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The implementation of subsonic boundary conditions for the direct simulation Monte Carlo method in dsmcFoam

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ABSTRACT

New treatments of the subsonic constant flow rate boundary and porous outlet boundary used for the direct simulation Monte Carlo (DSMC) method are proposed. For the constant flow rate boundary, the total number of molecules inserted is calculated using the number of molecules that flow out of the boundary at previous time step, and the molecules inserted over the boundary are distributed according to the local mean flow velocity and number density. For the porous outlet, it is used to simulate the vacuum pump, and the deleting probability is calculated using the number of molecules that impinge on the boundary, the local pressure and the pump speed. Except for the constant flow inlet and porous outlet, the pressure inlet/outlet and the outgassing wall boundaries are implemented in dsmcFoam and verified. The results of different treatments of the boundary are compared with each other, it shows that the new treatment of the constant flow rate boundary can achieve a more accurate flow rate, and the non-uniform distribution of the inserted molecules can decrease the averaging effect at the inlet; the porous outlet can achieve the desired pressure at the outlet when just giving the pump speed, but there is an averaging effect compared with the pressure outlet due to the uniform deleting probability. The results are also compared with that of DS2V when the boundary conditions are available, it shows that the constant pressure boundary can achieve a more accurate pressure in dsmcFoam than in DS2V, and the results of the outgassing wall are almost the same with both solvers.

1. Introduction

The DSMC method [1] was originally developed for the simulation of external, hypersonic flow fields. The most frequently used boundary conditions for supersonic flows are “free stream” and “vacuum” boundary conditions. Now DSMC method has been extended to subsonic flow problems, for example, flows in micro-channels and micro-tubes [2,3], MEMS devices [4], vacuum systems and material processing devices [5–7]. When applied in subsonic and internal flow applications, new boundary conditions should be developed.

In subsonic applications, the flow rate through a surface, the pressure at a surface, the pump speed of a pump, and the outgassing rate of a wall are always given. These are the well-developed subsonic boundaries in DSMC [4,8–15]. In the available DSMC program DS2V [16], we can specify constant pressure and outgassing wall boundaries, but the constant pressure boundary can only be defined at the boundary of the computation region and only two of them can be defined. In the official version of the open source program dsmcFoam [17], only the “vacuum” and “free stream” boundaries can be specified. There is no subsonic inlet available, and the wall can only be defined as a reflecting wall without outgassing. In the new and unofficial version of the dsmcFOAM [18], a lot of subsonic boundary conditions, including the pressure inlets mentioned in Refs. [8,12], the pressure outlets mentioned in Refs. [8,14], and the mass flow rate inlet mentioned in Refs. [13,15], are implemented. But the outgassing wall is still not available and all the subsonic boundary conditions in the new version of dsmcFOAM need to be verified. Except for the available programs, a lot of studies have also been reported for these subsonic boundaries. In Ref. [13], different treatments of the subsonic boundaries were summarized, including the pressure inlet, the pressure outlet, the constant flow rate inlet and the porous outlet. As to the constant flow rate inlet, it used the macro speed and number density to calculate the total number of molecules inserted, and the net number of molecules inserted was evenly distributed over the surface. As to the porous outlet boundary, it was used to simulate the vacuum pump, the deleting probability was

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calculated using the local macro speed and pump speed, and the desired pressure should be provided when substituting the constant pressure outlet.

In this article, new treatments of the constant flow rate inlet and the porous outlet are proposed. The total number of molecules inserted for the constant flow rate inlet is calculated using the number of molecules flow out of the boundary at previous time step, and the net number of molecules inserted over the boundary is non-uniformly distributed. The porous outlet is used to simulate the vacuum pump, and the pump out probability for the outlet is calculated using the number of molecules impinge upon the boundary at previous time step, the local pressure and the pump speed. Then with the most frequently used constant pressure boundary and outgassing wall, they are implemented in the open source solver dsmcFoam. Last, verification simulations are conducted, the results are compared with analytical solution and the results from DS2V, and different treatments of the boundaries are also compared with each other.

2. The theory

2.1. The DSMC method

The DSMC method is a statistical approach that widely employed in rarefied gas dynamics [1,17,19,20], and it provides a probabilistic physical simulation of a gas flow by simultaneously following the motion of representative model molecules in physical space [21]. The simplest form of the DSMC method can provide a solution of the Boltzmann equation [22]. But unlike the Boltzmann equation which has a lot of restrictions, the DSMC method can deal with physical effects that are beyond the Boltzmann formulation. Physical effects such as chemical reactions, evaporation, ionization and thermal radiation are more readily and realistically incorporated into DSMC method than into a mathematical model [16,21].

In DSMC, the motion of representative model molecules always includes molecular movements and intermolecular collisions, which are uncoupled in a small time step Δt, and a typical non-reaction DSMC simulation is achieved by the repetition of following procedures:

1. Generate a specific number of new molecules at the inlet boundaries where there are inward flux (including the outgassing wall), and specify the position and velocity of each molecule.
2. Calculate the positions of the molecules within Δt based on their velocities. If the trajectory intersects with the boundary, the gas-surface interaction is performed according to the given law, and the movement of the molecule is calculated within the residual time after gas-surface interaction.
3. Compute a representative number of collisions corresponding to Δt and the number of molecules in the cell. The velocities of the molecules after collision are replaced by post-collision values in accordance with the given law of the intermolecular interaction.

2.2. The inlet boundary

As shown in Section 2.1, the first step of a typical DSMC calculation is inserting molecules at the inlet boundaries. To do that, three parameters should be provided. 1) The total number of molecules N_{in} inserted within Δt; 2) the velocity $\mathbf{U}$ of every molecule, including the macro velocity $\mathbf{V}$ and thermal velocity $\mathbf{u}$ ($\mathbf{U} = \mathbf{V} + \mathbf{u}$); 3) the inserting position $\mathbf{P}$ of every molecule.

For an inlet boundary, when the number density n and macro velocity $\mathbf{V}$ are known, the total number N inserted for the inlet within Δt can be expressed as [1]:

$$N = \frac{A\Delta t n}{2\beta\pi^{1/2}}\left[\exp\left(-s^2\cos^2\theta\right) + \pi^{1/2} s\cos\theta\{1 + erf(s\cos\theta)\}\right]$$
$$s = V\beta = V/(2kT/m)^{1/2},\ \cos\theta = -\mathbf{V}\cdot\mathbf{n}/V,\ erf(s) = \frac{2}{\sqrt{\pi}}\int_0^s e^{-t^2}dt, \tag{1}$$

where A is the face area of the inlet, m is the mass of the molecule, k is the Boltzmann constant, T is the temperature of the inlet, and $\mathbf{n}$ is the unit normal vector of the inlet surface which points to the outer of the flow region.

2.2.1. Constant flow rate inlet

The parameter assigned for a constant flow rate inlet is the mass flow rate Q_m [kg/s] or the volume flow rate Q_V [Pa·m^3/s], they can be converted into number flow rate Q_N [/s], and

$$Q_N = \frac{Q_m}{m} = \frac{Q_V}{kT}. \tag{2}$$

Here Q_N is the net number of molecules inserted within unit time, and the total number inserted within Δt is

$$N_{in} = Q_N\Delta t + N_{out}, \tag{3}$$

where N_{out} is the number of molecules that flow out from the inlet within Δt.

The constant mass flow rate inlet has already been reported in the previous studies [13,15]. In Ref. [15], velocity magnitude and mass flux across the inlet surface were assumed to be uniform, and the number density was sampled from the neighboring cells, $n_{in} = \bar{n}_1$. In Ref. [13], only mass flux was assumed to be uniform, the macro velocity was sampled from the neighboring cell, $V_{in,i} = V_{1,celli}$, and the number density was calculated by Eq. (4). In both of the treatments, $N_{in,\,i}$ was calculated by Eq. (1).

$$n_{in,i} = \frac{Q_N}{V_{in,i}\sum A_{in,i}}. \tag{4}$$

Here new treatments of the constant flow rate boundary without the uniform assumption are proposed, and three different treatments of the constant flow rate inlet are achieved in DSMC.

a) Constant flow rate inlet type 1 (cf1)

At each time step, the total number of inserted molecules for the whole inlet surface within Δt can be calculated from Eq. (3). Since N_{out} is not known at the current time step k, it is replaced by the number sampled at previous time step $k-1$, and

$${N_{in}}^k = Q_N\Delta t + {N_{out}}^{k-1}. \tag{5}$$

Then, calculate the total number of molecules inserted for each inlet face $N_{in,\,i}$ by the distribution function. The distribution function is sampled from the neighboring cells of the inlet surface, and the number of molecules inserted for each inlet face i can be expressed as

$$N_{in,i} = \frac{N_{1,celli}}{\sum N_{1,celli}} N_{in}, \tag{6}$$

where $N_{1,\,celli}$ is calculated by Eq. (1) using $n_{1,\,celli}$ and $V_{1,\,celli}$. With the assumption that the molecules are evenly distributed over the single inlet face, the position $\mathbf{P}$ of each molecule can be sampled.

Lastly, assume that the number density at the inlet face is equal to the number density of the neighboring cell $n_{in,i} = n_{1,celli}$ and the macro velocity $\mathbf{V}_{in,\,i}$ of the flow is perpendicular to the inlet face ($\theta = 0^\circ$), then the magnitude of the macro velocity $V_{in,\,i}$ can be obtained by solving Eq. (1). Because DSMC is a stochastic method and the number of molecules in the cell is always not large enough, the calculated values of macro parameters always fluctuate around the mean value. So here weighted average of the instantaneous value