Journal of Statistical Physics, Vol. 71, Nos. 5/6, 1993

Boundary Conditions for Lattice Boltzmann Simulations

Donald P. Ziegler[1]

Received November 17, 1992

A heuristic interpretation of no-slip boundary conditions for lattice Boltzmann and lattice gas simulations is developed. An improvement is suggested which consists of including the wall nodes in the collision operation.

KEY WORDS: Lattice gas; lattice Boltzmann; hydrodynamics; boundary conditions.

1. INTRODUCTION

Cornubert *et al.*[1] have recently examined boundary conditions for lattice gas simulations of fluid flow. They show that for the parallel flow configuration, application of the "bounce-back" boundary condition is, to first order, equivalent to a no-slip wall halfway between the first row of nodes in the fluid and the first row outside.

Another discussion of appropriate boundary conditions for lattice gas models was provided by Lavallee *et al.*[2] On the basis of results of numerical simulations of a developing flow they suggest that the bounce-back condition is not the only one appropriate, but that a mixture of some fraction of "slip" can also give no slip at long times. Unfortunately, their work is marred in that the flow that they simulated has zero shear stress as its long-time asymptotic wall condition. Thus, no matter what fraction of slip they used, they would always get no motion at the boundary at long times.

In this report, the same result as obtained by Cornubert *et al.* is developed by examining the symmetry near the boundary of simple flows, and a new technique is suggested that should provide a higher order of accuracy.

[1] Chemical Systems Division, Alcoa Technical Center, Alcoa Center, Pennsylvania, 15069.

0022-4715/93/0600-1171$07.00/0

2. THEORETICAL DEVELOPMENT

The usual method of applying a no-slip condition is reviewed with reference to Fig. 1. The usual approach has been direct reflection of particles arriving at the wall. Particles will arrive at node *A* from nodes *B* and *C*. Whenever a particle going in direction 3 arrives from node *B*, a direction-6 particle is sent back to node *B* the following time step, and similarly for direction-2 particles from node *C*. Consequently, the time average of the population at node *A* has an equal number of direction-3 and direction-6 particles and an equal number of direction-2 and -5 particles, and so the average velocity at node *A* is zero. This result is the basis of the logic of using direct reflection at the walls.

The same technique has been used for lattice Boltzmann simulations, and it is in this context that the present argument is developed. As an illustrative example, suppose that there are no gradients in the streamwise direction and the velocity at the location of nodes *B* and *C* is such that the distribution function of 3-direction particles arriving at node *A* from *B* has a value of 0.19, while that of the 2-direction particles arriving from *C* is 0.17. Using the "bounce-back" algorithm, the distribution function of 6-direction particles leaving node *A* will be 0.19 and that of the 5-direction particles will be 0.17. So, from the point of view of nodes *B* and *C*, they are receiving particles from a population identical to their own, but traveling in the opposite direction. This is clearly different from the intended result of having a no-slip wall at *A*.

The alternate interpretation pointed out by Cornubert *et al.* is that the "bounce-back" condition corresponds to a zero-velocity boundary condition that is applied at a wall halfway between nodes *A* and *B*–*C*. The velocity at *A* in the opposite direction is the symmetric reflection of the state at *B*–*C* through the no-slip wall halfway between. This is a major improvement in the understanding of these simulations that permits use

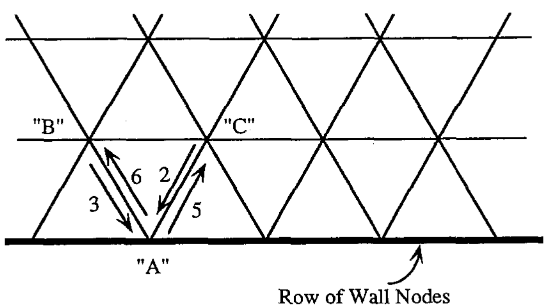

Fig. 1. Wall boundary condition schematic.

of the same general algorithm and gives much improved accuracy in the interpretation of the flow near the walls.

An additional improvement is available, however. It will be illustrated through a discussion of the meaning of the nonequilibrium contributions to the distribution functions.

In the usual discussions of the lattice Boltzmann method, the terms equilibrium and nonequilibrium are used to indicate two contributions to the values of the particle density distribution functions. In terms of the flow physics, however, these terms refer to the contribution of velocity gradients. For steady uniform flow, the state of all of the nodes is the same, equal to the equilibrium distribution given by the usual formulas. When there are velocity gradients, the distribution functions are no longer the equilibrrium values. In this situation, the particle population arriving at a node will have contributions from neighborhoods having higher and lower velocities than the nodal velocity. The collision operator, representing the action of viscosity, operates on the deviations of the populations from their zero-gradient values and moves them toward the equilibrium values. For high viscosity, the nonequilibrium values are adjusted very little, so that the momentum deficit or excess carried by the particles can propagate through a given node to the next neighbors. Conversely, for low viscosity, the operator moves the nonequilibrium contribution strongly toward zero.

Returning now to the boundary condition illustration, the remaining problem with interpreting the bounce-back condition as a wall halfway between the node rows is seen: The populations coming from nodes A and being received by the nodes at B–C, while corresponding to zero velocity halfway between, will not in general carry accurate gradient information. This procedure will be first-order accurate, and in case the velocity gradient is not changing, as for plane Couette flow, will be completely accurate. However, for cases where the velocity gradient is not constant, as in Poiseuille flow, second-order errors will remain.

A more accurate alternative is proposed as follows: The boundary is kept coincident with the first line of nodes, rather than being halfway between. For the boundary nodes, after the propagation step, the distribution functions of the directions complementary to those of arriving particles are set equal to the arriving distribution functions. This sets the normal velocity to zero. The remaining directions then have their distribution functions set to the average of the incoming directions, thus setting the tangential velocity to zero. During the collision phase, the collision operator is applied to the boundary nodes as well as to the fluid nodes, and the resulting distribution functions are then propagated normally in the next cycle.

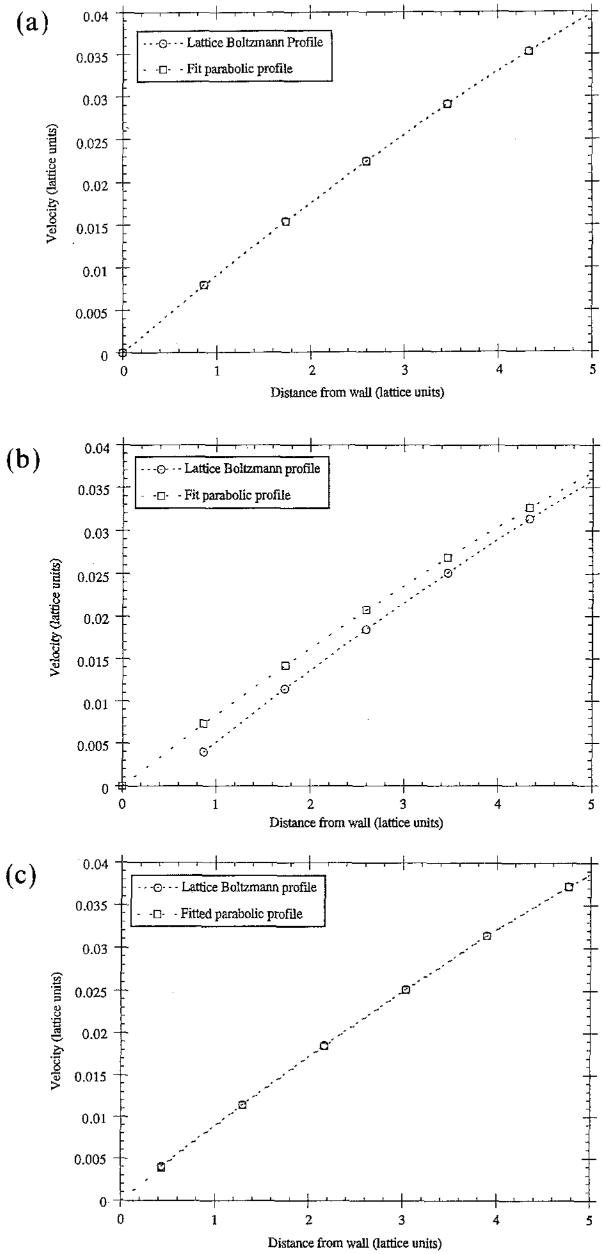

Fig. 2. Velocity profiles for various boundary condition implementations. (a) Velocity profile with proposed boundary condition. (b) Velocity profile for bounce-back condition. (c) Velocity profile for reinterpreted bounce-back condition.

3. NUMERICAL RESULTS

The improvement achieved with this technique is illustrated in the following numerical example. These results were calculated with a one-dimensional simulation of plane Poiseuille flow. Periodic boundary conditions are applied in the streamwise direction, except that a body force representing the pressure gradient is also applied in this direction, as practiced by Succi *et al.*[3] The symmetry of the flow was not exploited, i.e., the entire profile was simulated from one wall to the other. The collision operator was constructed in accordance with the FHP-II seven-bit model[4–6] at an average density per site of 0.18. The simulation was started with all of the densities set to the average density, and the model operated until steady state was reached, from 3000 to 6000 iterations, depending on the number of lattice points. The average velocity was then calculated by integrating the velocity across the flow.

The calculated velocity profiles near the walls are plotted in Fig. 2. Each figure contains two curves, one being the lattice Boltzmann results for that run and the other being a parabola constructed using the average velocity for that run. Figure 2a was calculated using the proposed new boundary condition, Fig. 2b with the bounce-back condition and the older interpretation of the wall at the node *A* line, and Fig. 2c with the wall moved to the midplane between the first and second nodes. The problem with the bounce-back condition is apparent, as is improvement occasioned with either of the other methods. The difference between the reinterpreted bounce-back and the new method is more clearly seen in Fig. 3, which shows the relative error in the velocity for the three boundary conditions. Even though the reinterpreted bounce-back (Cornubert *et al.*) and the new

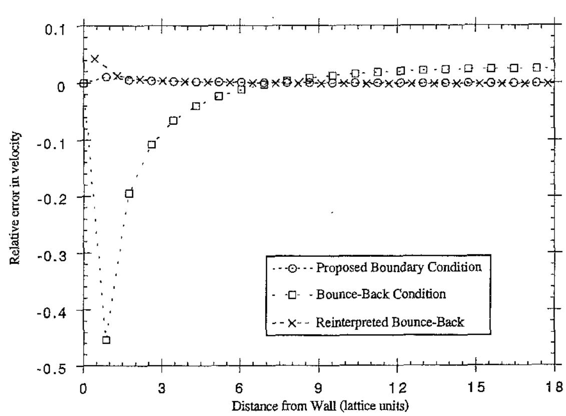

Fig. 3. Relative error in velocity for various boundary condition implementations.

Table I. Wall Shear Stress (Lattice Units ×1000) Calculated by Momentum Change and Velocity Gradient for Three Boundary Conditions for Mesh Sizes of 39 and 78

	Wall collision		Bounce-back		Reinterpreted bounce-back	
	39	78	39	78	39	78
Momentum	1.84	3.59	1.84	3.59	1.83	3.56
Velocity gradient	1.89	3.69	0.944	1.85	1.96	3.87
Difference	2.7%	2.8%	49%	49%	7.1%	8.7%

method are much better than the older interpretation of bounce-back, the new method is superior adjacent to the wall.

The interpretation of these results is consistent with the discussion of velocity gradients. The drag on the walls can be calculated using two methods. In the first, the momentum difference between the particles arriving and those leaving the wall is calculated. In the second, the velocity gradient at the wall is calculated and multiplied by the viscosity to give the shear stress. In principle, both methods should give the same result, which should also be consistent with the overall force on the system given by the product of the pressure gradient and channel width. Using the momentum difference method, each of the boundary implementations produces a wall shear stress in accordance with the imposed pressure gradient, to within several percent. However, when the velocity gradient method is used, the calculated shear stress does not match that calculated from the momentum change, by nearly 50% in the case of the bounce-back condition. This is shown in Table I, where the differences between the two shear stresses are given for each of the three boundary implementations. As can be seen, the reinterpreted bounce-back (i.e., wall halfway between node rows) is not as good as the new method of applying the collision operator at the wall nodes. The improvement results because applying the collision operator at the wall correctly applies the effect of viscosity and changing velocity throughout the calculation domain.

Incidentally, some of the difference between the momentum and velocity gradient methods may be attributed to the evaluation of the viscosity. Here the value was calculated from the theoretical kinematic viscosity and the real density based on the lattice used. A slightly different value would be obtained were the density based on an infinite lattice without edge effects.

4. CONCLUSION

Application of heuristic reasoning has led to the conclusion that the usual bounce-back boundary condition corresponds to a no-slip wall halfway between the row of fluid nodes and the row where the condition is applied. This is in agreement with the formal theoretical development of Cornubert *et al.*[1] The logic has been extended to suggest an improvement which accurately represents the viscosity and velocity gradients to the edges of the flow domain. The suggested technique returns the wall location to the first row of nodes. It involves application of the relevant symmetry conditions to assure zero normal and tangential velocity at the walls followed by application of the usual collision operator to the wall nodes. The proposed method is shown through a numerical example to give a more accurate near-wall velocity than the interpretation of the bounce-back condition given by Cornubert.

Although this method is discussed in the context of lattice Boltzmann simulations, it is expected that a similar approach could be applied to lattice gas simulations with equal effect.

REFERENCES

1. R. Cornubert, D. d'Humieres, and D. Levermore, A Knudsen layer theory for lattice gases, *Physica D* **47**:241 (1991).
2. Paul Lavallee, Jean Pierre Boon, and Alain Noullez, Boundaries in lattice gas flows, *Physica D* **47**:233 (1991).
3. S. Succi, E. Foti, and F. Higuera, Three-dimensional flows in complex geometries with the lattice Boltzmann method, *Europhys. Lett.* **10**:433 (1989).
4. Dominique d'Humieres and Piere Lallemand, Numerical simulations of hydrodynamics with lattice gas automata in two dimensions, *Complex Syst.* **1**:599 (1987).
5. Andrew K. Gunstensen, Daniel H. Rothman, Stephane Zaleski, and Gianluigi Zanetti, Lattice Boltzmann model of immiscible fluids, *Phys. Rev. A* **43**:4320 (1991).
6. F. J. Higuera and J. Jimenez, Boltzmann approach to lattice gas simulations, *Europhys. Lett.* **9**:663 (1989).

822/71/5-6-22