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An Efficient Hydrodynamic Cellular Automata for Simulating Fluids with Large Viscosities

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A hydrodynamic cellular automata (HDCA) for simulating two-dimensional fluids with large viscosities is proposed. The model is characterized by a mean free path which is of the same size as in the FHP-II model, but with a viscosity more than 10 times larger. This new model should make simulations of flows at low Reynolds number more efficient.

KEY WORDS: Cellular automata; hydrodynamics; lattice gases; high viscosity.

Hydrodynamic cellular automata (HDCA), also called "lattice gases," are by now a well-established tool to simulate hydrodynamics.[1-10] Previous researchers have concentrated on developing HDCA possessing very low viscosities in an attempt to study fluid flows at high Reynolds number.[1,2] Such models offer, at present, the best hope for examining the way in which macrostructures in hydrodynamics form from microscopic motions. Another application of the HDCA method is in low-Reynolds-number flow through complicated geometries, e.g., flows in porous media[3-5] or through porous membranes.[6] Both of these problems are especially important in the oil and chemical industries. However, for these problems, HDCA models with very low viscosities are inefficient for several reasons. First, the typical relaxation time τ of a system with characteristic length scale l_0 and viscosity ν scales like $\tau \sim l_0^2/\nu$.[7] Hence, the lower the viscosity, the longer one must wait for the system to come into equilibrium. Second, the velocity fluctuations increase as the viscosity is lowered, so that long-time or large spatial averages are need to smooth out these fluctuations.[6] Finally, in the

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previous models, the viscosity and the mean free path were correlated, so that any attempt to increase the viscosity led to an increased mean free path and, consequently, the need to simulate large systems.[3,5] In this paper an attempt is made to overcome these problems, by introducing a new model which has a relatively large viscosity but at the same time a relatively small mean free path.

The starting point for the present model rests upon the observation that the derivation of Navier–Stokes behavior from HDCA models is dependent only upon ensemble averages and not upon the detailed microstates.[8] More precisely, if $P(s_i, t, \mathbf{r})$ is the probability for obtaining configuration s along direction i at node $\mathbf{r}$ of a two-dimensional triangular lattice, then the only quantity of importance for studying hydrodynamic motions on macroscopic scales is the mean population $\mathcal{N}_i(t, \mathbf{r})$, defined as

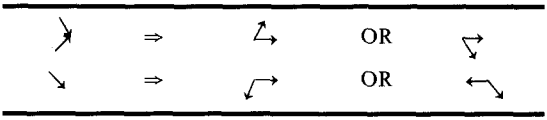
$$\mathcal{N}_i(t, \mathbf{r}) \equiv \sum_{s_i(\mathbf{r}) \in \Gamma} n_i(s_i, t, \mathbf{r})\, P(s_i, t, \mathbf{r}) \tag{1}$$

where $n_i(s_i, t, \mathbf{r})$ is the number of particles in configuration s along direction i at node $\mathbf{r}$ and Γ is the phase space of the fluid flow.[8] (As usual, we are working with a triangular lattice.) The particular consequence of Eq. (1) which is of interest here is that momentum conservation, defined by

$$\sum_i \mathbf{c}_i \mathcal{N}_i(t+1, \mathbf{r}+\mathbf{c}_i) = \sum_i \mathbf{c}_i \mathcal{N}_i(t, \mathbf{r})$$

(where the $\mathbf{c}_i$ represent the six possible lattice momenta) has meaning only for the ensemble average and not for each microscopic state. Hence, a set of collision rules which conserves momentum at the level of ensemble averages, but not at the level of the individual collision rules, should also yield behavior in agreement with the Navier–Stokes equations. Now, this is not to say that such collision rules will not have other consequences, indeed, since the viscosity is a function of the collision rules, such rules will yield viscosities which differ from the those found in the normal FHP

Table I. Collision Table for the Present Model[a]



[a] In addition to the collisions explicitly shown, those collisions obtained by reflection symmetry and time reversal are also included. The latter are needed to ensure exact detailed balance.

models and could in principle yield velocity-dependent viscosities, i.e., fluids with non-Newtonian behavior. In this paper, a set of collision rules which does not appear to have any of these undesired side effects will be presented.

The collision rules for this model are presented in Table I. Note that the rules satisfy exact detailed balance, that there are exactly as many rules which gain momentum as lose momentum, and that in each case the magnitude of the nonconserved momentum $\Delta\mathbf{p}$ is equal to one, $|\Delta\mathbf{p}| = 1$. A constant value for $|\Delta\mathbf{p}|$ appears to be necessary and sufficient to prevent the viscosity from acquiring a speed dependence. Rather than relying on the Boltzmann approximation[8] to demonstrate this point, we use numerical simulations, because any nonlinearities missed by the Boltzmann approximation will show up in computer experiments. It should be mentioned here that use of numerical techniques explicitly assumes the equivalence between time averages and ensemble averages. Although this remark also holds for the FHP models, it is important to note for the present models that the momentum is not conserved between successive time steps at each site. However, for times scales over which the time average approaches the ensemble average, momentum will be conserved at each site.

A sensitive test of the above model can be made by simulating a flow driven between two fixed plates by a linear pressure gradient (Poiseuille flow). The results of a typical two-dimensional simulation are presented in Fig. 1 for a system of $L = 1536 \times H = 512$. The system was allowed to equi-

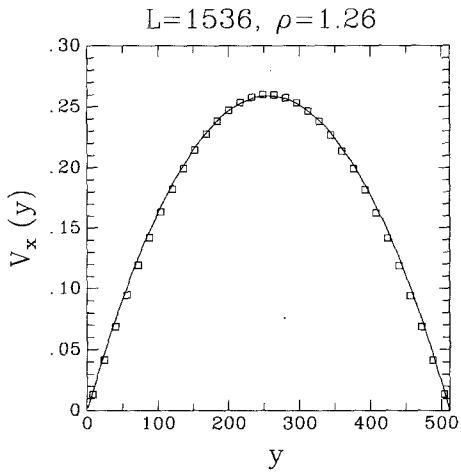


Fig. 1. Velocity profile for a flow driven by a linear pressure gradient. The system size is 1536×512. The solid line is the best fit to the one-parameter Poiseuille velocity profile.

librate for 50,000 time steps before measurements, which used another 50,000 time steps, were started. The solid line is the best fit to the one-parameter Poiseuille velocity profile: $v_x(y) = \text{const} \times y(H - y)$. These data alone support the claim that there are no velocity dependences entering into the viscosity. Further simulations at varying pressure gradients are represented in Fig. 2, which shows a plot of the maximum channel velocity versus pressure gradient. (As a check on the method, the results for similar simulations with the duality invariant version of the FHP-I model are also included.) The clear linearity in this plot demonstrates that the viscosity is independent of velocity.

Since the slope is inversely proportional to the viscosity, it can be immediately seen that the viscosity of the new model is much larger than that of the FHP-I model. Using a linear least squares fit to the data in Fig. 2, one can calculate the viscosity, and the results are shown in Fig. 3 along with similar data at different densities. For comparison, the viscosity of the duality invariant versions of the FHP-I and FHP-II models is also presented. These data demonstrate that the viscosity of the present model is an order of magnitude larger than that of the FHP-II model and nearly three times larger than that of FHP-I.

The next quantity of interest which concerns the efficiency of the simulations is the mean free path.[3,5] The mean free path λ can be estimated by dividing the total number of particles by a sum over all different types of collisions, with each type of collision being weighted by the number of particles involved in that collision. The mean-free-path

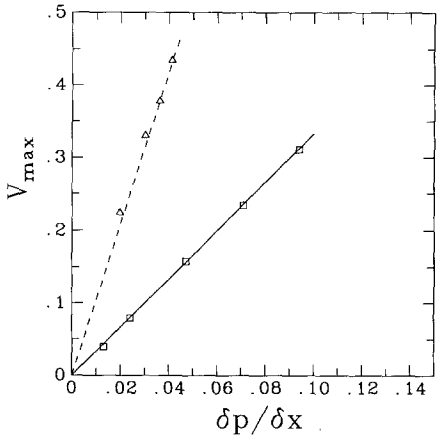


Fig. 2. Maximum channel velocity versus pressure gradient. The system size is the same as for Fig. 1. The squares are for the present model and the triangles for the duality invariant version of FHP-I.

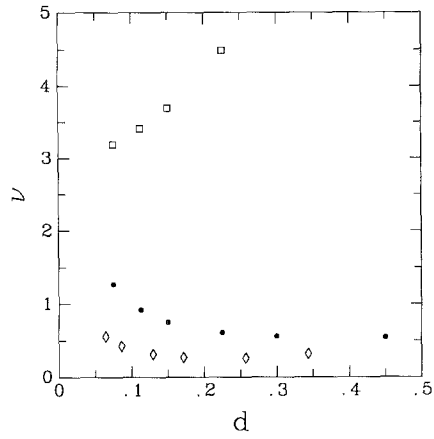


Fig. 3. Viscosity as a function of density for various models. The squares are for the present model, and the filled circles and open diamonds for the duality invariant versions of FHP-I and FHP-II, respectively.

results for the present model and duality invariant versions of the FHP-I and FHP-II models are presented in Fig. 4. From this figure it can be seen that the present model has a mean free path which is about as small as that for the FHP-II model and about three times smaller than that of the FHP-I model.

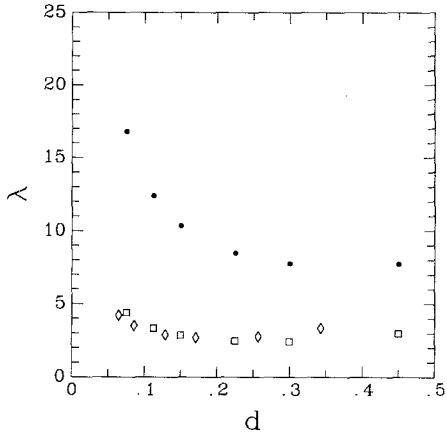


Fig. 4. Mean free path as a function of density for various models. The symbols have the same meaning as in Fig. 3.

These results taken together lead to the conclusion that the present model should be more efficient at low-Reynolds-number flows than the older models. An estimate of the efficiency of the present model in such flow regimes can be made by noting that, because the system size must be much greater than λ in order for hydrodynamic correlations to have time to develop,[3,5] the Reynolds number at constant velocity is bounded from below by λ/v. From Fig. 3 and 4, this lower bound can be estimated and it is approximately one order of magnitude smaller in the present model than in the FHP models.

As a further check on the question of how the hydrodynamic correlations build up with system size, we have performed the same channel experiment with the present model as was performed previously with the FHP-I[5] and FHP-II[11] models, in order to determine how the finite size effects scale with the channel width, R. Figure 5 shows a plot of the scaled permeability ($\kappa \equiv$ flux/pressure gradient) as a function of, λ/R, for the three models. The present model has the same finite size behavior as the FHP models in terms of λ/R; thus for a fixed R its finite size errors are smaller.

No model is of much use if it needs an inordinate amount of computer time for actual simulations. The present model can be implemented with Boolean operations on vector or SIMD computers. Its update speed is about 460 site updates per μsec on the NEC-SX3/11. This is about 10% slower than the implementation of the FHP-I model discussed in ref. 9 and

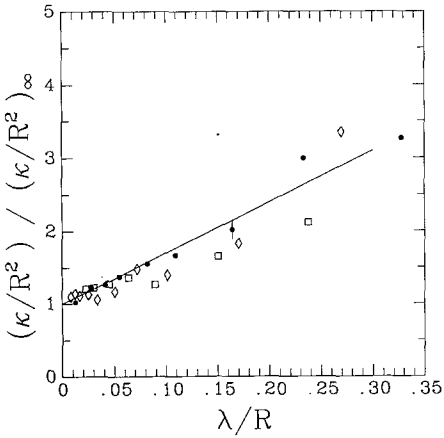


Fig. 5. Scaled permeability as a function of the mean free path divided by the channel size. The filled circles are for the FHP-I model, the diamonds for the FHP-II model and the squares are for the present model. The experimental setup is described in Refs. 5 and 11. The density is 0.9 particles per site.

about 30% faster than a similar Boolean implementation of the FHP-II model. Hence, in terms of computer speed and memory, it is competitive with the FHP models.

In summary, a new HDCA model has been presented, and computer simulations have demonstrated that this model possess a mean free path which is approximately the same size as that of the FHP-II model, although the viscosity is more than ten times larger. This new model should be very useful for studying low-Reynolds-number fluid flows through complicated geometries. Furthermore, the new model may be of use for studying problems in two-phase fluid flows where the viscosities differ by an order of magnitude.[10] Previous attemps to deal with this problem used fluids whose mean free paths differed considerably. The present model would reduce the complications introduced by such unphysical approximations.

Finally, we have also performed simulations in which the collision rules of the FHP-I model were combined with those of the present model. Such a set of collision rules violates the condition that $|\Delta \mathbf{p}| = \text{const}$. Indeed, using this set of rules, we were unable to establish a constant pressure gradient and, consequently, no Poiseuille velocity profile. Such models could be of use in describing non-Newtonian fluids, although more work is needed in this area before such an assertion can be sustained.

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