Application of Modified DSMC Algorithm to Inviscid Flow Calculation

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Abstract. Newly modified DSMC algorithm for inviscid flow calculations is introduced to save the computational costs. By using this algorithm, two examples are tested. In both of the example tests, the calculation time is shortened approximately twice. The results obtained with the modified DSMC algorithm correspond well to the results obtained with the finite-difference method or analytical solution.

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INTRODUCTION

The use of Direct Simulation Monte Carlo method (DSMC) in rarefied gas dynamics now is widely accepted approach [1]. The reason is that by continuum equations it is impossible to describe rarefied regimes [2]. But, it will be interesting that for continuum flows calculations DSMC method can be effectively used.

The first try was done by Pullin in 1980. In his paper [3], the method of modeling of compressible inviscid gas flow on the basis of local Maxwellian distribution function is described. He also mentioned the advantage and disadvantage of such a method. Advantage of this method is the possibility to simulate various physical processes. On the other hand, disadvantage is high computational cost comparing with the finite-difference methods. There are two solutions for these disadvantages; the first one is the parallelization and second one is the modification of algorithm. Here we suggest variant of solution for this problem based on modification of the algorithm.

In paper [4] possibilities to calculate rarefied gas flows in a wide range of rarefaction on the basis of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{\xi}\Delta f = I(f) \tag{1}$$

are discussed (here f is the probability distribution function, $\vec{\xi}$ is the particle velocity, $I(f)$ is the collision integral) and the examples of modeling of rarefied gas flows up to continuum regime on the basis of postulated probability distribution function are shown.

For the DSMC algorithm, the «transition – relaxation» scheme is used. During the time step Δt, this scheme splits the common algorithm into two independent physical processes:

1. Collisionless transition of modeling particles between spatial cells (2)
2. Spatially homogeneous relaxation in each cell (3)

Therefore, the Boltzmann equation could be divided into as below:

$$\frac{\partial f}{\partial t} + \vec{\xi}\Delta f = 0\,, \tag{2}$$

$$\frac{\partial f}{\partial t} = I(f)\,. \tag{3}$$

For the modeling of inviscid flow, Maxwellian distribution function f_0 (4) can be used:

$$f_0 = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{m(\vec{\xi}-\vec{U})^2}{2k_B T}\right). \tag{4}$$

Modeling algorithm consists of the following stages:

1. Division of the calculation domain into cells and definition of initial density (ρ), velocity ($\vec{U}$), temperature (T). The number of particles in each cell is proportional to the gas density.
2. Coordinates of particles ($\vec{x}_i$) are calculated according to the uniform spatial distribution in cell volume. The particle velocities ($\vec{\xi}_i$) are calculated according to the Maxwell probability distribution function f_0 (4).
3. All particles are moved according to their velocities during time step Δt. New positions ($\vec{x}_i'$) are calculated as

$$\vec{x}_i' = \vec{x}_i + \vec{\xi}_i \Delta t\,. \tag{5}$$

   Boundary conditions are taken into account at this stage.
4. New macroscopic parameters are calculated in each cell.
5. Steps 2 – 4 are repeated till the end of the calculation time.

Using this algorithm, we need to calculate velocities of particles according to Maxwellian distribution function at each time step. Therefore it consumes lots of computation time.

MODIFICATION OF ALGORITHM

The idea of modification of algorithm is to change the way of computation of random velocities. Particularly, before calculation we can compute a fixed set of random velocities according to the Maxwellian distribution function with unit temperature and zero average velocity. This number of modeling particles is constant and corresponds to the unit density. Further we can use this set of random velocities in cells with appropriate weighting factors that are proportional to the real density.

With this idea, newly modified DSMC algorithm for inviscid flow calculation is as follows:

1. Division of the calculation domain into cells and definition of initial density, velocity, temperature.
2. The number of modeling particles in each cell is constant; weighting factor is assigned to each particle proportional to the local gas density. Coordinates of particles are calculated according to the uniform spatial distribution in cell volume. The particle velocities are chosen from the prescribed set, simple transformations are made to take into account the local temperature and the average velocity.
3. All particles are moved according to their velocities during time step, new positions are calculated. Boundary conditions are taken into account at this stage.
4. New macroscopic parameters are calculated in each cell with weighting factors taking into account.
5. Steps 2 – 4 are repeated till the end of the calculation time.

This modification can save the calculation time substantially. Because the set of random velocities with unit temperature and zero average generated once, then in each cell this ensemble is used with appropriate weighting factors. Note that the procedure of random distribution of particles coordinates over cell volume allows to avoid possible and undesirable correlations. The method of weighting factors is well known [1]; it ensures that mass, momentum and energy conservation laws in each cell are satisfied.

ONE-DIMENSIONAL NON-STATIONARY PROBLEM

Firstly, this modified DSMC algorithm is applied to one-dimensional non-stationary problem, called decay of discontinuity problem [5]. Initial discontinuity in gas parameters at $t = 0$ is evolving at $t > 0$ with creation of centered waves and discontinuities.

Two gas states under the conditions

$$\frac{P_1}{P_2} = 4; \frac{\rho_1}{\rho_2} = 4; U_1 = U_2 = 0; \gamma = 1.4$$

are separated by some impenetrable interface. After removing of the interface, the evolution begins with self-consistent gasdynamic parameters distributions formation depending on the initial conditions.

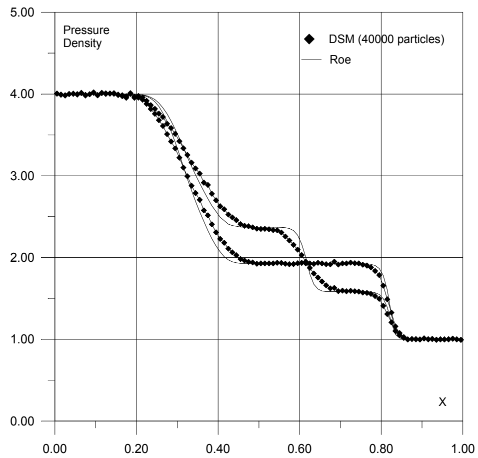

FIGURE 1. Distributions of density and pressure (100 cells)

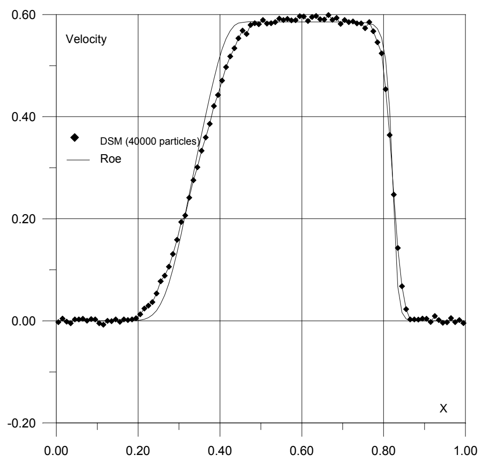

FIGURE 2. Distributions of velocity (100 cells)

Figure 1 shows distribution of density and pressure. For the DSMC simulation, 40,000 particles are used and the domain is uniformly divided into 100 cells. The pressure and density in the left half of the cells are taken to be 4 times higher than those in the right half. The resulting flow will be from left to right. To show the validity of the DSMC result, it is compared with one obtained with the Roe finite - difference method [6]. Figure 2 shows the distribution of velocity, formed after decay of the initial discontinuity. Shock and rarefaction wave are visible in the velocity distribution, while the contact discontinuity is moving with gas and consequently doesn't create gaps in the pressure and velocity distributions. Here the DSMC result is also compared with the finite - difference solution.

TWO-DIMENSIONAL STATIONARY PROBLEM

The second example is two-dimensional stationary problem of supersonic flow around a flat plate.

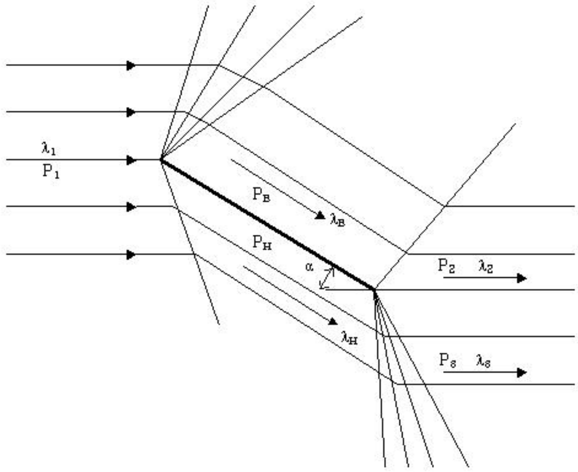

FIGURE 3. Drawing of supersonic flow around flat plate

In Figure 3, the flow comes from left to right, the flow Mach number M > 1 and the plate is placed at the angle of attack α. At the upper front and lower rear of flat plate, there will be a sudden decrease of pressure and increase of flow velocity due to passing through the rarefaction wave. Due to passing through the shock wave at the lower front and upper rear of flat plate, the velocity increases and the pressure decrease along streamlines.

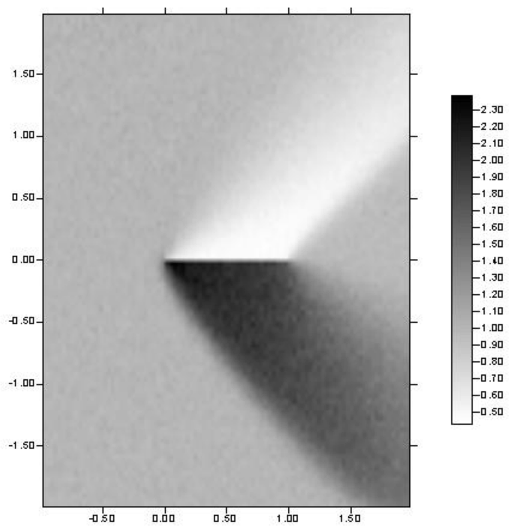

FIGURE 4. Field of density, α = 15º, M = 1.5

Figure 4 shows the density field obtained with the modified DAMC algorithm in the case of two-dimensional inviscid flow around a flat plate. For simulation, computation domain was divided into 90×90 cells and 500,000 particles were used.

If real foil is thin enough and angle of attack is not large, one can use analytical expressions for aerodynamic coefficients C_x and C_y [5]:

$$C_x = \frac{4\alpha}{\sqrt{M^2 - 1}}, C_y = \frac{4\alpha^2}{\sqrt{M^2 - 1}} . \tag{6}$$

Figure 5 shows distributions of $C_x(\alpha)$ and $C_y(\alpha)$ for a flat plate with the fixed Mach number M = 1.5. Figure 6 also indicates dependencies C_x(M) and C_y(M) for a flat plate with the fixed angle of attack α =15º.

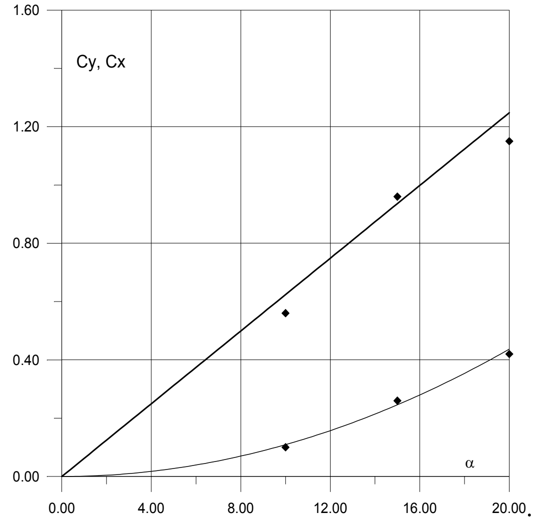

FIGURE 5. $C_x(\alpha)$ and $C_y(\alpha)$ at M = 1.5

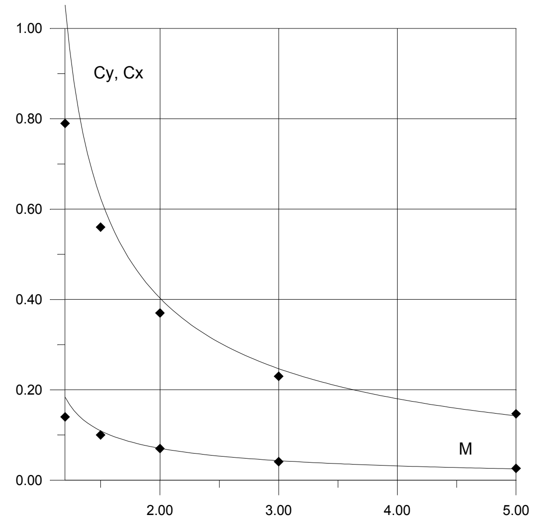

FIGURE 6. C_x(M) and C_y(M) at α =15º

CONCLUSIONS

Modified DSMC algorithm for inviscid flows is developed, allowing to obtain reliable results for correct problems of inviscid gas dynamics with increased efficiency.

The DSMC numerical results for non-stationary one-dimensional problem are in good agreement with the theory and results obtained with the finite-difference method. In the case of two-dimensional problem, better agreement with theory is achieved when the angle of attack is not too small and too large (5º < α < 20º) and the Mach number is greater than 1.5, in these cases the DSMC results are in good agreements with the linear theory. If we need a rough estimate for aerodynamical characteristics we can use small number of modeling particles in each cell and quickly obtain desired result.

In the both cases, the time of calculation is essentially reduced (by a factor of approximately two) comparing with the traditional algorithm.

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