PHYSICAL REVIEW E VOLUME 51, NUMBER 4 APRIL 1995

Reply to "Comment on 'Simulation of a two-dimensional Rayleigh-Bénard system using the direct simulation Monte Carlo method'"

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(Received 31 October 1994)

In response to the preceding Comment by Garcia, Baras, and Mansour [Phys. Rev. E **51**, 3784 (1995)], we evaluate the Rayleigh number by taking the temperature jump at the wall into consideration. It is shown that a good agreement between the direct simulation Monte Carlo results and the linear stability theory is obtained by using the diffuse boundary condition, while there is a slight discrepancy in the case of the semislip boundary condition.

PACS number(s): 47.11.+j, 47.20.Bp, 47.45.Gx, 47.70.Nd

The authors of the preceding Comment [1] criticize the results of our paper [2] in which we performed the simulation of not only the Rayleigh-Bénard (RB) convection but also the heat conduction using the direct simulation Monte Carlo (DSMC) method. The objective of our systematic simulation was to study the macroscopic flow instability by a molecular-level computation. In this sense, our simulation was a trial using a particle method. They claim that the difference in critical Rayleigh number between the linear stability analysis and the DSMC method with the semislip boundary condition is due to the temperature jump near the wall. They also state that the semislip condition is more economical than the diffuse condition.

The existence of the temperature jump near the wall in rarefied gas is well known. In DSMC calculations, it is significantly large when the semislip boundary condition, in which only the normal component of velocity is thermalized, is used even in the continuum region at a low Knudsen number. On such a condition, the Rayleigh number may be defined not by the wall temperatures but by the calculated fluid temperatures at the wall. On the other hand, if we use the diffuse boundary condition, in which all the velocity components are thermalized based on the equilibrium Maxwellian distribution, such a modification is not necessary since the temperature jump is small under the same condition. In this case, we can compare the DSMC results with the hydrodynamic theory directly.

In response to the preceding Comment, we evaluate the Rayleigh number by taking account of the temperature jump. The temperature difference used for the evaluation of the Rayleigh number is defined not by the wall temperatures but by the calculated fluid temperatures at the wall. The midelevation temperatures obtained by the diffuse boundary condition and the semislip boundary condition are shown in Figs. 1 and 2, respectively. For a

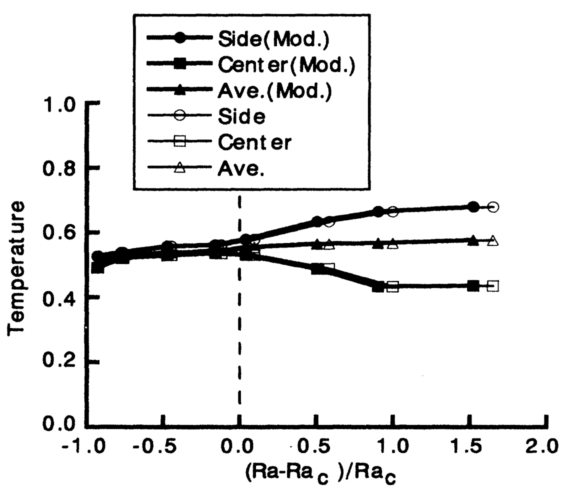

FIG. 1. Midelevation temperatures obtained by using the diffuse boundary condition. The temperatures are normalized so that the temperatures of the top and bottom walls are 0.0 and 1.0, respectively. The temperatures near the side wall (side) and at the center (center) are plotted together with the horizontal average (Ave.). The case with the modified Rayleigh number taking account of the temperature jump is denoted by "Mod."

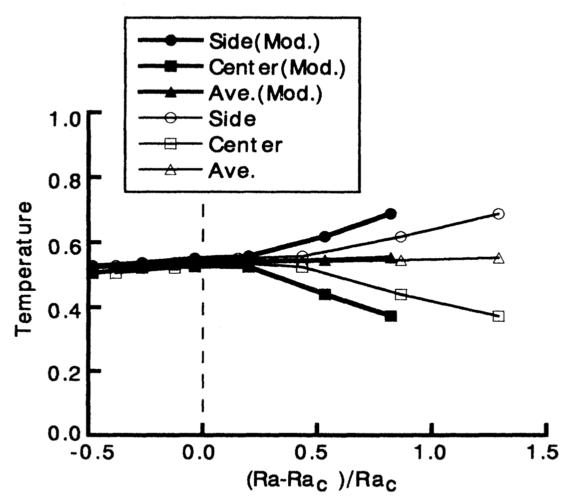

FIG. 2. Midelevation temperatures obtained using the semislip boundary condition. See caption to Fig. 1.

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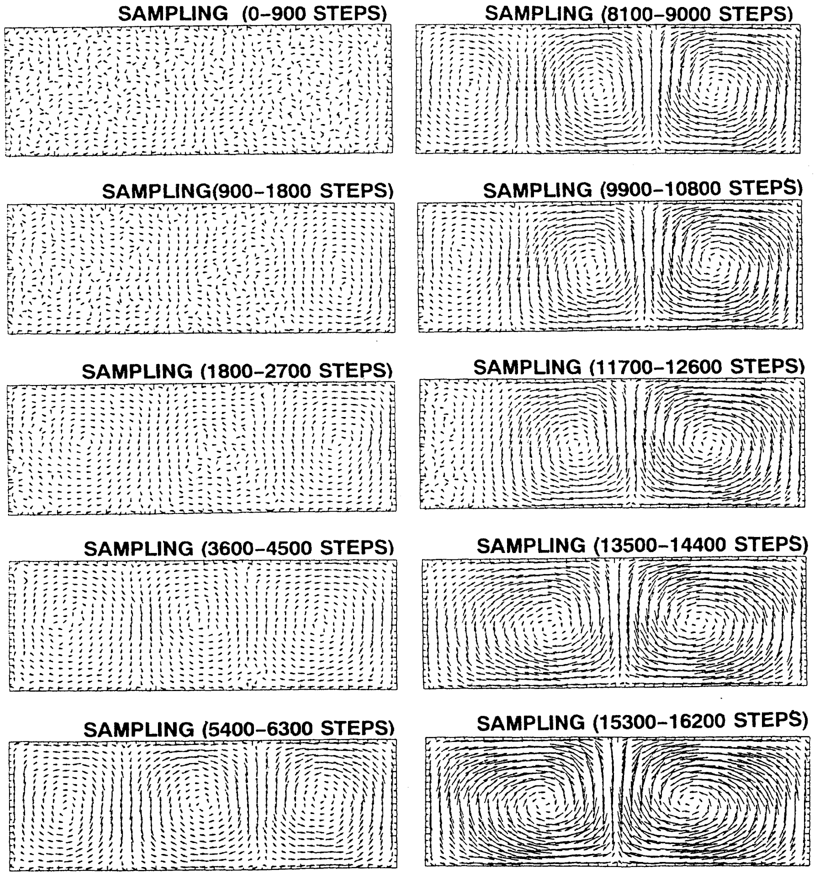

FIG. 3. An example of the transient of the velocity field using the semislip boundary condition.

clearer comparison of the DSMC results and the hydrodynamic theory, the nondimensional temperatures are plotted against the parameter $(\mathrm{Ra}-\mathrm{Ra}_c)/\mathrm{Ra}_c$, where Ra is the Rayleigh number in the DSMC calculation, and Ra_c is the critical Rayleigh number obtained by the linear stability theory. The temperatures near the side wall and at the center are denoted by "side" and "center," respectively, and the average temperature is denoted by "Ave." in these figures. The data points using the Rayleigh number taking account of the temperature jump are indicated by "(Mod.)."

As shown in Fig. 1, the temperature jump is almost negligible under the diffuse boundary condition. This is because our simulation condition with the Knudsen number of 0.016 almost corresponds to the continuum region. The temperature bifurcation is observed at around $(\mathrm{Ra}-\mathrm{Ra}_c)/\mathrm{Ra}_c=0$, and the agreement between the DSMC results and the hydrodynamic theory is still good. On the other hand, in the case of the semislip boundary condition, the temperature bifurcation is shifted towards $(\mathrm{Ra}-\mathrm{Ra}_c)/\mathrm{Ra}_c=0$ by taking account of the temperature-jump effect as shown in Fig. 2. It is, however, seen that there is a slight discrepancy between the DSMC results and the hydrodynamic theory.

As for the computational cost using the semislip boundary condition, the statement of the authors of the preceding Comment is not always the case. For instance, the transient of convection rolls using the semislip boundary condition is shown in Fig. 3 at a Rayleigh number sufficiently higher than the critical value. In this figure, three convection rolls appear first, and then the two of them grow into stable rolls. More than 15 000 time steps are necessary in this case to get a stable convection. On the other hand, the stable convection rolls are obtained only after 3000 time steps using the diffuse boundary condition [2]. The transient behavior of macroscopic flow field is affected by the boundary and initial conditions. Although the study of the transient flow is of importance, a longer transient is not necessary when the field variables in steady-state convection rolls are of main interest, and thus the semislip boundary condition is not always "more economical."

[1] A. L. Garcia, F. Baras, and M. M. Mansour, preceding paper, Phys. Rev. E **51**, 3784 (1995).

[2] T. Watanabe, H. Kaburaki, and M. Yokokawa, Phys. Rev. E **49**, 4060 (1994).