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Short Note

Highly efficient volume generation reservoirs in molecular simulations of gas flows

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1. Introduction

DSMC (Direct Simulation Monte Carlo) method pioneered by Bird is a stochastic molecular simulation method that can be used for simulations of rarefied gas flows [1]. In DSMC method, each DSMC molecule represents a large number of physical gas molecules. DSMC molecules carry position, velocity and, if applicable, internal energy information on them. Molecule movements and collisions are decoupled from each other. Moving molecules either fly freely or interact with boundaries. In the collision step, translational and internal energies are re-shared between molecules according to the collision model chosen.

Molecules interact either with wall or with stream boundaries. In case of wall boundaries, molecules are reflected back according to the reflection model chosen. When molecules cross stream boundaries, they leave the domain without any further interaction. At the same time new molecules are introduced into the flow area.

The number of molecules introduced into the gas flow area and their velocity components depend on the boundary conditions. In the case of Pressure Boundary Conditions (PBC), temperature (T_i), pressure (p_i) and stream velocity components parallel to the boundary (V_i, W_i) are predetermined properties on upstream boundaries. On the downstream boundary only the pressure (p_o) is predetermined. All missing boundary conditions can be calculated with extrapolation from the gas flow area [2]. Particle flux conservation technique by [3] can also be used to calculate the stream velocity components normal (U_i, U_o) to the stream boundaries. Molecule number density (n) at the boundary can be calculated from the perfect gas equation of state.

$$n = \frac{p}{k_B T} \tag{1}$$

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where k_B and T are Boltzmann constant and temperature respectively. The number, position and velocity of entering molecules are modeled via fictitious reservoirs placed on the boundaries. These reservoirs, representing entrance and exit conditions, are either surface or volume generation molecule reservoirs [4]. Molecule generation reservoirs are also used in hybrid molecular-continuum solvers and Brownian systems [5].

Surface and volume generation methods have various advantages and disadvantages in terms of computational efficiency and accuracy. In this study, a novel implementation of the volume method is presented and compared with surface and conventional volume generation reservoir methods.

2. Surface generation reservoir method

This method is usually considered as the standard method [4]. It is called surface generation reservoir method because molecules are launched from a virtual surface located on the stream boundary. For the Maxwell–Boltzmann distribution, the theoretical molecule number flux $\dot{N}$ is calculated in non-dimensional form [1].

$$\frac{\dot{N}\beta}{n} = \frac{1}{2\sqrt{\pi}}\left[S\sqrt{\pi}(1 + erfS) + exp(-S^2)\right] \tag{2}$$

Here β is reverse of the most probable molecular speed $\left(=\sqrt{2RT}\right)$ where R is the specific gas constant; S is the molecular speed ratio $(=\beta U)$ where U is the gas flow velocity normal to the boundary.

Molecule velocity consists of two parts. These are the thermal velocity part and the gas stream velocity. The molecule thermal velocity components parallel to the boundary are calculated using the inverse-cumulative method [1]. Calculation of the normal component, on the other hand, requires the acceptance–rejection method explained in detail in [1]. The application of the acceptance–rejection method greatly increases the computational effort.

Furthermore, in the standard surface generation reservoir method, the velocity range is usually limited between $u_{min}\beta = max(S-3,0)$ and $u_{max}\beta = max(S+3,1)$ [4]. Consequently, molecules with higher and lower velocity values are not generated with this method. Although the probability for these velocity values to exist is almost four orders of magnitude lower than accepted velocity values, this is still a deficiency of the standard surface generation reservoir method.

Lately new formulations have been developed. Instead of employing a box type envelope used in the standard surface generation reservoir method, new types of envelopes are used in surface generation reservoir methods. These new formulations are several times faster than generators in common use and additionally they are exact methods, which produce all possible values of velocities unlike the standard surface generation reservoir method [5].

Another issue with the surface generation method is that the number of molecules generated by the surface method is obtained from Eq. (2), and it is constant in time for steady conditions. However this is not realistic since it resembles a Poisson distribution. Unless particles are supplied to the system at a Poisson distributed rate, surface generated reservoirs cause non-equilibrium behaviors, such as anomalous fluid velocity [6].

3. Volume generation reservoir method

This method is usually called the alternative method [4]. The volume generation reservoir method is implicit in hybrid molecular-continuum methods [4,7] and in non-equilibrium reservoirs in which particles are generated using the Chapman–Enskog distribution [9]. In this method, fixed volume molecule reservoirs are formed on stream boundaries and filled with molecules. The number of molecules in the reservoirs is calculated from boundary conditions

$$N = \frac{p}{k_B T} V_R \tag{3}$$

Each molecule is assigned velocity components calculated from a velocity distribution function. Molecule positions in the reservoir are determined randomly. During the simulation each molecule changes its position according to its velocity ($\mathbf{c}$) and simulation time step (Δt).

$$\mathbf{r}_2 = \mathbf{r}_1 + \mathbf{c}\Delta t \tag{4}$$

These molecules are tested as to whether new positions are inside the flow area or not. The ones crossing the boundary towards the flow area are added to the molecule data structure as new molecules. The others are just removed. This procedure is repeated at each time step throughout the simulation.

Molecule production rates generated by the volume generation reservoir method at each time step (Δt) are not constant unlike those generated by surface generation reservoir method. Although the particle rate distribution is expected to be a Poisson distribution, it is reported that there are noticeable deviations in the distribution [6]. Yet non-equilibrium behavior of volume generation reservoir method is an order of magnitude better than surface generation reservoir method.

The volume generation reservoir method presents two distinct disadvantages compared to the surface generation reservoir method. Firstly, in terms of computational efficiency, the volume generation reservoir method is less efficient than the surface generation method [5]. Secondly, it is reported that the mean number of molecules generated by the volume method is slightly less than the theoretical number due to the depleted population of high-speed particles. Two new implementa-

tions of the volume generation reservoir method are proposed to obtain the correct number flux [4]. However the new implementations do not involve correction of the depleted population of high-speed particles.

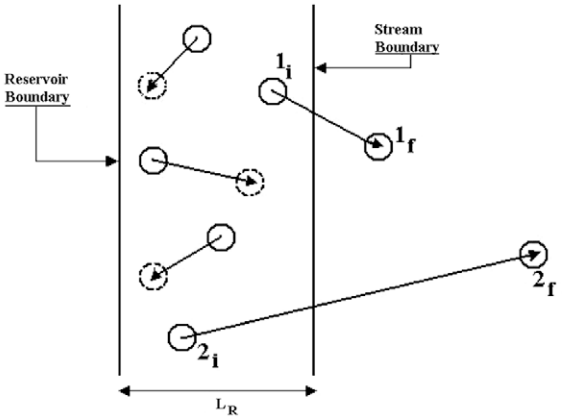

Fig. 1. Molecules number 1 and 2 starting from initial positions (i) cross the stream boundary toward final positions (f) in the flow zone.

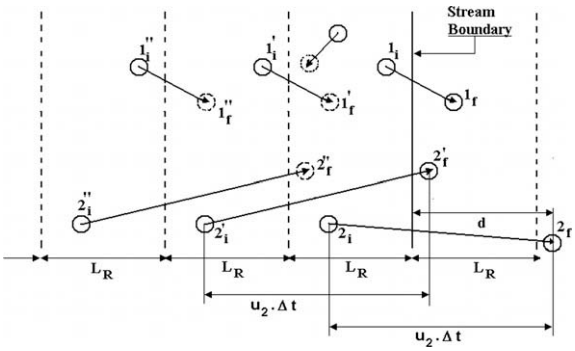

Fig. 2. If periodic reservoirs are implemented, some additional fast velocity molecules (such as molecule number 2') can cross the stream boundary into the flow zone.

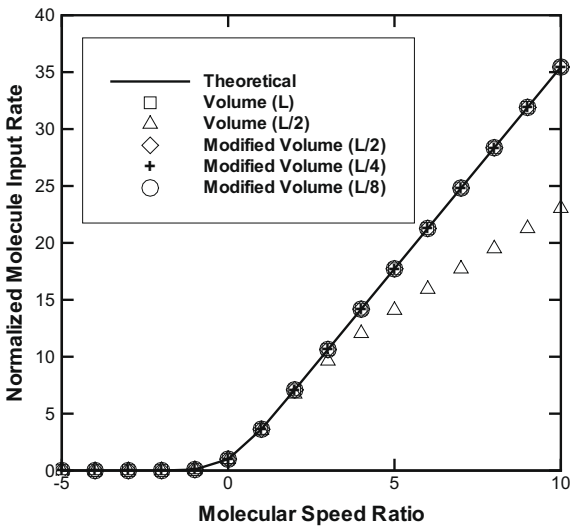

Fig. 3. Comparison of molecule input rates.

4. Modified volume generation reservoir method

In this study, the volume generation reservoir method has been modified slightly to include the correct number of high-speed particles within a computationally more efficient algorithm. As it can be seen from Fig. 1, the length of the reservoir (L_R) is an important parameter affecting the number and velocity distribution of molecules entering the domain.

If this reservoir's length is extended further, there is a possibility that additional high-speed molecules cross the boundary into the flow area, whereas low-speed molecules located away from the boundary will remain in the reservoir, changing the number and velocity distribution of the inflow. To reach the theoretically correct molecule number flux given by Eq. (2), the reservoir length should be extended to infinity, which is computationally impossible. It is suggested that a reservoir length of $L = (U + 3\beta^{-1})\Delta t$ should be used to include an acceptable number of high-speed particles with a reasonable computational efficiency [4].

Assuming translational periodicity in the direction normal to the stream boundary, multiple copies of the first reservoir with a length of L_R can be used to extend the reservoir length arbitrarily, as shown in Fig. 2. If the conventional volume generation procedure is applied to the first reservoir, there will be molecules with relatively low velocities (e.i. molecule 1 in

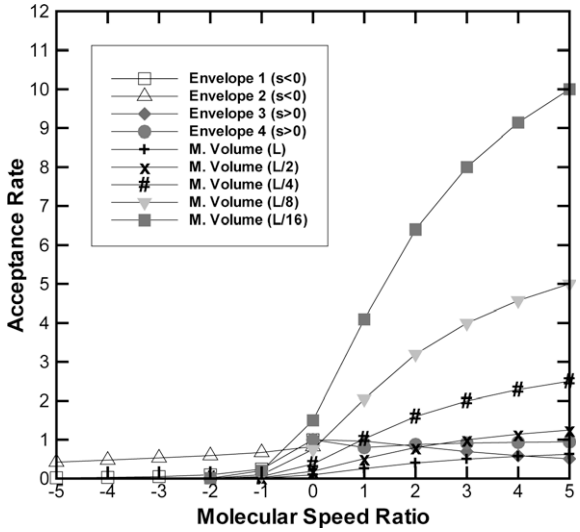

Fig. 4. Acceptance rates for modified volume generation reservoir method with different reservoir lengths and surface method with Envelopes 1–4.

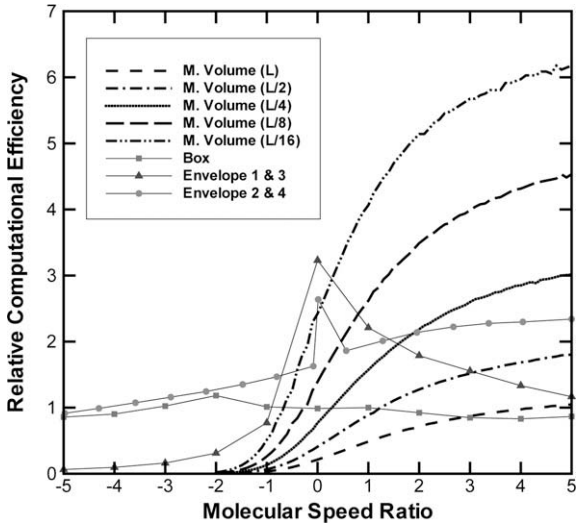

Fig. 5. Computational efficiencies for modified volume generation reservoir method with different reservoir lengths and surface method with Envelopes 1–4 and box ($\alpha_1 = 1$).

Fig. 2) entering the domain through the stream boundary. There will also be molecules with relatively high velocities (e.i. molecule 2 in Fig. 2) entering the domain and traveling a longer distance (d) from the stream boundary within the time step. If the volume generation procedure would have been applied to the second reservoir, the high-speed molecule ($2'$) would also enter the domain reaching its final position $2'_f$. Utilizing periodicity of the reservoir, the total number of copies of an accepted molecule entering the domain can be determined from Eq. (5) without processing all the periodic copies of the first reservoir. Here *int* is a special function that returns the greatest integer less than or equal to its argument.

$$N_1 = int\left(\frac{d}{L_R}\right) + 1 \tag{5}$$

This approach practically extends the reservoir length to infinity in a very efficient way, eliminating the limitation on the length of the reservoir required for the conventional method. It shall be noted that, although for each additional copy of a high-speed molecule the velocity component normal to boundary is the same, velocity components parallel to the boundary should be sampled separately. Otherwise, all copies of the high-speed molecules will be identical and this will adversely effect the collision rates. Simulations are performed to demonstrate the suitability of the new approach. Results obtained, and their comparisons with surface and volume generation methods are presented in the following section.

5. Results

The molecule input rates, obtained by using the surface reservoir method, the conventional volume reservoir method with different reservoir lengths and the modified volume reservoir method with different reservoir lengths are compared

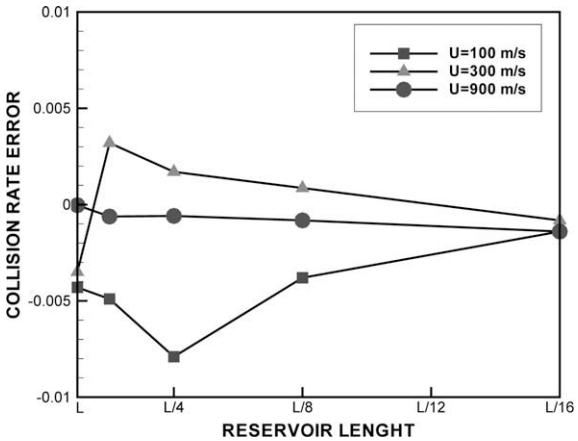

Fig. 6. Collision error rates for different reservoir lengths and gas flow velocities.

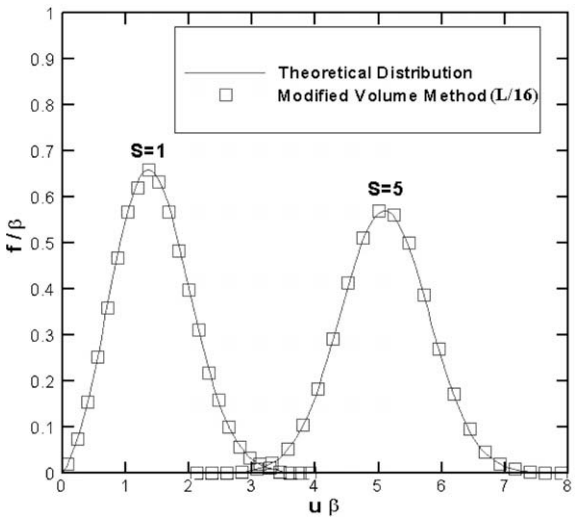

Fig. 7. Theoretical velocity distribution and distribution generated with modified volume method for $S = 1$ and $S = 5$.

in Fig. 3. As seen, the surface reservoir method (theoretical) and the volume reservoir methods with the a suggested reservoir length of $L = (U + 3\beta^{-1})\Delta t$ yield the same input rates. The input rates shown on the vertical axis are normalized with the molecule input rates at $S = 0$. If the reservoir length is reduced to half, the input rates calculated with the conventional method deviate considerably from the theoretical one, especially for $S > 2$. However, it is seen that the molecule input rates obtained with the modified volume reservoir method agree well with the theoretical values for all of the reduced reservoir lengths. The results represent an average of 10,000 samples per case.

As an indicator of computational efficiency, acceptance rates, which are the ratio of the number of accepted molecules to the number of generated molecules, are compared in Fig. 4 for $-5 < S < 5$. The results obtained with the modified volume reservoir methods using different reservoir lengths are compared with the highly efficient envelopes proposed by [5] to be used within the surface generation method. It can be seen that the acceptance rate of the proposed method increases with a reduced reservoir length. Furthermore, the acceptance rates of the proposed method with short reservoirs are considerably higher than for the surface method on inflow boundaries.

The computational efficiencies achieved by various methods are presented in Fig. 5. The relative computational efficiency [4], defined as the CPU time per accepted molecule is normalized by the CPU time requirements of the surface method with box type envelope [1] at $S = 0$. Relative computational efficiencies for the modified volume method and surface method with envelopes 1, 3, box ($\alpha_1 = 1$) are obtained by implementing the algorithms. Uniformly distributed random numbers are produced by the Fortran version of the Mersenne Twister generator [8]. The Box–Muller method is used for Gaussian distributed random numbers. The codes are written using Fortran 90 and compiled with /O1 optimization using the Intel FORTRAN 8.1 compiler and run on an Intel Centrino 1.4 GHz. processor. The efficiency figures for envelopes 2, 4 are read directly from [5], as the implementation of the algorithm has yielded slightly lower efficiencies. As seen from Fig. 5, the modified volume method gives higher computational efficiencies, as the reservoir length gets shorter.

In order to observe possible adverse effects of the shorter reservoir lengths on the collision rates, 1-dimensional bulk flow with the same reservoir values on each side are simulated and collision rate errors, as calculated in [1], are recorded. Bulk flow is sampled in 10,000 time steps with an average of 100 DSMC molecules in each cell for three different gas flow velocities. As seen in Fig. 6, collision rate errors are in an acceptable range and decrease with increasing gas velocity.

Finally, the theoretical distribution and the distributions generated by the modified volume method with a reservoir length of $L_R = L/16$ are compared in Fig. 7. 5×10^5 and 7×10^5 samples are used for $S = 1$ and $S = 5$ respectively. Distributions generated by the modified volume method are in excellent agreement with the theoretical distribution.

6. Conclusions

Generally, two different methods are employed to generate molecules on stream boundaries. These are the surface generation reservoir (standard) method, which uses acceptance–rejection algorithms with different envelopes and the volume generation reservoir (alternative) method. In this study a modification to the conventional volume generation reservoir method is proposed. The proposed method extends the reservoir length to infinity using periodic reservoirs. As a result, the problem of depleted population of high-speed particles is solved. It is also shown that the proposed method used with short reservoirs has higher acceptance rates than the surface generation reservoirs for inflow boundaries. The computer implementation further reveals that the relative computational efficiency of the proposed method is higher than the surface generation reservoir methods for $S > 0.3$ when used with a reservoir length of $L_R = L/16$.

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