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A Modification Technique of Collision Probability in the Direct Simulation Monte Carlo Method

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Abstract

In Direct Simulation Monte Carlo (DSMC) method, it is difficulty to keep grid size smaller than local mean free path, that influences calculation accuracy much. In this paper, a new modification technique of collision probability with least square method and sub-relaxation technique is introduced to improve simulation accuracy in DSMC with coarse grid size. The new method is applied to direct simulation Monte Carlo method based on unstructured tetrahedral cells, which can be easily used for other grid topology. A numerical example with different grid size is implemented to validate the method discussed here, and the numerical results confirm feasibility of the modification technique.

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Keywords: DSMC; Unstructured grid; Collision probability correction; Least square method

1. Introduction

As the development of hypersonic vehicles, star exploration and satellite technique[1-3], rarefaction becomes more and more important. In numerical simulation methods for forecasting the rarefied aerodynamics, Direct Simulation Monte Carlo(DSMC) method is the most effective one than others[4,5]. Direct simulation Monte Carlo(DSMC)method had been formulated by Bird [6] in 1970,and it marked a milestone in the evolution of fluid mechanics. Although probably not appreciated then, the method had enormous power, and, as time went on, it was

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extensively adopted at solving very complex rarefied flows involving chemical reactions, ionization, and high degrees of molecular non-equilibrium [4,5].The basic steps in DSMC[6]simulation are that the position, velocity, andinternal energy of each simulated particle which represent real gas particles are stored and can be changed as colliding with each other and reflecting off surfaces. Lastly, the macroscopic quantities of the flow can be obtained by sampling.

One of the fundamental assumptions of the DSMC method is that particle movement can be decoupled from collision behavior.The probability of a collision occurring is dependent on the collision model and selection scheme being employed and is a function of the relative velocity, collision cross section and the gas number density in that cell.

No time counter (NTC)scheme of Bird[7] for collision pair selection in the Direct Simulation Monte Carlo(DSMC) is used to determine the number of potential collision pairs in a cell. The number of potential collision pairs in a cell is related to the cell-averaged number density, and collision probability for each pairs is not related to local position within a cell. However, when grid size is coarse, internal density variation within a cell will introduce collision probabilities error if using the cell-averaged number density for collision probability. Correction of the binary collision probability for effects of spatial density variation need to be done.

From above all, collision probability of potential collision pairs in a coarse cell is very different from that in a dense grid cell. To correct the collision probabilities error of a collision pairs in a coarse cell, linear reconstruction for number density in a cell can be made, and local collision probability of the collision pairs in a cell can be modified with local number density.Burt[8] has used this method in Cartesian grid. However, it can be found that Burt's method is easy to use in Cartesian grid, but that is difficult for other mesh topology. In this paper, this difficulty can be overcame by using least square method and sub-relaxation method.

2. Present approach

2.1 DSMC methods[6]

The variable hard sphere model was used for molecular collisions. The Larsen-Borgnakke model[9]was assumed for energy transfer between translational and internal molecular modes. The rotational energy was only considered in the internal modes. The acceptance- rejection method was applied for the division of energy. Diffuse reflection condition is used at wall.

2.2 collision probability correction method

For NTC methods, the number of collisions in Δt time step is computed by

$$N_{coll} = \frac{W\bar{N}^2}{2V}\Delta t(\sigma g)_{\max} \tag{1}$$

Where σ is collision cross section，g is relative velocity，$\bar{N}$ is the time-averaged molecular number，N_{coll} is collisions number，Δt is time step，W is particle weight，V is cell volume。

In DSMC method，the collision probabilities of a collision pairs in a cell is given by

$$p_{ij} = \frac{\sigma_{ij} g_{ij}}{(\sigma g)_{\max}} \tag{2}$$

Substituting Eqs. (1-2) to Eq. (3), the averaged collision frequency in a cell can be computed by

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