Information Preservation Modeling of Rayleigh-Bénard Transition from Thermal Conduction to Convection

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Abstract. Onset and evolution of the Rayleigh-Bénard (R-B) convection are investigated using the Information Preservation (IP) method. The information velocity and temperature are updated using the Octant Flux Splitting (OFS) model developed by Masters & Ye based on the Maxwell transport equation suggested by Sun & Boyd. Statistical noise inherent in particle approaches such as the direct simulation Monte Carlo (DSMC) method is effectively reduced by the IP method, and therefore the evolutions from an initial quiescent fluid to a final steady state are shown clearly. An interesting phenomenon is observed: when the Rayleigh number (Ra) exceeds its critical value, there exists an obvious incubation stage. During the incubation stage, the vortex structure clearly appears and evolves, whereas the Nusselt number (Nu) of the lower plate is close to unity. After the incubation stage, the vortex velocity and Nu rapidly increase, and the flow field quickly reaches a steady, convective state. A relation of Nu to Ra given by IP agrees with those given by DSMC, the classical theory and experimental data.

Keywords: Hydrodynamic instability; Rayleigh-Bénard flows; DSMC; IP Method
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INTRODUCTION

The onset of convection in an initially quiescent fluid confined between two parallel horizontal walls and heated from below is a classical problem known in hydrodynamics as the Rayleigh-Bénard (R-B) flow [1]. It is often taken as a standard model to analyze hydrodynamic instability, self-organization and transition to turbulence in fluids [2-5].

Compared to enormous works on R-B flows in the continuum viewpoint during more than one century, kinetic studies in this aspect are at a young stage. Garcia [8] firstly applied the direct simulation Monte Carlo (DSMC) [6, 7] method to the R-B flow. After many efforts [9-12], the DSMC method was extended to calculate the chaotic fluid motions at large Rayleigh numbers [13], and the DSMC results compared well with those given by the finite difference method solving the Navier-Stokes equations.

A R-B transition from thermal conduction to convection occurs very quickly in a macroscopic sense, but it is considerably long in a microscopic sense that lasts about 10^4 mean collision time at Ra=3190, as shown in Sec. IV. To resolve clearly and efficiently the evolution of the R-B flow patterns at low Mach number, the information preservation (IP) method [14, 15] is employed here. The IP method has been successfully applied to many micro-scale gas flows [16-20] that efficiently overcome the statistical scatter of DSMC, but this is the first time for IP to solve a hydrodynamic instability problem. Therefore, it is quite interesting to test if it can correctly predict some important phenomena such as the critical Rayleigh number and evolving spatiotemporal structures. The answers given by the following calculations are very positive, which encourage more investigations in this aspect using the IP method.

INFORMATION PRESERVATION METHOD

In kinetic viewpoint, fluid flows are determined by molecular motions and initial and boundary conditions. In the IP method [14, 15], the initial IP velocity and temperature of each simulated molecule are given based on the initial conditions of a problem interested. They transport along with molecular motions. When a simulated molecule

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collides with another, they exchange the IP quantities in the meantime. When a simulated molecule encounters a computational boundary during its movement, the IP velocity and temperature take the boundary velocity and temperature. In the IP method, the flow field is obtained through sampling and averaging the IP velocity and temperature. This treatment avoids the computational noise arising from the molecular thermal motions.

The IP method was originally proposed to solve micro gas flows where the motions of simulated molecules can be described very well using the DSMC method [6, 7]. Because the transport processes of the IP quantities are carried out directly through molecular motions, the IP method works over the entire Knudsen regime [14-20]. The IP method can also be extended to other situations such as liquid using molecular dynamics instead of DSMC to simulate molecular motions.

Some important advancements of the IP method were achieved. Base on the Maxwell transport equation, Sun and Boyd [19] developed a theoretical frame to update the IP quantities. For monatomic molecules, it may written as

$$\frac{\partial}{\partial t}\left(nm\right) = -\nabla\cdot\left(nm\overline{\mathbf{V}_{IP}}\right), \tag{1}$$

$$\frac{\partial}{\partial t}\left(nm\overline{\mathbf{V}}_{IP}\right) + \nabla\cdot\left(nm\overline{\mathbf{c}\mathbf{V}_{IP}}\right) = -\nabla\cdot\left(nm\overline{\mathbf{c}'\mathbf{c}'''}\right) + nm\mathbf{F} + \Delta\left[m\mathbf{c}\right], \tag{2}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}nm\overline{(\mathrm{V}_{\mathrm{IP}}^2 + 3R\mathrm{T}_{\mathrm{IP}})}\right) + \nabla\cdot\left(\frac{1}{2}nm\overline{\mathbf{c}(\mathrm{V}_{\mathrm{IP}}^2 + 3R\mathrm{T}_{\mathrm{IP}})}\right) = \nabla\cdot\left(\frac{1}{2}nm\overline{\mathbf{c}'(\mathrm{V}_{\mathrm{IP}}^2 + 3R\mathrm{T}_{\mathrm{IP}} - c^2)}\right) + nm\mathbf{F}\cdot\overline{\mathbf{V}_{IP}} + \Delta\left[\frac{1}{2}mc^2\right]. \tag{3}$$

where the over bar denotes averaging over a volume element, $\mathrm{V_{IP}}$ and $\mathrm{T_{IP}}$ are the IP velocity and temperature of a simulated molecule, $\mathbf{c}' = \mathbf{c} - \mathbf{c}_0$ is the thermal velocity, $\mathbf{c}_0 = \overline{\mathbf{c}} = \overline{\mathbf{V}}_{IP}$ is the stream velocity, $\mathbf{c}''' = \mathbf{c} - \mathbf{V}_{IP}$, and $\mathrm{T_{IP}} = \left(\overline{c^2} - \mathrm{V_{IP}^2}\right)\Big/3R$.

The first terms on the right hand side of Eqs. (2) and (3) reflect the correlations between the IP quantities and molecular motion. To calculate these correlated terms, a Flux Splitting (FS) model was suggested in Ref. [19], and it was extended by Masters and Ye [20] who developed an octant flux splitting (OFS) model. Using the OFS model, several thermal transpiration phenomena were successfully solved by the IP method [20].

Eqs. (1-3) and the OFS model are employed here to update the IP quantities in simulation of R-B flows.

COMPUTATIONAL CONDITIONS

This paper considers a two-dimensional R-B problem. Linear perturbation analysis of the N-S equations shows that its stability is determined by a non-dimensional parameter, namely the Rayleigh number (Ra)

$$\mathrm{Ra} = \frac{\alpha g \Delta T d^3}{\nu\kappa}, \tag{4}$$

where α, ν, κ are the coefficients of volume expansion, kinetic viscosity and thermal diffusivity, respectively, g is the acceleration of gravity, $\Delta T = T_l - T_u$, T_u and T_l are the temperatures at the upper and lower plates, respectively, and d is the distance between the lower and upper plates.

Substitution of the kinetic transport coefficients for a hard-sphere gas into Eq. (4) yields [13]

$$\mathrm{Ra} = \frac{2048}{75\pi}\times\frac{1-r}{(1+r)^2\,\mathrm{Kn}^2\mathrm{Fr}}, \tag{5}$$

where $\mathrm{Kn} = \lambda/d$, $\mathrm{Fr} = c_m^2/gd$, $c_m = \sqrt{2kT_l/m}$ is the most probable thermal speed of molecules, and the temperature ratio $r = T_u/T_l$.

Eq. (5) shows that Ra depends upon Kn, Fr and r. In our calculations, the required Ra is obtained through adjusting Fr, while the Knudsen number and the temperature ratio are fixed to be 0.01 and 0.1, respectively, and the length-to-width ratio of the computational domain ($\Gamma = L/d$) is also fixed to be 2.

The simulation gas is argon. Each simulation starts from a uniform state at rest, gas temperature is the same as T_l, and the number density is 2.45×10^{25}. The boundary conditions are assumed to be diffusively reflecting at the upper and lower plates, and specularly reflecting at the left and right sides. The computational domain is divided into 64×32 sampling cells, and each sampling cell contains 4×4 sub-cells [6] within which collision pairs are selected. The time step Δt equals to $0.1\tau_c$, where τ_c is the mean collision time of the gaseous molecules. The evolution of R-

B flow patterns are described through short time averaging. The averaging period t_s is taken as $200\,\Delta t$ that is much smaller than the time scale of unsteady flows investigated here.

RESULTS AND DISCCUSION

IV.1 Case A: Ra=1509

Fig. 1 shows the velocity vector distributions in the initial stage given by the IP method at Ra=1509, while Fig. 2 presents the Nusselt numbers (Nu) versus time given by IP and DSMC, respectively, which agree well with each other. In this paper, $Nu = q_t / q_c$, where q_t is the heat flux through the lower plate, and $q_c = \kappa \Delta T / d$ is the heat flux in thermal conduction. Because the initial temperature of gas is the same as the lower plate that is 10 times the upper plate, a drastic upward motion appears around the upper plate immediately (Fig.1a). Such an upward motion gradually extends to the whole domain after $4\,t_s$ (Fig.1b) that corresponds to the maximum total heat flux through the lower plate (Fig.2a). Limited by the upper and lower plates, the upward motion becomes to oscillate up and down at t=$5\,t_s$ (Fig.1c). This oscillation lasts about $50\,t_s$, and its amplitude gradually decreases due to the gas viscosity (Fig.2a). The flow field reaches a steady state of thermal conduction without macroscopic motions after about $100\,t_s$, and the heat flux through the lower plate becomes constant since then (Fig.2b).

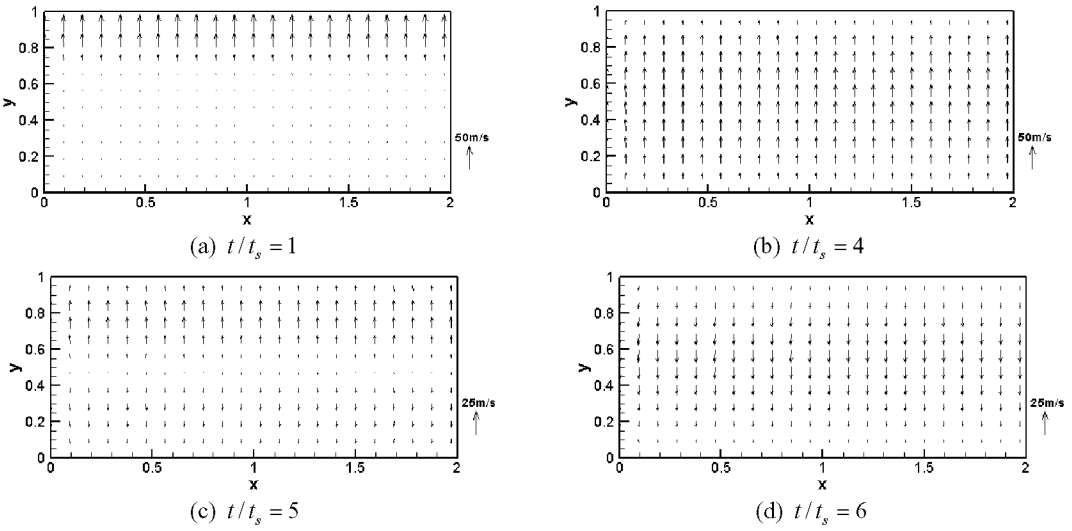


FIGURE 1. Evolution of the velocity field given by IP at Ra=1509.

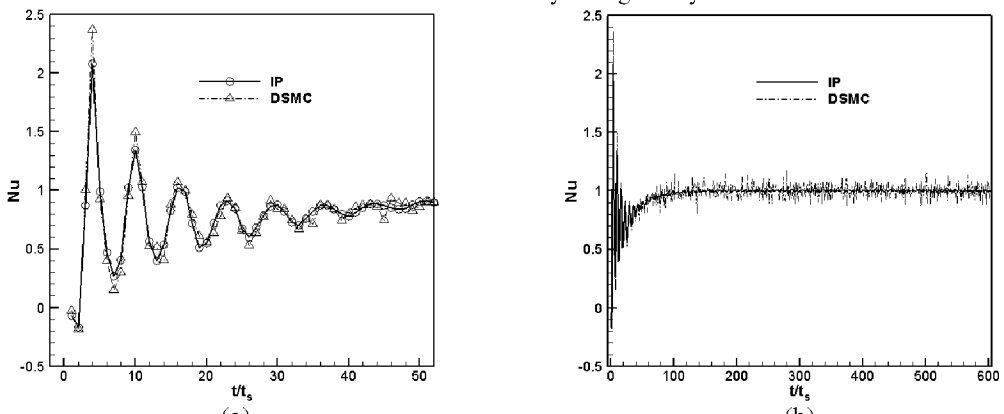


FIGURE 2. Nu versus time given by IP and DSMC at Ra=1509. (a): the initial stage; (b): the whole process.

IV.2 Case B: Ra=3190

Fig. 3 presents Nu versus time at Ra=3190. The IP and DSMC profiles are in good agreement, and they show that the evolution consists of three stages.

The first stage is similar to that at Ra=1509. When it ends at about $100\,t_s$, the Nusselt number is close to unity (Fig.3), and the amplitude of oscillation almost vanishes.

The second stage is from $100\,t_s$ to $250\,t_s$. This can be regarded as an incubation stage of the R-B transition. The values of Nu almost remain unity (Fig. 3), but the vortex structures and slight temperature variations are clearly demonstrated by the IP method (Fig.4a-4d). The vortex velocity is of the order of 1 m/s at $110\,t_s$, and increases to about 2m/s at $200\,t_s$, and 4m/s at $250\,t_s$, while the three vortices at $110\,t_s$ evolve and combine to be two vortices at $250\,t_s$. It is difficult for DSMC to catch these phenomena at the low Mach numbers because of its statistical fluctuation.

In the third stage, the vortex velocity rapidly increases about 10 times from 4m/s at $250\,t_s$ to 40m/s at $400\,t_s$ (Fig.4d-4g), accompanied by a jump of Nu (Fig. 3). When the transition is finished at about $400\,t_s$, the flow field reaches a steady, convective state.

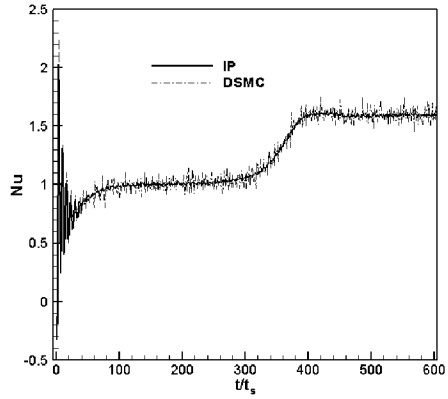
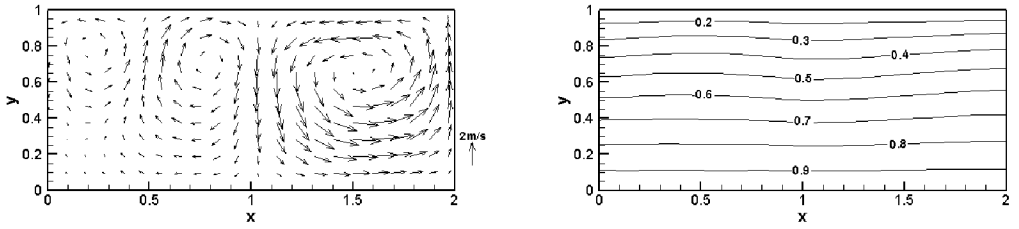
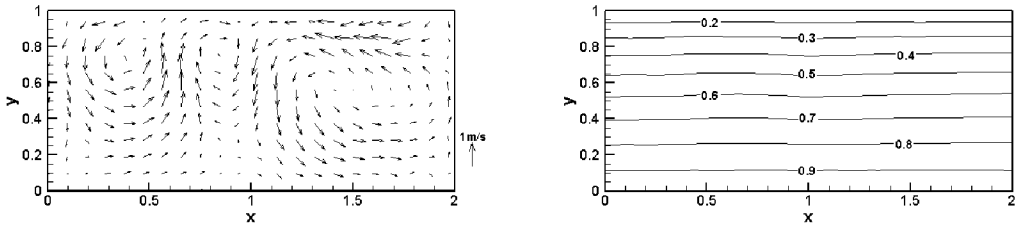


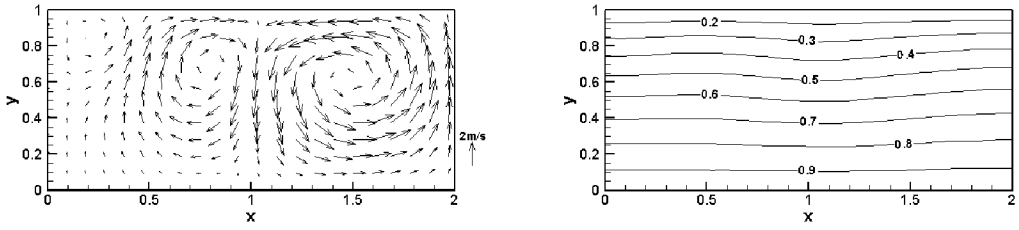
FIGURE 3. Nu versus time given by IP and DSMC at Ra=3190.



(a) $t/t_s = 110$

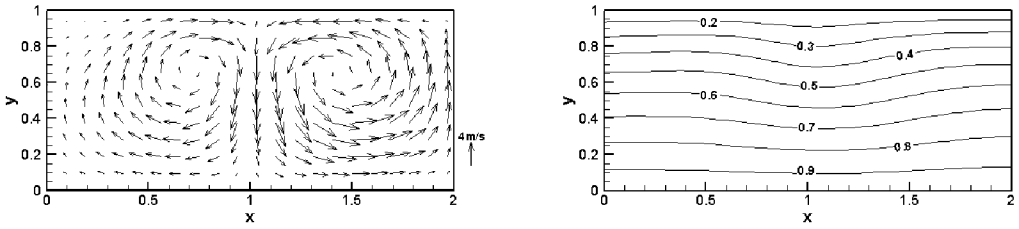


(b) $t/t_s = 150$

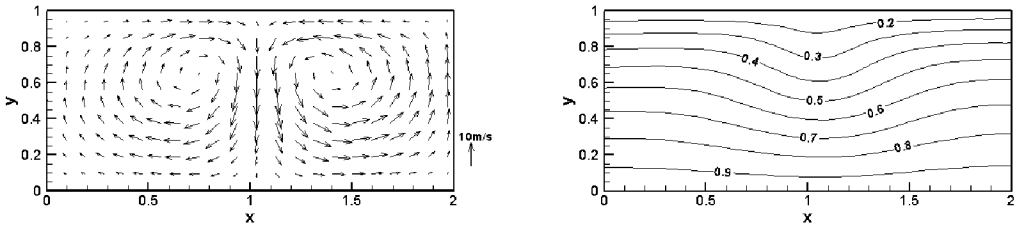


(c) $t/t_s = 200$

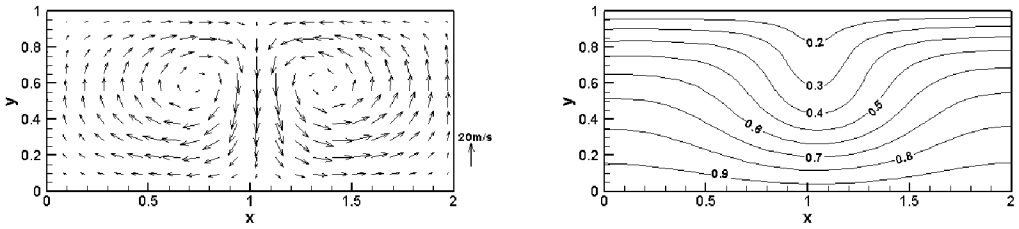
FIGURE 4. Evolution of velocity and temperature fields given by IP at Ra=3190.



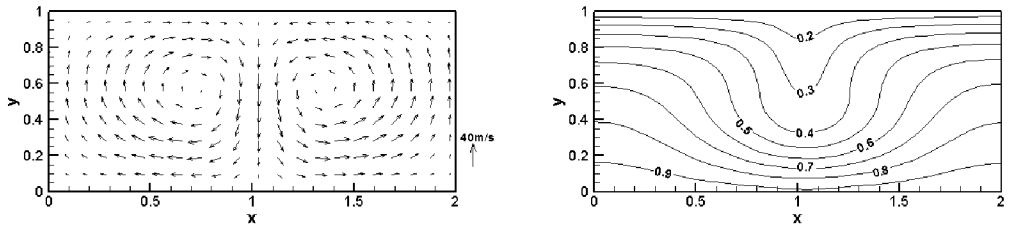
(d) $t/t_s = 250$



(e) $t/t_s = 300$



(f) $t/t_s = 350$



(g) $t/t_s = 400$

FIGURE 4. (cont.).

IV.3 Relation of Nu to Ra

After the R-B flows evolve and reach a steady state, the total heat flux through the lower plate is related to Ra in Fig.5. The IP and DSMC results are in excellent agreement, and in general they are supported by the classical theory of Schlüter, Lortz and Busse [21] and experimental data of Koschmieder and Pallas [22]. The theoretical solution [21] based on the Navier-Stokes equations for small Prandtl number after the onset of convection in the

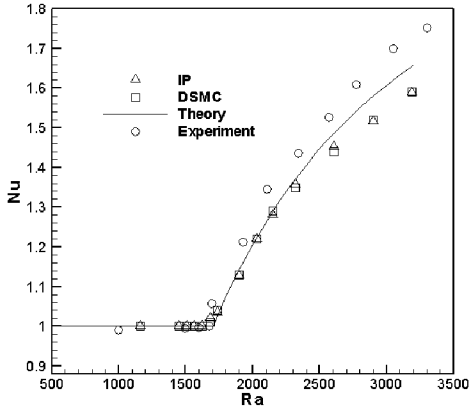


FIGURE 5. Relation of Nu to Ra when R-B flows reaches a steady state.

form of rolls may be written as:

$$\mathrm{Nu} \cong \begin{cases} 1.0 & \mathrm{Ra} < \mathrm{Ra}_c \\ 2.41 - 1.41\mathrm{Ra}_c/\mathrm{Ra} & \mathrm{Ra} \geq \mathrm{Ra}_c \end{cases}, \tag{6}$$

where the critical Rayleigh number $\mathrm{Ra}_c \cong 1708$.

According to the Schmidt-Milverton principle [1], the onset of thermal instability takes places when the measured data of the total heat flux through the lower or upper plate abruptly increases. The values of Ra_c determined in this principle from the IP and DSMC calculations are about 1680.

CONCLUSION

In this paper, The R-B transitions from thermal conduction to convection are efficiently simulated by the IP method, which clearly depicts the incubation stage where the vortices firstly appear and gradually form the convective pattern. The IP method provides a promising tool to study the microscopic origin of hydrodynamic instability.

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