BOUNDARIES IN LATTICE GAS FLOWS

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Abstract

A one dimensional lattice gas model is used to study the interaction of fluid flows with solid boundaries. Various interaction mechanisms are examined. Lattice Boltzmann simulations show that bounce-back reflection is not the only interaction that yields "no-slip"boundary conditions (zero velocity at a fixed wall) and that Knudsen type interaction is also appropriate.

Introduction

A large class of problems in fluid mechanics involves solid boundaries. Standard analysis require that the velocity of the fluid be zero at a fixed boundary, in agreement with experimental observation at the hydrodynamic level: this is known as "no-slip" condition. This condition is satisfactory for simulation of the Navier-Stokes equations with traditional computational methods, but obviously it does not shed any light on the mechanisms that effectively reduce the velocity to zero on the wall . On the other hand, there are very few experiments that explore the interaction of fluids and solid boundaries at the molecular level. In this respect, lattice gas methods prove useful because even though lattice gas automata are constructed as fictitious microworlds, their operational algorithms

must include the proper basic microscopic mechanisms in order to produce correct hydrodynamic behavior. Therefore the lattice gas approach to the boundary flow problem requires a model interaction mechanism with solid boundaries. We present a simple lattice gas model, for the study of flows near walls; the model is easily implemented on a small computer and is free of the usual Monte-Carlo noise inherent to a description at the microscopic level, so that computations run fast.

The latttice gas model

We consider the six-particle FHP model [1]: this automaton runs on a triangular lattice with hexagonal symmetry; all particles have unit mass, move with unit velocity in one of the six possible directions of the lattice (fig. 1a) and are subject to an exclusion principle, (at a given node, no two particles occupy the same link at a given time); thus, the maximum number of particles per node is six; when two particles meet at a node, they collide at integer times. There are essentially two collision rules, one involving head-on binary collisions and one involving three particles converging symmetrically towards a node (fig. 1b).The presence of three particle collisions is essential in order to remove a non-physical conservation law [2] so that the only conserved quantities are mass and momentum. All other collisions leave the particle configuration unchanged, and so do not contribute to momentum transfer. After the collision, particles move one lattice link length per unit time in the direction of their velocity. These are the simplest rules that produce correct hydrodynamic behavior at the macroscopic level.Specific collision rules are used to model interactions of particles with solid boundaries; for instance, particles are either specularly reflected or bounced back as shown in figure 2. Collision rules can be conveniently written as a collision table. In the simple six particle FHP model, the collision table has 64 input states (the number of possible input configurations is 2^b, where b is the number of sites per node).

The equations governing the evolution of the gas can be written by inspection. The position of a lattice node is denoted by $\mathbf{r}$. The occupancy variable n_i (direction i = 0, 1, 2, ...,5) is either 0 or 1(because of the exclusion principle) and n_i is a function of position $\mathbf{r}$ on the lattice and of time t. The evolution of the automaton in space and time proceeds by sequences of two consecutive events: propagation followed by collision. During propagation, all particles move one lattice unit in the direction of their velocity $\mathbf{c}_i$, and during collision , all nodes are updated i.e. particles are reorganized according to the collision rules. Note that after a large number of updates, it does not matter wether collision or propagation occurred first [2].

In establishing the equations governing the evolution of the lattice gas obeying the simple FHP collision rules (fig. 1b) given above one must account for the fact that there are two possible output configurations for binary head-on collisions which are assigned complementary probabilities a and (1-a). The value a =1/2 is most common, that is on the average every other collision leads to one of the possible configurations. The microdynamical equations are [2]:

$$n_i(t+1, \mathbf{r} + \mathbf{c}_i) = n_i(t,\mathbf{r}) + \Delta_i(n), \qquad i = 0,1, \ldots, 5, \tag{1}$$

where $n_i(t,\mathbf{r})$ is the propagation term and $\Delta_i(n)$ is the collision term:

$$\Delta_i(n) =$$

$$a\, n_{i+1} n_{i+4} \bar{n}_i \bar{n}_{i+2} \bar{n}_{i+3} \bar{n}_{i+5} + (1-a)\, n_{i+2} n_{i+5} \bar{n}_i \bar{n}_{i+1} \bar{n}_{i+3} \bar{n}_{i+4} - n_i n_{i+3} \bar{n}_{i+1} \bar{n}_{i+2} \bar{n}_{i+4} \bar{n}_{i+5}$$

$$+ n_{i+1} n_{i+3} n_{i+5} \bar{n}_i \bar{n}_{i+2} \bar{n}_{i+4} - n_i n_{i+2} n_{i+4} \bar{n}_{i+1} \bar{n}_{i+3} \bar{n}_{i+5} \qquad \bar{n}_i = 1-n_i \tag{2}$$

The first line on the right hand side of (2) refers to collisions involving two particles and the second line to those involving three particles; terms with a plus (minus) sign represent populating (depopulating) contributions to $n_i(t+1, \mathbf{r} + \mathbf{c}_i)$. A lattice gas obeying the microdynanical equations;

1- has an equilibrium state, and the equilibrium distribution is of the Fermi-Dirac type, resulting from the exclusion principle [2].

2- evolves according to the Navier-Stokes equations in the incompressible hydrodynamic limit.

The set of equations (2) defines the cellular automaton to be implemented for simulation purposes. These equations are well suited for efficient implementation since all variables are boolean. All particles on the lattice are first propagated in the direction of their velocity; then each node is updated according to the collision rules. This operation is most conveniently performed by means of at look up table, that yield directly the output configuration resulting from a given input configuration. All variables are thus updated by "boolean processors" of the cellular automaton type.

As appealing as this method may seem, it may not be the optimal computation technique for investigating boundary flow mechanisms, because it is by essence inherently noisy. Therefore to obtain a velocity profile with the required degree of accuracy one needs long times for the average velocities to emerge from the noise. So it appears more efficient to use averaged quantities N_i for the occupancy rather than the boolean microscopic quantities n_i. This is accomplished by standard of statistical mechanical methods

One defines a probability distribution P that assigns each microstate a probability of occurrence in phase space Γ of all possible assignments $\{n_i = \{n_i(\mathbf{r})\}, \mathbf{r} \in \text{Lattice}\}$ of the boolean field $n_i(\mathbf{r})$ [2]. Averaged quantities can then be defined; in particular, macroscopic probabilities of occupancy Ni are given by:

$$N_i(r_*) = \langle n_i(r_*) \rangle = \sum_{\{m_j\} \in \Gamma} n_i(r_*) P(\{m_j\}) \qquad (3)$$

The averaging process defined above applied to the microdynamical equations (1) yields:

$$N_i(t+1, \mathbf{r} + \mathbf{c}_i) = N_i(t, \mathbf{r}) + \Delta_i(n), \qquad (4)$$

where $\Delta_i(n) =$

$$\begin{aligned} & a\langle n_{i+1} n_{i+4} \bar{n}_i \bar{n}_{i+2} \bar{n}_{i+3} \bar{n}_{i+5} \rangle \\ & + (1-a)\langle n_{i+2} n_{i+5} \bar{n}_i \bar{n}_{i+1} \bar{n}_{i+3} \bar{n}_{i+4} \rangle - \langle n_i n_{i+3} \bar{n}_{i+1} \bar{n}_{i+2} \bar{n}_{i+4} \bar{n}_{i+5} \rangle \\ & + \langle n_{i+1} n_{i+3} n_{i+5} \bar{n}_i \bar{n}_{i+2} \bar{n}_{i+4} \rangle - \langle n_i n_{i+2} n_{i+4} \bar{n}_{i+1} \bar{n}_{i+3} \bar{n}_{i+5} \rangle) \end{aligned} \qquad (5)$$

With the factorization hypothesis (Boltzmann approximation) applied to (5), (4) becomes the lattice Boltzmann equation where the collision term (for the FHP model) reads:

$\Delta_i(N) =$

$a\, N_{i+1}N_{i+4}\,(1-N_i)(1-N_{i+2})(1-N_{i+3})(1-N_{i+5}) + (1-a)\, N_{i+2}N_{i+5}\,(1-N_i)(1-N_{i+1})(1-N_{i+3})(1-N_{i+4})$

$- N_iN_{i+3}\,(1-N_{i+1})(1-N_{i+2})(1-N_{i+4})(1-N_{i+5})$

$+ N_{i+1}N_{i+3}\,N_{i+5}(1-N_i)(1-N_{i+2})(1-N_{i+4}) - N_iN_{i+2}\,N_{i+4}(1-N_{i+1})(1-N_{i+3})(1-N_{i+5})$ (6)

The local observables, such as the density ρ and the velocity $\mathbf{U}$ are obtained as :

$$\rho = \sum_i N_i \qquad\qquad \rho\mathbf{U} = \sum_i N_i\mathbf{c}_i \tag{7}$$

For the type of problem considered here, computation from the lattice equation is quite straightforward; the lattice Boltzmann method is then particularly fast and convenient, as compared to microscopic simulations and to conventional numerical techniques.

Flow near a flat wall

We consider the interaction of a moving fluid with an infinitely long flat boundary; however because of translational invariance, it suffices to consider a short section of the boundary (actually, a single column of nodes perpendicular to the wall). The system is initialized as a fluid with density ρ (or link density $d = \rho/6$) at rest near along the wall. At time $t = 0$, the fluid is made to flow instantaneously with velocity Uo and the bulk of the fluid is in the stationary state corresponding to density ρ and velocity (Uo,0) (fig.3).

After the first time step, only the layer adjacent to the wall will experience the influence of the boundary and the velocities at all nodes in that first layer will have decreased by an equal amount ΔU. All subsequent layers (labeled second layer, third layer,...) remain at the free flow velocity Uo. After the second time step, not only has the first layer been further slowed down by the wall, but now the velocity gradient imposed between the first and third layers has slowed down the second layer. Because of the initial

conditions in the simulation, all the nodes of the second layer are slowed down by an equal amount. Again all layers beyond the second one remain at velocity Uo.

After the n^{th} time step, friction effects from the wall affect all layers up to the n^{th} layer. All velocities within a given layer will be reduced by an equal amount and all nodes above the n^{th} layer have velocity Uo. Thus,the velocity profile of the gas is translationally invariant: for flat boundaries of infinite extent, we have a one dimensional problem. Such a problem can be easily implemented. Each new computation step adds a new layer to the simulation, while all layers beyond are at the stationary velocity Uo.

We define the boundary layer thickness δ as the distance from the wall where the velocity is 0.99 Uo. δ increases with time at a much slower rate than the rate at which the number of layers involved in the computation increases.

Because of translational invariance, there is no velocity gradient along the wall and the Navier-Stokes equation for the flow considered reduces to (in the incompressible limit):

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} \qquad (8)$$

where ν is the kinematic viscosity, u is the velocity in the x direction along the wall and y denotes the axis orthogonal to the wall. If the velocity on the wall is zero, the boundary condition are $u(0,t) = 0$, and $u(\infty,t) = Uo$, and the solution to (8) reads [4]:

$$u(y,t) = \frac{U_o}{\sqrt{\pi \nu t}} \int_0^y \exp\left(\frac{-y'^2}{4\nu t}\right) dy' = U_o \, \mathrm{erf}\left\{\frac{y}{\sqrt{4\nu t}}\right\} \qquad (9)$$

Two important properties emerge from this solution;

1- velocity profiles have a space-dependent scaling property;

2- the boundary layer thickness δ increases as the square root of time.

Note that when the free flow velocity is constant, time can be converted into distance along the wall (x=Uot) and the variation of d with respect to t can be equally expressed in terms of x. In classical laminar boundary theory applied to flow along a semi-infinite plane [4] (Blasius), δ increases as $(x)^{1/2}$, where x is the horizontal distance from the leading edge

of the wall. Since Uo is constant, we can interpret the successive velocity profiles as profiles at increasing distance along the wall whose edge is located at x = 0 (i.e. at t=0).

Lattice Boltzmann Simulations

Simulations with zero velocity boundary condition obtained by the bounce-back rule on the wall (fig. 2b) match very well the theoretical prediction, equation (9), for the velocity profile (fig. 4) and for the growth of the boundary layer thickness (fig.5). The velocity profiles are also quite close to the classical Blasius profile (fig. 4).

When the assumption of zero velocity on the wall is relaxed, one no longer has an error function type velocity profile. In this respect, we now specifically address the question tof the relationship between the velocity profile and the particle-wall interaction. Bounce-back reflection with solid bodies is (fig. 2b) is commnly used in lattice gas simulations; however, there are good reasons to examine other types of reflections. One reason stems from consideration of experiments at the molecular level. In his book published in 1934, Knudsen [5] describes an experiment where molecules are directed towards a wall at a fixed angle of incidence; he observes that the molecules are randomly scattered in all directions. In a lattice gas, this would correspond to a combination of specular and bounce back reflections in equal proportions. A second reason is that, with purely deterministic interactions with the wall, the Boltzmann assumption of no correlation between particles prior to collision is not valid; note however that the hypothesis is correct in a statistical sense for a 50% combination of bounce-back and specular reflections.

In a lattice gas, zero velocity at the boundary is obtained (in a strict sense) only with pure bounce back reflection. If bounce-back reflection is present (in any proportion), more fluid particles will be reflected in the backward direction than the forward direction. This results in a friction effect that slows down the fluid near the wall until its velocity vanishes; in other words, the velocity on the wall should go as close to zero as we want, if we wait long enough.

Our model is particularly well suited to verify this assertion. We define a reflection coefficient r as the ratio of bounce-back to specular reflections in the interactions with the wall: r=1 corresponds to pure bounce-back reflection and r=0 to pure specular reflection. Figure 6 shows the velocity profiles obtained for different values of r, all other parameters (computation time, particle density and free flow velocity) being kept constant. As expected, velocity on the wall is found to be zero for r=1, and increases progressively to Uo as r decreases to zero. However, for long computation times (with all other parameters kept constant), (fig. 7), the velocity on the wall decreases and goes arbitrarily close to zero.

In order to support the claim that zero velocity on the wall can be obtained in the long time limit, figure 8 shows the computation time required to obtain the velocity value 0.1 Uo on the wall as a function of r (all other parameters being kept constant). We find that the velocity on the wall can be expected to go close to zero very rapidly for $r > 0.4$ (60% specular reflection proportion or less); for $0.1 > r > 0.35$, the computation time increases exponentially with (1-r).

The validation of lattice gas modelling of physical phenomena requires knowledge of these phenomena at the hydrodynamic level, but also, to some extent, at the molecular level. Conversely, lattice gas simulations can be useful in providing information as to what simple models can do and how simplified microdynamics can provide correct hydrodynamics. Boundary interactions are a good example of such a situation. In a real gas there are no "layers" and molecules do not move in discrete time steps. However, if we imagine layers of thickness dy parallel to the wall, and if we assume that all molecules in each layer have the same average velocity, then a random redistribution of molecules colliding with a wall would not give a zero velocity stricto sensu; to first approximation the redistribution would result in a velocity on the wall with value equal to one half the velocity in the first layer. Of course, as dy --> 0, this value would go infinitesimally close to zero.

However, even without going to this limit, the velocity on the wall is expected to get closer to zero in the course of time because of viscosity effects. This suggests that r = 0.5 might be an alternate choice to r=1 for boundary condition .

The situation discussed above is different from Couette channel flow (one side of the channel moves with velocity Uo) where the flow effectively reaches a steady state.With r=1 on fixed wall, theory predicts a steady-state velocity profile increasing linearly from zero on the wall at rest to Uo on the moving wall. For the semi-infinite Poiseuille system, the profile never reaches a steady state and the boundary layer grows indefinitely. Lattice gas simulations of Couette flow show the expected linear profile. The velocity on the fixed wall is zero for a reflection coefficient r =1. However, for r <1, the velocity on the fixed wall reaches a non zero steady state value which increases as specular reflection becomes more important; indeed one should not expect zero velocity on the boundary since along the wall momentum transferred from the adjacent layers cannot be be transferred back to the fluid at each time step and consequently there is a constant velocity on the wall. This effect is expected to be negligible when the width of the channel is large compared to the mean free path.

Conclusion

We have shown that in a lattice gas flow along a fixed solid boundary, pure bounce-back reflection is not the only type of interaction that yields no-slip condition at the boundary. Zero velocity on the wall can be reached when bounce-back reflection is combined with specular reflection in any proportion. However the time required to obtain no slip condition increases considerably when the reflection coefficient becomes smaller than 0.4 . These results validate the use of the Knudsen interaction (r=0.5) model which is in agreement with actual experimental observation.

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Figure captions

Figure 1. (a)Indices for velocity orientations on lattice nodes ; (b)Collision rules

Figure 2. Collision rules for wall interactions (a)Specular reflection ; (b)Bounce back reflection

Figure 3: Configuration of the lattice near the wall (layer indices)

Figure 4: Velocity profile for flow along a fixed wall. Theoretical error function, Blasius profile, and lattice gas simulation data after 150 time steps (particle density d = 0.1833, free flow velocity Uo = 2.72, bounce back reflection coefficient r = 1). y norm is the normalized space coordinate measuring the distance from the wall. y norm = 4.99 j/jo where jo is the interpolated row index value corresponding to U = 0.99Uo. The factors 4.99 and 0.99 are standard in boundary layer theory [4]

Figure 5: Boundary layer growth with distance (up to 41 distance units). Same conditions as given in caption of figure 4. y norm is defined in caption of figure 4. The distance from the leading edge is t U*. Since the boundary layer thickness is defined at U* = 0.99 Uo, we define x by converting directly t into distance (ignoring the constant factor U*)

Figure 6: Velocity profiles for various bounce back reflection ratios. (gas density: d = 0.233; free flow velocity: Uo = 0.500). The data shown were obtained after 20 time steps

Figure 7; Velocity at the boundary as a function of time for various reflection coefficient values

Figure 8; Logarithm of the number of computation steps versus reflection coefficient. (d=0.25, Uo = 0.4).

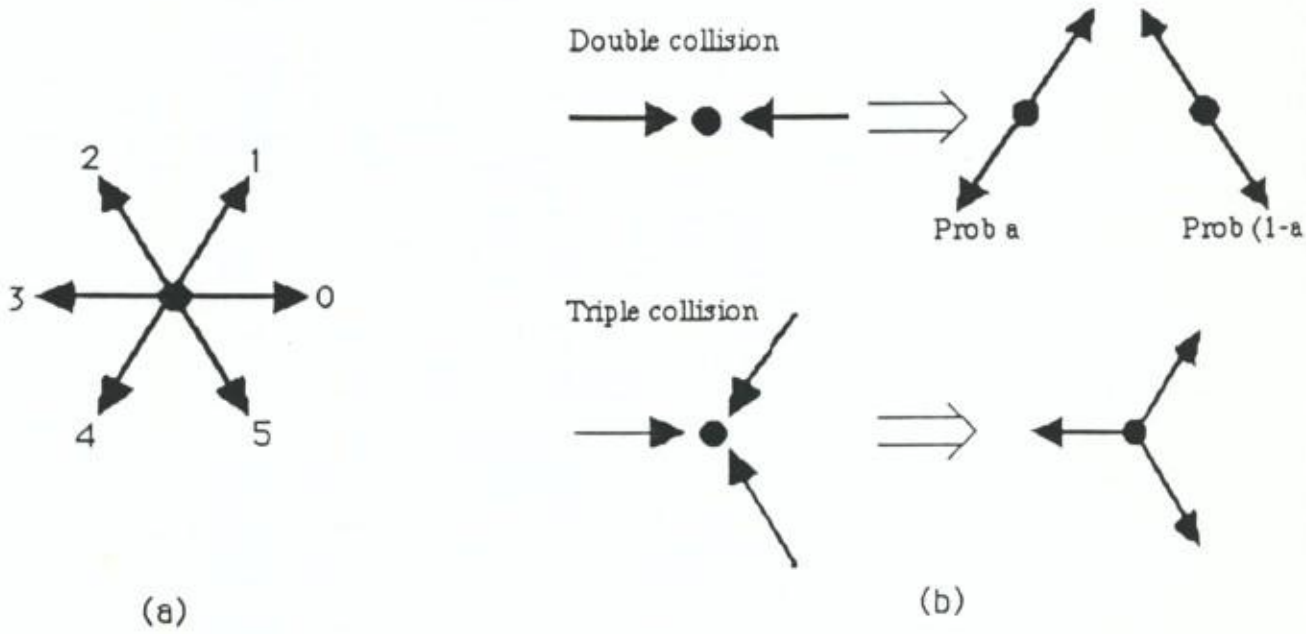


Figure 1

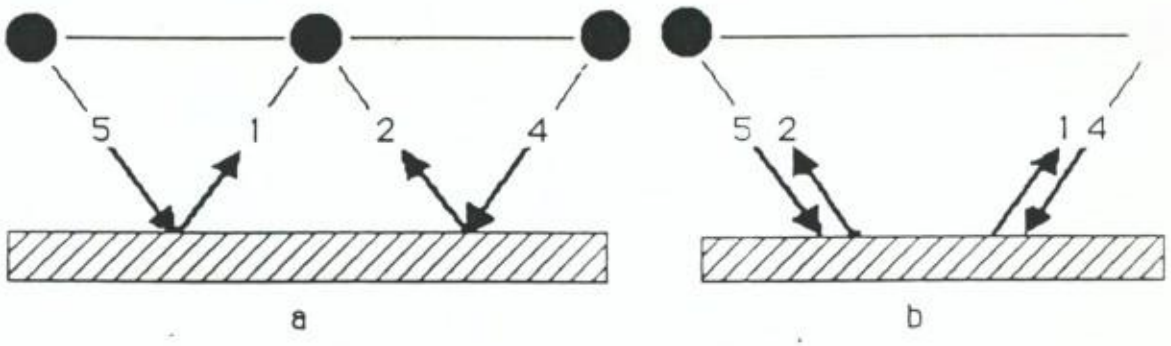
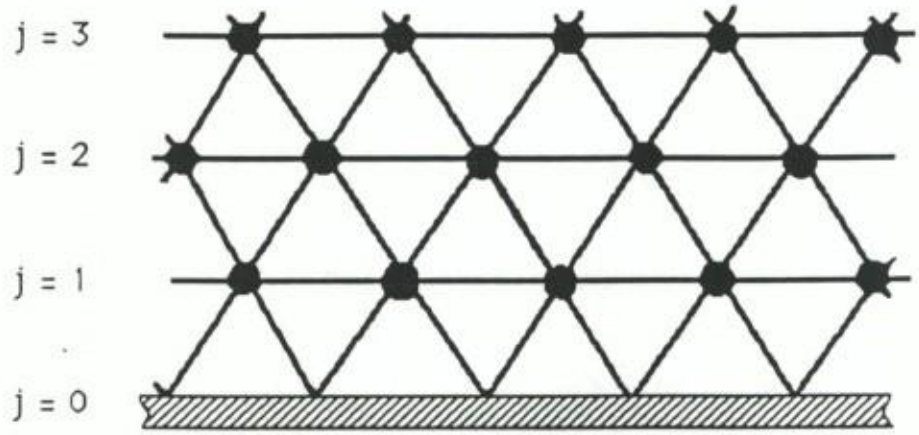


Figure 2



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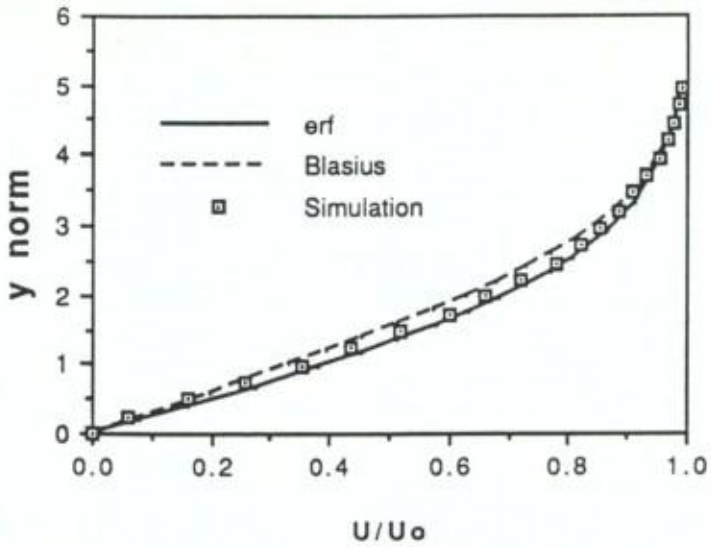

Figure 4

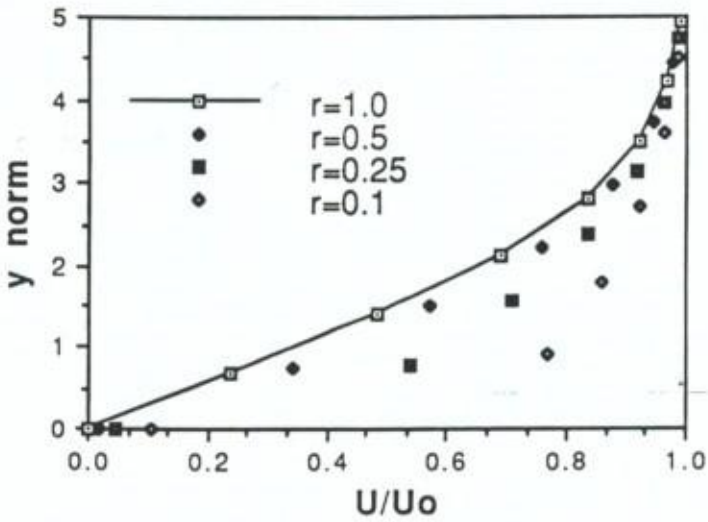

Figure 5

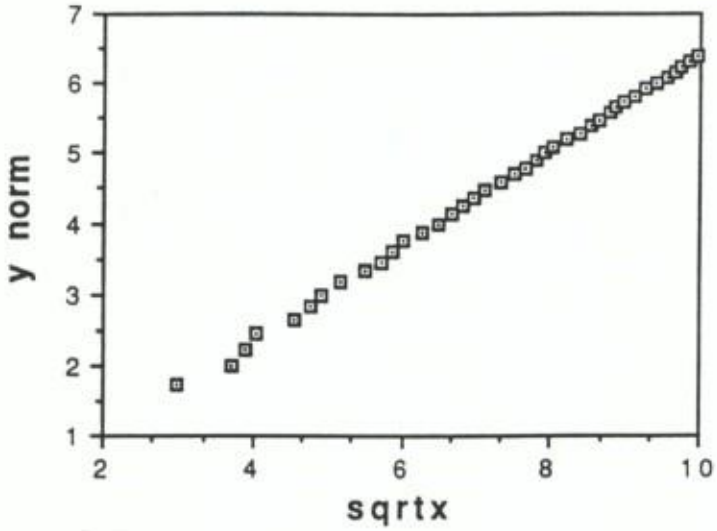
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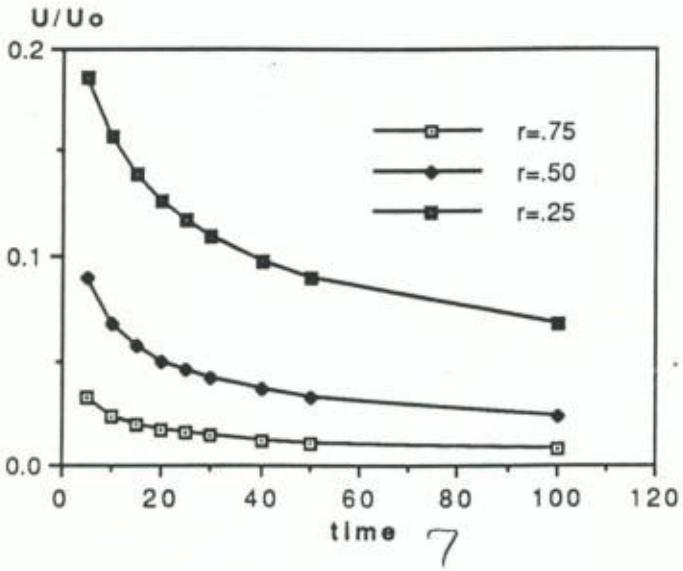
Figure 6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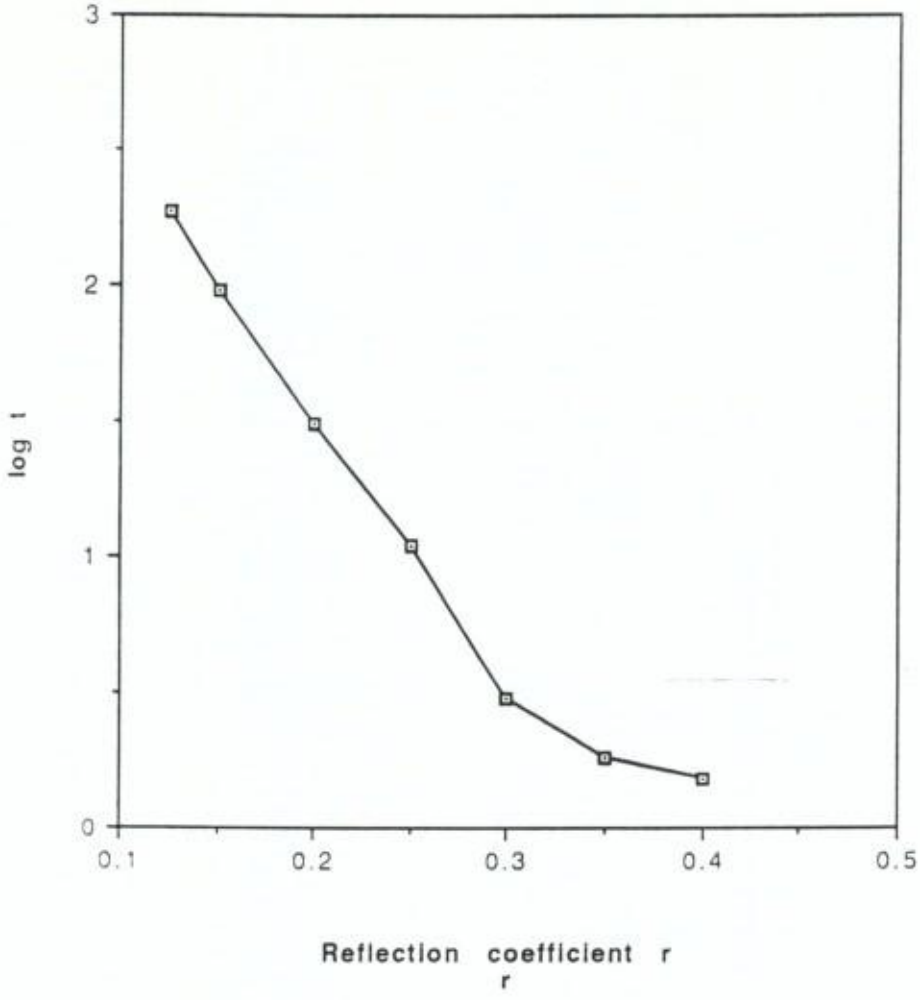
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