IMPROVEMENT OF THE METHOD OF STATISTICAL TRIALS (MONTE CARLO) FOR CALCULATING FLOWS OF RAREFIED GASES

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Abstract

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IMPROVEMENT OF THE METHOD OF STATISTICAL TRIALS (MONTE CARLO) FOR CALCULATING FLOWS OF RAREFIED GASES

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In paper ([1]) a general description was given of the application of the method of statistical trials (Monte Carlo) to the calculation of stationary flows of rarefied gases. The random walk of a single molecule was simulated. To calculate collisions, the distribution function of molecules was stored; in general, it depends on 6 variables, which imposes severe requirements on the amount of computer random-access memory. Therefore the application of the Monte Carlo method was limited to the simplest one-dimensional problems (heat transfer between parallel planes and the structure of a shock wave), and also to nearly free-molecular flows.

It is shown below that one can dispense with storing the complete distribution function if one uses a quasi-Maxwellian model of molecules, for which the total effective collision cross section of two molecules with velocities $\mathbf{v}$ and $\mathbf{v}_1$ is equal to

$$\sigma = \sigma(g) = \sigma_1/g, \tag{1}$$

where $\sigma_1 = \text{const}$ and $g = |\mathbf{v}_1 - \mathbf{v}|$ is the magnitude of the relative velocity of the molecules before collision.

Consider a stationary flow of a monatomic rarefied gas. We shall follow one molecule, which we shall call the *test* molecule. The remaining molecules we shall call *field* molecules. Let $f(\mathbf{r}, \mathbf{v})$ be the molecular distribution function, and $n = n(\mathbf{r}) = \int f(\mathbf{r}, \mathbf{v})\, d\mathbf{v}$ the number density of the gas.

The collision frequency of a test molecule having velocity $\mathbf{v}$ at a given instant is ([2])

$$\mathcal{P} = \mathcal{P}(\mathbf{v}) = \int g\sigma(g) f(\mathbf{v}_1)\, d\mathbf{v}_1 = \sigma_1 n, \tag{2}$$

i.e., for the quasi-Maxwellian model of molecules it depends only on the density.

Fig. 1

Figure 1: Fig. 1

Fig. 2

Figure 2: Fig. 2

The normalized collision frequency of a test molecule $\mathbf{v}$ with field molecules whose velocities belong to a small element $\Delta\mathbf{v}_1$ of velocity space around $\mathbf{v}_1$ is

$$p(\mathbf{v}, \mathbf{v}_1)\Delta\mathbf{v}_1 = g\sigma(g)f(\mathbf{v}_1)\Delta\mathbf{v}_1/\mathcal{P}(\mathbf{v}), \tag{3}$$

which for model (1) gives

$$p(\mathbf{v}, \mathbf{v}_1) = p(\mathbf{v}_1) = f(\mathbf{v}_1)/n, \tag{3a}$$

i.e., to calculate the free-flight time of the molecule $\mathbf{v}$ it is necessary to know only the gas density, while the velocity distribution of the "collision partners," instead of the complicated expression (3), turns out to be proportional to the distribution function.

The test molecule enters the given geometrical cell (for simplicity of analysis, a spherical one), having a velocity close to $\mathbf{v}$, with a frequency proportional to $vf(\mathbf{v})$. Storing this velocity with probability propor-

proportional to $1/v$, we shall store it with a frequency proportional to $f(\mathbf{v}) \sim p(\mathbf{v})$, i.e., instead of the complete distribution function $f(\mathbf{v}_1)$ or $p(\mathbf{v}_1)$, for the calculation of a possible collision in a given geometrical cell it is sufficient, at each exit from it of a test molecule having velocity $\mathbf{v}$, to store this velocity with probability $q \sim 1/v$, $\mathbf{v}_1^{(k+1)} = \mathbf{v}$, forgetting

Fig. 1

the preceding value $\mathbf{v}_1^{(k)}$, and with probability $1-q$ to leave $\mathbf{v}_1^{(k+1)} = \mathbf{v}_1^{(k)}$. The singularity at the point $v = 0$ is easily eliminated by several almost obvious methods.

The amount of machine memory required is thereby reduced by three orders of magnitude. This method permits several modifications, which are easily adapted to the particular features of the problem. The following procedure is more effective: when a test molecule with velocity $\mathbf{v}$ leaves a cell, we store in this cell $\mathbf{v}_1^{(k+1)} = \mathbf{v}$ with probability $q = \Delta t/(\Delta t + \Delta t_1)$, where Δt and Δt_1 are the residence times in this cell of molecules with $\mathbf{v}$ and $\mathbf{v}_1^{(k)}$, respectively, and with probability $1-q$ we leave $\mathbf{v}_1^{(k+1)} = \mathbf{v}_1^{(k)}$. Intermediate methods are possible, in which in each geometrical cell several velocities of field molecules are stored.

Fig. 2

The method described above was illustrated on the simplest problem of heat transfer between parallel planes. For comparison, the parameters of the problem were taken the same as in work ([1]): the ratio of the plate temperatures $T_1 : T_2 = 4 : 1$, the effective Knudsen number

$$\mathrm{Kn} = 3(P_{xx}/2m)^{1/2}/\sigma_1 d\bar{n}^{3/2},$$

where d is the distance between the planes, $\bar{n}$ is the mean number density of the gas, and m is the molecular mass.

In work (1) the phase space was divided into 2880 cells. Since two iterations must be stored, the amount of computer memory for numerical material was 5760 words. In the present work the number of geometric cells is 10, as in (1). In each cell, 24 velocities of field molecules $v_m^{(k)}$, $m = 1, 2, \ldots, 24$, were stored. In this way the amount of memory for numerical material was reduced by a factor of 8. The free-molecular flow was taken as the initial approximation. Figures 1 and 2 show the results of calculations for the first iteration. Figure 1 shows the change in heat flux as a function of the number N of sampled collisions of a test molecule with field molecules. The cross denotes the result of work (1). Figure 2 gives the gas-density profile between the plates for $N \approx 4 \cdot 10^5$. The quantities q and ρ are referred to their free-molecular values. The dashed line marks the data of work (1) for $N \approx 5 \cdot 10^4$. In the subsequent calculations the number of molecules in a geometric cell was reduced to 7.

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Note: Figure translations are in progress. See original paper for figures.