A PARTICLE COLLISION SELECTION METHOD BASED ON MONTE CARLO METHOD

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Keywords Monte Carlo Method, Particle Collision Selection, Optimization

Abstract Calculation of rarefied gases most adopts discrete method. The number of simulated particles is an important parameter of discrete algorithm. The lighter the mass of simulated particles is, the more the number of simulated particles is, the higher the accuracy of the corresponding calculation results, and the more difficult the calculation is. Therefore, how to set the appropriate simulated particle mass has always been an important problem to be solved by discrete algorithm.

There is no solution to set the appropriate simulated particle mass in this paper, but by optimizing the conventional particle collision selection method, this paper indirectly reduces the dependence of the accuracy of calculation results on the setting of simulated particle mass, and then reduces the difficulty of calculation, so as to determine the appropriate simulated particle mass equivalently.

The particle collision selection method proposed in this paper is explained by the two-particle collision selection method in a grid in Monte Carlo method: The basic parameters of the grid and the particles in the grid are known, the original Monte Carlo method calculates the number of collision particle pairs n first, and then randomly chooses n for collision calculation; And the method in this paper is to add an influence factor m greater than 1 and select n*m pairs of particles, each pair of particles chooses whether or not to collide through probability 1/m, then the collision pairs calculated by probability are calculated. Others such as mesh generation and boundary reflection and so on, follow the original Monte Carlo method.

Assuming that the mass of the simulated particle is 1, by adding the particle collision selection method (m=2) in the Monte Carlo method, and comparing with the original Monte Carlo method to reduce the particle mass, it is found that adding the influence factor m=2 is equivalent to the original Monte Carlo method with the particle mass of 0.6 under the same convergence accuracy and the particle mass of 0.8 under the same convergence time.

It can be seen that the particle collision selection method proposed in this paper is added to the Monte Carlo method, which improves the calculation accuracy but increases the computational difficulty. However, the increase of computational difficulty is less than that of computational accuracy, which shows that this method is useful to optimize the Monte Carlo method.

1 INTRODUCTION

Calculation of rarefied gases most adopts discrete method. The number of simulated particles is an important parameter of discrete algorithm. The lighter the mass of simulated particles is, the more the number of simulated particles is, the higher the accuracy of the corresponding calculation results, and the more difficult the calculation is. Therefore, how to set the appropriate simulated particle mass has always been an important problem to be solved by discrete algorithm.

There is not yet an internationally recognized method in Monte Carlo to set the mass of simulated particles, which makes the calculation difficulty minimum to achieve the appropriate convergence accuracy.

2 OBJECTIVE

In this paper, a new method is proposed to optimize the conventional particle collision selection method. It is assumed that it can indirectly reduce the dependence of the accuracy of calculation results on the setting of simulated particle mass, and then reduces the difficulty of calculation, and the difficulty of "setting appropriate simulated particle mass" is reduced equally.

3 METHOD

In conventional Monte Carlo calculation, the computational region needs to be meshed first, and then the initial value is given. Then the trajectory of the simulated particle is calculated step by step according to the time step. The changes of various fields composed of the trajectory of the simulated particle in the computational region are counted continuously, and the calculation is completed when the fields are stable to the computational requirements. Among them, the trajectory of the simulated particle is calculated separately by each grid according to the time step, which includes four calculation parts: the number of collision pairs, the selection of collision pairs, the collision and the new trajectories.

The calculation method presented in this paper is applied to the calculation part of the selection of collision pairs, while the rest of the calculation method remains unchanged. By optimizing the method of collision pair selection, the quality of collision pair selection is improved, so as to indirectly reduce the dependence of the accuracy of calculation results on the mass of simulated particles. The specific methods are as follows.

The number of simulated particle collision pairs calculated in the previous step is set to n , and n is integrative up to n_{ceil}, and the original method is:

$$N_n = f(n) \tag{1}$$

Where N_n is an array of 2 rows and n_{ceil} columns, each column represents a pair of simulated particles corresponding to the next collision calculation.

Assuming that the optimization factor proposed by this method is m □ $m > 1$ □,the number of simulated particle collision pairs of the original method is transformed into $k = n \cdot m$, and k is integrative up to k_{ceil}. Using the original collision pair selection method, we can calculate:

$$N_k = f(k) \tag{2}$$

N_k is an array of 2 rows and k_{ceil} columns.

The simulated particle pairs corresponding to each column in the N_k array are re-sampled and selected for the next collision calculation. The sampling method is random sampling by

means of (0, 1) average distribution. When the sampling result is less than $\frac{n}{k_{ceil}}$, it is selected, on the contrary, it is excluded.

4 RESULT

Assuming that the calculation area is a cylinder with a radius of 30 cm and a height of 30 cm. when looking down along the central axis, the cylinder rotates clockwise with a rotating speed of 500 Hz, each wall of the cylinder is isothermal for 300 K, the working gas is nitrogen, the inlet is a circular hole with a radius of 1mm at the center of the upper cover of the cylinder, the inlet velocity is 0.72 mg/h, the inlet position is random with the average area of the circular hole, the particle velocity is 0.5 times the sound velocity, and the particle velocity direction is average random in the lower half of the sphere, the outlet is a circular ring with a radius of 250-251 mm under the cylinder cover, and the outlet pressure is 2 Pa. The computational area diagram is shown in Figure1.

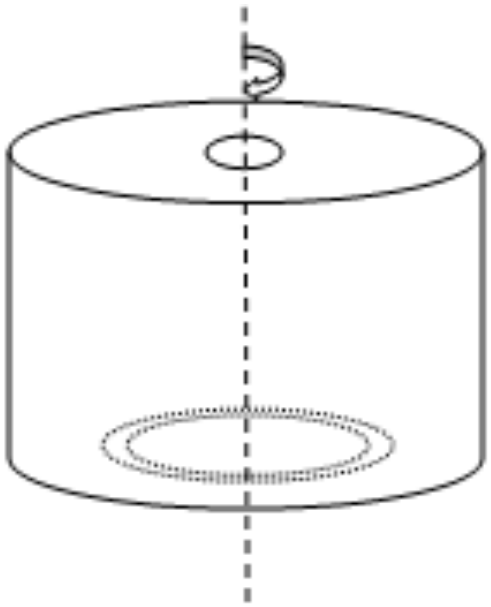

Figure 1: Computational area diagram

The computational area is meshed by approximate cubes with a height of 1 mm, a radius difference of 1 mm and a ring area of less than 1 mm^2.The initial value of gas is according to the pressure of 2 Pa at radius 250.5 mm, the pressure and density of each region can be calculated by using isothermal rigid body model. The number of simulated particles is calculated according to the set mass of the particles, the positions of particles are averagely distributed in the grid, the particle velocities are 0.5 times the sound velocities, and the direction of the particle velocities is spherical average random. The time step is 10^{-5} s, the particle collision model is elastic soft sphere collision, the solid reflection model is diffuse reflection, and the convergence accuracy is the average value of relative deviation of density of 100 step of each grid in the calculation area.

Using the method proposed in this paper, the particle mass is 10^{-14} g, the optimization factor is 2. The particle mass is 6×10^{-15} g and 8×10^{-15} g by the original method. The relationship between convergence accuracy and calculation time is calculated respectively. The calculation results are shown in Figure 2.

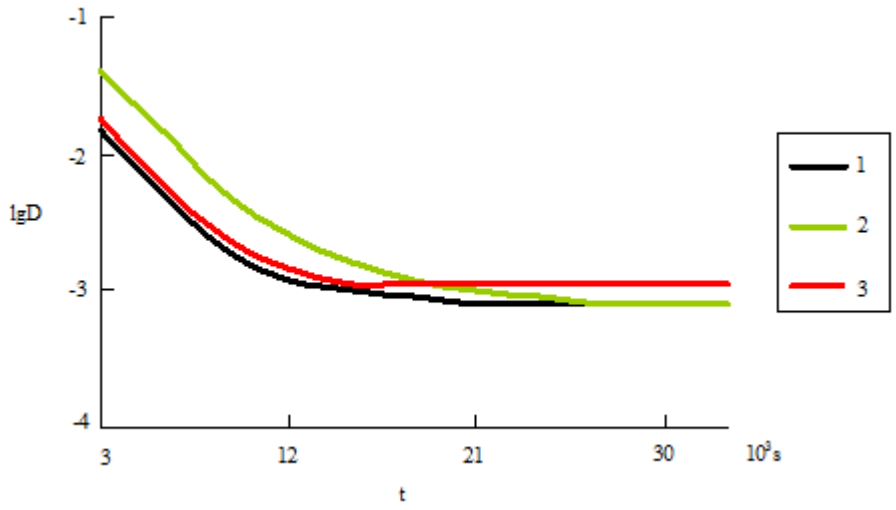

Figure 2: Calculation results of optimization method and original method

Among them, curve 1 is the data of 10^{-14} g particle mass selected by the method proposed in this paper, curve 2 is the data of 6×10^{-15} g particle mass selected by the original method, curve 3 is the data of 8×10^{-15} g particle mass selected by the original method. It can be seen from the graph that the convergence speed of curve 1 and curve 3 is nearly same, but the highest convergence accuracy that curve 1 can achieve is higher; the highest convergence accuracy that curve 1 and curve 2 can achieve is nearly same, but the convergence speed of curve 1 is faster.

5 CONCLUSION

The particle collision selection method proposed in this paper is added to the Monte Carlo method, which not only improves the calculation accuracy, but also increases the computational difficulty. However, the increase of computational difficulty is lower than that of computational accuracy, which shows that this method has a certain role in optimizing Monte Carlo method.

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