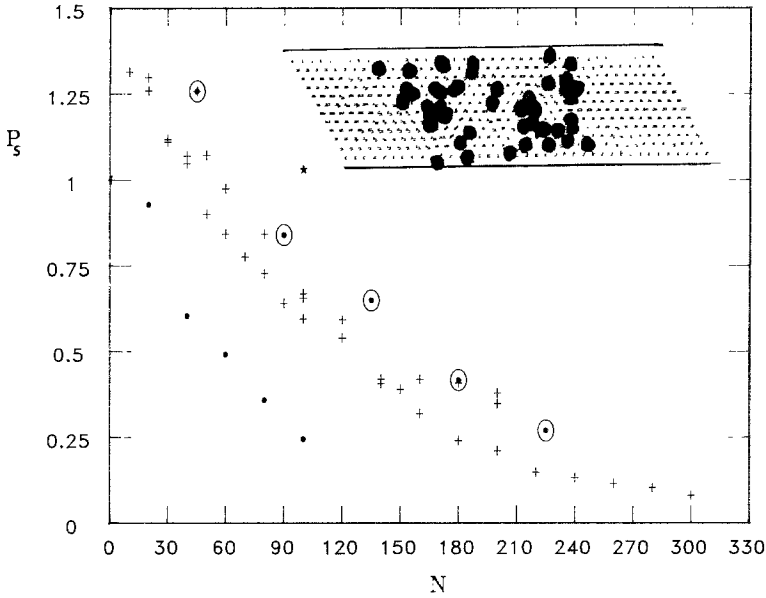

Fig. 1. Scaled permeability as a function of the number N of circles; geometry as in the top part. (The units are chosen such that the scaled permeability is one for a single circle in the center of the lattice and is on average 1.5 for well-separated obstacles.) Dots: 900 * 300, crosses: 2000 * 666, circles: 3000 * 1000, star: 4800 * 1600. The percolation threshold[14] is near $N = 550$. The upper right inset shows a model of porous medium flow with 50 solid circles of radius 20 placed randomly in a 2000 * 666 triangular lattice; no circles were placed close to the ends.

larger lattices, with circle radius 20 and 30, the results are not much different. (Our size dependence presumably is too large to be explained by the logarithmic divergence of the two-dimensional viscosity.[18]

It would be nice if model experiments[15] analogous to these computer simulations would be made in two dimensions to test their accuracy; the overall behavior of our data seems reasonable. The fractal behavior near the percolation threshold, and scaling laws for the dependence, still need to be investigated. A modification of the algorithm, to keep track of the identity of single particles, will be needed to study hydrodynamic dispersion.[16]

From the theoretical point of view it would be nice to have analytic theories similar to those of ref. 17 which give the leading nontrivial order of the cooperation between different obstacles. For porosities p above 3/4 our figure gives a permeability roughly proportional to $(p-2/3)/(1-p)$: How to explain our factor $p-2/3$?

Note. Since the completion of this work, M. Sahimi and D. Stauffer (*Chem. Eng. Sci.*, in press) have applied the method to layered porous

media; and G. A. Kohring has improved the speed by a factor of six (*J. Stat. Phys.* **80**:411 (1991) and investigated the size dependence of porous permeability [*J. Phys.* (Paris) **II**:L87 (1991)].

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