

Rarefied Gas Flow Analysis by Direct Simulation Monte Carlo Method in Body-Fitted Coordinate System

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A new method is proposed for the rarefied gas flow analysis by the direct simulation Monte Carlo (DSMC) method in a multidimensional flow. In this method, a body-fitted coordinate system is used and therefore the DSMC method can be applicable to a flow-field analysis around the body of arbitrary configuration. Through an application to the rarefied supersonic flow around the circular cylinder, the present method was found to be reliable and time-saving in computation time. © 1989 Academic Press, Inc.

I. INTRODUCTION

Recently the aerodynamics about a vehicle in a rarefied flow regime attracted much attention in relation to the aero-assisted orbital transfer vehicle (AOTV) and/or the reentry vehicle [1]. In a simulation of a rarefied gas flow, the direct simulation Monte Carlo (DSMC) is a powerful numerical simulation method [2]. An application of DSMC to vehicle aerodynamics, however, has been restricted to a vehicle of simple geometry since an implementation of a boundary condition at a vehicle surface of complex geometry into the simulation program is a rather complex problem. Furthermore, the simulation program thus obtained must be modified corresponding to the modification of the vehicle configuration.

In a numerical simulation of a continuum flow in which the Navier-Stokes equation or the Euler equation is solved, the body-fitted coordinate system is employed so that the numerical simulation program can be applicable to a flow-field analysis around a body of arbitrary configuration [3]. In this method, the flow field is calculated at a rectangular space which is transformed from the physical space around a body, i.e., at the body-fitted coordinate system. Hence the flow field around the body of arbitrary configuration can be easily calculated when the body-fitted coordinate system is determined. In the present paper, we propose the DSMC method using the body-fitted coordinate system. This method is shown to overcome the above mentioned problem. That is, the present method makes it possible to analyse the rarefied gas flow around the vehicle of arbitrary shape by generating a body-fitted coordinate. Furthermore, it is shown that the computation time is much reduced in comparison with the standard method.

2. DSMC METHOD WITH BODY-FITTED COORDINATE

In the present paper, we consider 2-dimensional flow for simplicity although the extension to 3-dimensional flow is straightforward. In 2-dimensional flow, the body-fitted coordinate system (ξ, η) is introduced using

$$\begin{aligned}x &= x(\xi, \eta), \\y &= y(\xi, \eta),\end{aligned}\quad (1)$$

which transforms the rectangular region in the (ξ, η) space to the physical space around the body in the (x, y) coordinate. In this transformation, a line of $\eta = \text{constant}$, for example, is chosen to coincide with the body surface. Among a variety of transformations, the *O*-type grid is shown schematically in Fig. 1 in which the body surface coincides with a line of $\eta = 0$.

In the DSMC method, the physical space in which the simulation is conducted must be divided into cells. Since the direct discretization in the physical space is a complex problem, we consider this in the (ξ, η) space at first. The discretization of the (ξ, η) space can be conducted by discretizing ξ and η coordinates at equal intervals of $\Delta\xi$ and $\Delta\eta$, respectively. Hence the cells in the (ξ, η) space are rectangular with a uniform size of $\Delta\xi \times \Delta\eta$. Corresponding to this discretization, the discretization in the (x, y) space is done automatically. The cells in the (x, y) space cannot be rectangular in general.

In general, it is difficult to obtain the body-fitted coordinate system analytically for an arbitrary body configuration. Hence we assume that the transformation defined by Eq. (1) is obtained numerically; i.e., it is only defined at the discrete points on the (ξ, η) space. The body-fitted coordinate system defined numerically can be easily obtained, for example, by solving the Poisson equation with appropriate boundary conditions [3].

In the DSMC method, the particles move around in the region where the simulation of the flow field is conducted. Two types of the coordinate system are possible for describing the location of the particles; i.e., the (x, y) and (ξ, η) coordinate system. The standard method employs the (x, y) coordinate system. We consider

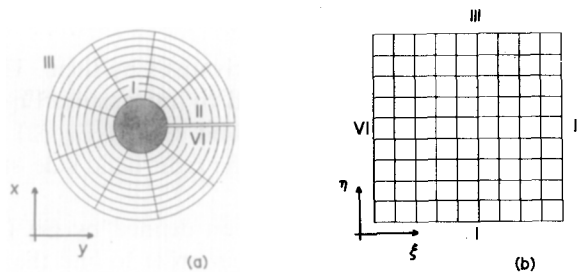


FIG. 1. Schematic figure for the transformation between the body-fitted coordinate system around a circular body and the rectangular coordinate system.

merits and demerits between both methods paying attention to the algorithm of the DSMC method.

The DSMC method comprises two different processes: (1) the collisions between the particles due to the intermolecular forces are counted (step I) and (2) the particles move freely (i.e., not being affected by intermolecular forces) (step II). In the step I of the DSMC method, the collisions are counted among the particles which reside in the same cell. To do this, the particle in each cell must be identified. This identification can be easily conducted in the (ξ, η) space, while it is a complicated problem in the (x, y) space [2]. That is, in the (ξ, η) space, the cell in which the particle resides can be easily identified by only dividing the ξ and η coordinates of the particles by the cell size $\Delta\xi$ and $\Delta\eta$ in the (ξ, η) space, respectively. In the (x, y) space, however, all the cells must be checked whether the particle resides or not until the cell in question is identified. In general, this process is more time-consuming in computation although several methods were proposed to solve this defect [2]. Hence, the (ξ, η) space is preferable for a coordinate system describing the particle location. Once the cells are identified for all the particles, the collision process can be counted in a manner similar to the standard method.

In step II of the DSMC, the particle moves under no influence of the intermolecular force according to the following equations;

$$\begin{aligned}\frac{dx}{dt} &= v_x, \\ \frac{dy}{dt} &= v_y,\end{aligned}\tag{2}$$

if there is no external force. Here v_x and v_y are the particle velocities in the x and y components. In the (ξ, η) space, these equations are rewritten as

$$\begin{aligned}\frac{d\xi}{dt} &= (v_x y_\eta - v_y x_\eta)/\Delta, \\ \frac{d\eta}{dt} &= -(v_x y_\xi - v_y x_\xi)/\Delta,\end{aligned}\tag{3}$$

$$\Delta = x_\xi y_\eta - x_\eta y_\xi,$$

where the suffices of ξ and η represent the derivatives by them. The motion of the particles in the (ξ, η) space can be determined by integrating Eq. (3). Although it is easy to integrate Eq. (2) (since the right-hand side of Eq. (2) is constant), the integration of Eq. (3) is rather complex since the right-hand side of Eq. (3) depends on the local (ξ, η) coordinate.

We must note here that if the transformation defined by Eq. (1) is determined analytically, it is of no use to integrate Eq. (3) in order to find the (ξ, η) coordinate of the particle. Instead, we can get the (ξ, η) coordinate by using the analytical transformation Eq. (1) after the movement by Eq. (2). On the other hand, when the

transformation is defined only numerically, it is not a good method to determine the (ξ, η) coordinate through the transformation (1). In this case, the (ξ, η) coordinate of the particle must be interpolated from the transformations of the nearest grid points. Hence the cell (in the (x, y) coordinate) in which the particle resides must be identified in order to employ the transformation (1). This process is more time-consuming in computation. Therefore, we can conclude that Eq. (3) must be integrated in order to obtain the (ξ, η) coordinate of the particle.

The boundary condition must be specified for the particles which move into the boundary of the computation (the body surface and/or the boundary of the area in which the simulation is conducted). Hence, for the particle which comes near the body surface or the boundary of the calculation region, it is important to know whether the particle hits on the body surface or goes out from the calculation region during the freely moving process (i.e., step II of the DSMC method). Apparently it is easy to know whether the particles enter into the boundary if the geometry of the boundary is simple. Especially, if the boundary is represented by a line in which some coordinate is constant, this process can be more easily conducted. In this view point, the (ξ, η) coordinate system is preferable in comparison with the (x, y) coordinate system, since four boundaries of a rectangular region in the (ξ, η) coordinate system coincide with all the boundaries of the region in the (x, y) coordinate system. On the other hand, the boundaries of the region in the (x, y) coordinate system are curved lines in general. Therefore it is a complex problem to check the particles which enter into the boundary in the (x, y) space. Besides the boundary condition for the particles which hit on the body surface and/or go out from the calculation region, the boundary condition for the particles entering the calculation region is important. As for the particles of this category, the way to give the boundary condition is similar to the one in the standard method. That is, the particles are selected in accordance with the boundary condition and are moved into the calculation region by an appropriate time step.

In the standard DSMC method, the movement of the particles is conducted according to Eq. (2) (i.e., in the (x, y) space). The integration of Eq. (2) is straightforward and simple. However, as noted above, the calculation step I is more time consuming. Furthermore, the way to give the boundary condition (i.e., at the surface of the body) is complex. In contrast to this, when the particle movement in the (ξ, η) space is employed, the calculation in step I is much easier and the way to give the boundary condition is rather simple, while the calculation for the particle movement might be rather complicated. Considering these merits, we propose the method using the (ξ, η) coordinate system to represent the particle location.

3. PARTICLE PUSHING TECHNIQUE

The collisions in step I of the DSMC method are counted during the time interval of Δt_c which is selected as $\alpha \tau_c$ in general. Here τ_c is the collision time and α is a constant which is smaller than 1 but not so small. In step II of the DSMC

method. Eq. (3) must be integrated during the time interval Δt_c , i.e., from a given time t^n to the next time $t^n + \Delta t_c$. This integration must be done numerically, since the right-hand side of Eq. (3) depends on the (ξ, η) coordinate and is defined only numerically. The time step Δt_c is not sufficiently small in general to maintain good accuracy in the numerical integration. Hence we employ a smaller time step Δt_i for integration of Eq. (3). The time step Δt_i is chosen to be sufficiently small in order to maintain good accuracy. While a variety of numerical integration methods are applicable, we employ here a simple difference form

$$\begin{aligned} \frac{\xi^{k+1} - \xi^k}{\Delta t_i} &= (v_x y_\eta - v_y x_\eta) / \Delta |^k, \\ \frac{\eta^{k+1} - \eta^k}{\Delta t_i} &= -(v_x y_\xi - v_y x_\xi) / \Delta |^k, \end{aligned} \quad (4)$$

where the superscript k represents the time step at the numerical integration. When Δt_i is chosen to be $\Delta t_c / K$ (K , integer), the coordinates ξ and η at the time $t^n + \Delta t_c$ can be obtained by using ξ, η values at $t = t^n$ as initial values and using Eq. (4) successively (i.e., K times). The right-hand side of Eq. (3) is a function of (ξ, η) ; i.e., the metrics $x_\xi, x_\eta, y_\xi,$ and y_η depend upon (ξ, η) . Since these metrics are specified at each grid point in the (ξ, η) space, the values of the metrics are determined during the integration by interpolating from the values at the nearest grid points. The symbol $|^k$ in the right-hand side of Eq. (4) indicates that these terms are evaluated at (ξ^k, η^k) .

4. APPLICATION

For an application of the present method, we consider the rarefied supersonic flow around a circular cylinder; i.e., the Mach number is 3.5 and the Knudsen number defined by λ/D is 0.25. Here λ is the mean free path and D the diameter of the cylinder. Hence the flow simulated is a supersonic flow in a transitional regime.

Since the flow is symmetric, the calculation is conducted at the upper half plane in the (x, y) coordinate system. The calculation region in the (x, y) coordinate system and the cells in it are shown in Fig. 2, where s is the coordinate which starts from the body surface and directs along the stagnation line. The representative cell size is about $\lambda \times \lambda$ while the cells near the body are rather small. The time step Δt_c is chosen as $0.25\tau_c$. The hard sphere model is employed for the intermolecular potential. As for the boundary condition at the body surface, specular reflection of the particles is assumed for simplicity. As for the outer boundary condition, uniform in-flow is assumed. Initially, the uniform flow is set around the cylinder in a whole region. The calculation is conducted up to $t = 25\tau_c$. The total number of particles employed in the simulation is about 2000 and the ensemble average is taken over 80 simulation runs.

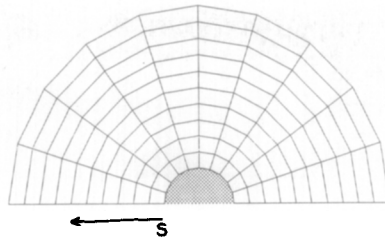


FIG. 2. Body-fitted coordinate system around a half-cylinder.

Before going to the simulation result, we show the example of the time integration of Eq. (3) by the method noted in Section 3. In Fig. 3, the example of the particle path in the coordinate system depicted in Fig. 2 is shown. In each path, the particle starts from the point represented by the symbol \rightarrow and its velocity is kept constant although the particle which hits the body is reflected from the body surface specularly. This example shows that the time integration of Eq. (3) is conducted quite accurately.

Initially the flow is uniform. As time goes on, the body generates compression waves and a steady shock wave is formed in front of the body. At the time $t = 25\tau_c$, a quasi-steady flow is expected to be attained. In fact, a rather broad shock wave is formed in front of the body at $t = 25\tau_c$ as shown in Fig. 4. This rather broad

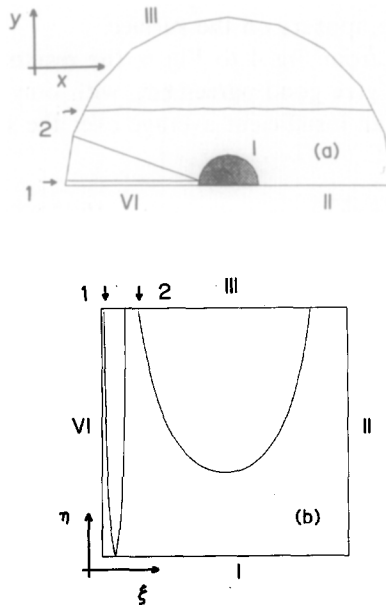


FIG. 3. Typical examples of time-integration of the particle path in (x, y) coordinates (a) and in (ξ, η) coordinates (b).

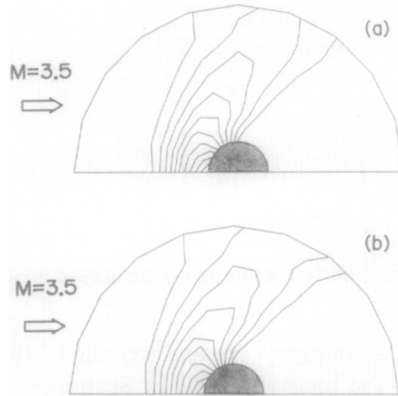


FIG. 4. Density contour around the cylinder in uniform flow in which the Mach number is 3.5. The results by the present method and the standard method are in (a) and (b), respectively.

shock wave is a merged layer where the shock layer and the shock wave are merged. The density and pressure variations along the stagnation line represent the structure of the merged layer (see Fig. 5). Formation of the merged layer is a characteristic feature of a transition regime. In Fig. 6, the velocity field is depicted by a vector the length of which is proportional to the magnitude of the flow velocity. This figure shows the deceleration along the stagnation line and the acceleration along the body surface takes place. The flow velocity near the surface suggests that sufficient slip appears on the surface.

Throughout the figures from Fig. 4 to Fig. 6, the results by the present method and the standard method give good agreement, with only a slight difference. This difference is attributed to an insufficient average over the simulation runs.

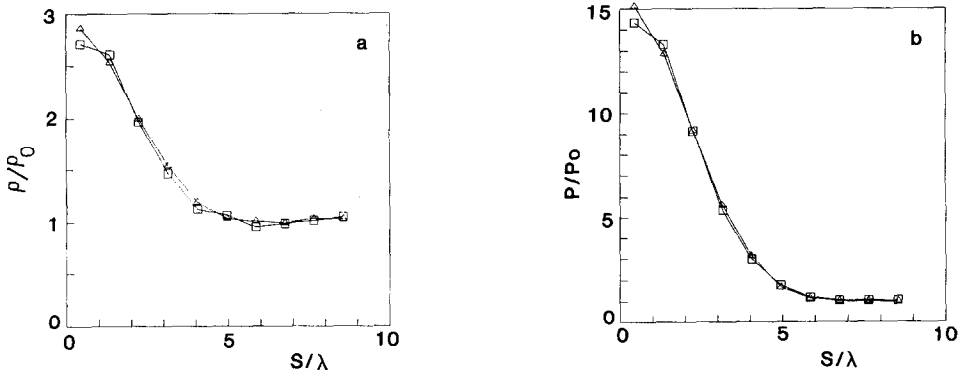


FIG. 5. Density (a) and pressure (b) distribution along the stagnation line. Results by the present method and the standard method are represented by the symbols \square and \triangle , respectively. The density and the pressure in the uniform flow is represented by ρ_0 and P_0 , respectively.

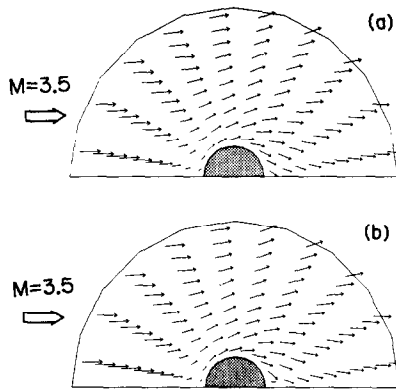


FIG. 6. Velocity field around the cylinder in the uniform flow in which the Mach number is 3.5. The results by the present method and the standard method are in (a) and (b), respectively.

As noted in Section 2, we can expect an economy of computation time in the present method in comparison to the standard method. This economy of computation time is expected from the effectiveness in selecting the cell in which the particle resides. As expected, the computation time is reduced to about $\frac{1}{3}$ the time that the standard method consumes.

For another example of the present method, we consider the rarefied supersonic flow around a non-circular cylinder. This non-circular cylinder shown schematically in Fig. 7a is defined appropriately free form. The symmetric supersonic flow is assumed as shown in Fig. 7a. Since the flow is symmetric, the calculation is

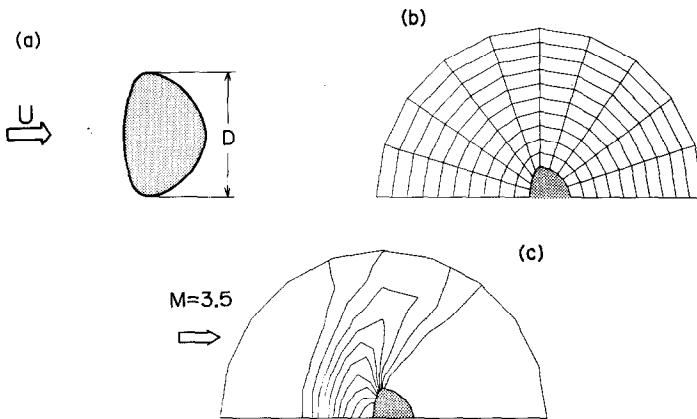


FIG. 7. Schematic figure for the non-circular cylinder (a), the body fitted coordinate system around it (b), and the density contour around it in the uniform rarefied supersonic flow (c). The minimum and the maximum density which the contour lines represent are $1.2 \times \rho_0$ and $3.0 \times \rho_0$, respectively. Here ρ_0 is the density in the uniform flow.

conducted at the upper half plane in the (x, y) coordinate system. The body fitted coordinate system around the body is shown in Fig. 7b. The conditions except the body shape are the same as the ones for the previous example. The density contour around the body is shown in Fig. 7c. The standing bow shock wave is formed in front of the body in a similar manner to the previous example. In the present method, we have assumed the numerical coordinate transformation; the transformation defined at the discrete cell vertices. Hence the example shown in Fig. 7 is easily calculated by using the common program but changing the numerical data defining the transformation.

5. CONCLUSIONS

We have proposed a new method of DSMC in the multidimensional flow. In this method, the body-fitted coordinate system is used. As a result, the standard DSMC method is improved so that the DSMC method can be applicable to a flow-field analysis around the vehicle of arbitrary configuration. Furthermore, the present method is more time-saving in comparison with the standard method.

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