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

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In a recent paper, Watanabe, Kaburaki, and Yokokawa [Phys. Rev. E **49**, 4060 (1994)] used a direct simulation Monte Carlo method to study Rayleigh-Bénard convection. They reported that, using stress-free boundary conditions, the onset of convection in the simulation occurred at a Rayleigh number much larger than the critical Rayleigh number predicted by a linear stability analysis. We show that the source of the discrepancy is their omission of a temperature jump effect in the calculation of the Rayleigh number.

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The direct simulation Monte Carlo method (DSMC), introduced by Bird, is a popular numerical scheme for computing rarefied gas flows [1]. The method is particularly useful in the simulation of flows with high Knudsen number (ratio of mean free path to characteristic length), where the conventional Navier-Stokes description of hydrodynamics breaks down. Numerical and experimental tests have confirmed the validity and accuracy of the DSMC algorithm in diverse scenarios [2]. Theoretical studies have also shown the mathematical convergence of DSMC methods to the solution of the fluctuating Boltzmann equation [3].

Consider a fluid confined between horizontal walls held at fixed temperatures T_L (lower wall) and T_U (upper wall), with $T_L > T_U$. When a critical value of the temperature gradient is exceeded, the purely conductive state becomes unstable and a transition to well structured convective behavior occurs [4]. This transition, known as the Rayleigh-Bénard (RB) instability, is governed by the Rayleigh number, Ra, defined as

$$\mathrm{Ra} = \frac{\alpha \Delta T g L^3}{\nu \lambda_T}, \tag{1}$$

where L is the distance between the horizontal boundaries, g is the gravitational acceleration, $\Delta T = T_L - T_U$ is the temperature difference, ν and λ_T are the kinematic viscosity and thermal diffusivity, respectively, and $\alpha = -(\partial \ln \rho / \partial T)_P$ is the thermal expansion coefficient.

In a recent paper, Watanabe, Kaburaki, and Yokokawa [5] discuss DSMC simulations of Rayleigh-Bénard convection in low Knudsen number systems. The study of RB convection using DSMC is not new [6–8] and numerous molecular dynamics (MD) studies have also appeared [9–11]. In their paper, Watanabe *et al.* considered two types of boundary conditions for the upper and lower boundaries: fully thermalizing and stress-free conditions. By varying ΔT they found that, for fully thermalizing boundaries, the onset of convection occurs at a Rayleigh number which roughly agrees with linear stability theory (see their Fig. 4). On the other hand, for stress-free boundaries (which they call "semislip") they found the onset of convection occurring at a significantly higher temperature difference than predicted by theory (see their Fig. 6). They concluded that the "semislip boundary condition, which has been frequently used in MD and DSMC simulations, was shown to be inadequate to simulate the thermal boundary condition."

Particle-based simulations of RB convection often use stress-free boundary conditions because convection occurs at a significantly lower Ra than with fully thermalizing boundaries. Since computational costs increase rapidly with Rayleigh number, it is more economical to study RB convection using stress-free boundaries. Furthermore, particle simulations with stress-free boundaries are found to be in excellent agreement with numerical solutions of the Navier-Stokes equations (e.g., see Fig. 6 in [7], Fig. 1 in [8], Figs. 2–5 in [10], and Fig. 7 in [11]). Thus the question arises: why did Watanabe *et al.* find disagreement between the linear stability prediction for the critical Ra and their DSMC simulations using stress-free boundaries? The answer is that they neglected to account for "temperature jump" in their calculation of Rayleigh number. It was first pointed out by Maxwell that in a gas with a temperature gradient the temperature of the gas near a wall does not match the wall's temperature. This phenomenon is known as temperature jump or temperature slip [12,13]. Specifically, the difference between the temperature of the wall and the temperature of the gas near the wall is $\delta \nabla_\perp T$ where $\nabla_\perp T$ is the temperature gradient normal to the wall. For fully thermalizing boundaries, $\delta \approx 2\lambda$ where λ is the mean free path in the gas [14]. For stress-free boundaries, where only the normal component of velocity is thermal-

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ized, the temperature jump can be significantly larger [15]. In some circumstances (e.g., the onset of explosion in exothermal gas-phase reactions [16]) the temperature jump effect can be dramatic.

For a dilute gas, the density profile in the conduction state goes as $\rho \propto T^{-c}$ where $c = 1 - mgL/k\Delta T$, m is the mass of a particle, and k is Boltzmann's constant. To maintain an approximately constant density, one often fixes the gravity in a simulation as $g = k\Delta T/mL$ and Watanabe *et al.* set g in this manner. Using the Chapman-Enskog expressions for ν and λ_T, we may write the Rayleigh number as

$$\mathrm{Ra} = \frac{256}{125\pi}\left(\frac{\Delta T}{T_0}\right)^2\left(\frac{L}{\lambda}\right)^2, \qquad (2)$$

where T_0 is the mean temperature in the system. From this expression one sees that, keeping all else constant, the Rayleigh number varies quadratically with ΔT.

The vertical temperature gradient measured in a DSMC simulation of RB convection using stress-free boundary conditions is shown in Fig. 1. The gas is convecting and the vertical cross section shown in Fig. 1 is centered on one of the rolls. The system size is $L = 40\lambda$ and the wall temperatures are $T_U = 0.5$ and $T_L = 2.0$. The important feature to notice is that the temperature gradient in the gas is significantly reduced due to the temperature jump at the walls. For this reason, linear stability analysis using $\Delta T = T_L - T_U$ will not correctly predict the onset of convection in the simulation. Previous work comparing MD or DSMC simulations to Navier-Stokes solutions *did* account for temperature jump and thus found no discrepancy. Even nonlinear stability analysis was shown to give quantitative agreement with hard disk MD simulations of RB convection provided the temperature jump was included in the analysis [11].

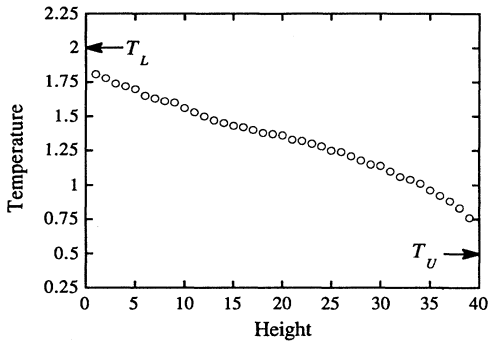

FIG. 1. Temperature profile measured in a DSMC simulation for a convecting Rayleigh-Bénard system with stress-free boundaries. Wall temperatures are $T_L = 2.0$ and $T_U = 0.5$; note that the temperature of the fluid near the wall does not match the wall's temperature.

For fully thermalizing walls, a temperature jump is present but its magnitude δ is smaller. In the Watanabe *et al.* simulations using this boundary condition, if the critical Rayleigh number was shifted by about 10%, the effect would not be noticeable in their data.

In conclusion, even at relatively low Knudsen numbers, microscopic effects, such as temperature jump, are important in particle simulations of fluids. Great care must be taken when comparing simulation results with continuum theory.

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