Molecular Dynamics Simulation of Gas Molecules Reflected from Rough Surface

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Abstract. Direct statistical Monte-Carlo simulation of rarefied gas molecular flow near a rough surface is studied on the base of analytical approximation of scattering function V and of the momentum and energy exchange coefficients [1-3]. The computation time is reduced due to the expansion of the roughness operator $\hat{S}$ [2-6], which is used to express the scattering function V on rough surface in the form $V = \hat{S}\ V_0$. The representation of the roughness operator is derived that is convenient to use both in numerical DSMC methods and in analytical investigations.

Keywords: Surface roughness, atoms scattering from surface, numerical computation, rarefied gas, flows in channels.
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INTRODUCTION

In [1], a review has been given of the papers of different authors in which the velocities of the gas atoms reflected from rough surface are computed using direct statistical Monte-Carlo simulation. Typical approach to this problem is based on the simulation of geometrical shape of surface roughness. If the roughness is modelled as a random field, then each step of Monte-Carlo computation requires the solution of the problem of statistical description of the intersection of gas atom trajectory with random field (or with random process) [2]-[7]. Analytical solution of this problem is obtained only in simplest cases having no practical applications.

Numerical solutions are very difficult, and computational realization of these algorithms requires much more calculation time than usual DSMC procedures in rarefied gas flow. Even if surface roughness is considered as nonrandom, and linear shapes like polygonal-line or conical-hole based models are considered [8], [9], computation time increases essentially in comparison with calculations near a smooth surface (without roughness).

Generally, three basic models of surface roughness were discussed:

- the deterministic model, assuming non-random expression of the shape;
- the statistical model, where the roughness is modelled as a homogeneous isotropic Gaussian random field;
- the fractal model that generalizes the approach of Blackmore and Zhou [10] and provides the analytical expression for geometrical shape of the surface.

Deterministic roughness is modelled by flat elements and sine waves. Here, as well as in the case of more involved models, such as conical holes [9], the point of intersection between the gas atom trajectory and the surface can be found analytically. Thus standard deterministic model allows simulating the geometrical shape of the surface in a Monte Carlo computation. However, simple non-random models cannot account for the contribution of micro-roughness. The influence of the irregularities at smaller scale (including nano-scale) is justified by experiment and plays an important role in aerodynamic computation. It becomes possible to compute the contribution of micro-roughness only by using fractal or statistical models for the surface roughness.

The advantage of the statistical model is the ability to work with a more general class of rough surfaces, which means that a more complex shape can be used. In this work, we offer a fast algorithm that allows simulation of scattering by these surfaces. The computation time in our method is even less than that of deterministic models.

New advanced method proposed in the present paper permits simulating the scattering of gas atoms from a more general class of rough surfaces. The expansion of the roughness operator $\hat{S}$ [2], which is used to express the scattering function in the form $V = \hat{S} V_0$, allows to reduce computation time using direct expansion of the velocities of scattered gas atoms. The physical and the chemical parameters of the gas and of the surface are accounted here by the local scattering function V_0, whereas the roughness operator $\hat{S}$ is fully determined by the geometrical shape of roughness and by the trajectory of the gas atom [3]-[4]. Within the statistical model of the roughness [5], $\hat{S}$ can be studied by means of the random-field and random-process theory. The most principal difficulty in statistical approach is the complexity of computation of continuum integrals, which must be approximated by the integrals of higher dimension [6]. To tackle this difficulty we apply Rice series [6], [7]. Especially important is here that the most difficult and time-consuming step of the computation should be performed prior to the simulation of gas atom trajectories. Such technique of the pre-computation of continuum integrals allows us to minimize computing time and at the same time to reduce the number of the parameters. Consequently, eliminating the need for the geometrical-shape simulation in the Monte-Carlo method, our algorithm outperforms all usual methods that apply geometrical models to simulate the shape of the rough surface, such as polygonal-line or conical-hole based models. Additional advantage of considered statistical approach is that real rough surfaces can be simulated in details since applied model of a Gaussian random fields builds a wider class of surface models than other models used in practice.

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Our main assumption is that the number of rough irregularities in a small area dS is large, so that the scale of these irregularities is smaller than the aerodynamic scale of the flow. Consequently, the characteristic scale of the roughness is smaller than the characteristic scale of the flow.

The scattering function of the rough surface can be represented in the form

$$\mathbf{V}(\mathbf{v}_1, \mathbf{v}) = \hat{S}\ \mathbf{V_0}(\mathbf{v}_1, \mathbf{v}, \mathbf{n}), \qquad (1)$$

where $\mathbf{v}_1$ and $\mathbf{v}$ are the velocities of incident and reflected gas atoms, $\mathbf{n}$ is the local normal, $\hat{S}$ is the roughness operator, and $V_0(\mathbf{v}_1,\mathbf{v},\mathbf{n})$ is the local scattering function on a smooth area on a surface.

The physical and the chemical parameters of the gas and of the surface are accounted by the local scattering function V_0; the roughness operator $\hat{S}$ is fully determined by the geometrical shape of roughness and by the trajectory of the gas atom. Within the statistical model, $\hat{S}$ can be studied by means of the random-field and random-process theory.

STATISTICAL MODEL OF ROUGH SURFACE

The most general statistical model of roughness is a homogeneous isotropic Gaussian random field $z(x,y)$, where the (x,y) plane of coordinate system corresponds to the plane of the average level of roughness, and z-axis is directed along the normal vector to this plane (different from local normal to the surface $\mathbf{n}$, fig.1).

Random field is characterized by the roughness parameter σ_1 and the normalized correlation function ρ.

Partial derivatives $z_x = \dfrac{\partial z}{\partial x}$ and $z_y = \dfrac{\partial z}{\partial y}$ of random field in directions x and y determine the parameter $\sigma_1 = \sqrt{Mz_x^2} = \sqrt{Mz_y^2}$ which is more relevant to rarefied gas dynamics than the square mean deviation of rough surface $\sigma = \sqrt{Mz^2}$ often used in other technical applications.

Consider the expansion of the roughness operator $\hat{S}$ in a series:

$$\hat{S} = \sum_{m=1}^{\infty} \hat{S}_m .$$

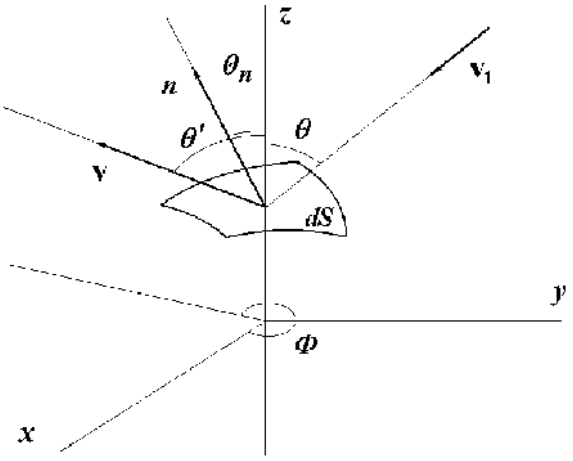

FIGURE 1. Scattering of gas particles from rough surface .

Traditionally the term $\hat{S}_m$ corresponds to the contribution of gas atoms that were m times reflected from the surface. In our approach another expansion of operator $\hat{S}$ is used, m is the number of reflections that happened before the considered reflection. This expansion is more convenient for computation.

Let $\Pi^{(1)}$ be the conditional (provided the given values of z, z_x, z_y) probability of absence of level-crossings between the random field $z(x,y)$ and the trajectory of the gas atom:

$$\Pi^{(1)}(\theta_1, \sigma_1, z, z_x, z_y) = P\{z(0,y) \le z + y \cdot \cot\theta_1 \mid z(0,0) = z, \\ z_x = z'_x(0,0), z_y = z'_y(0,0)\}. \quad (2)$$

The contribution of the first collisions to the surface scattering function has the form

$$\mathrm{V}^{(1)}(\mathbf{v}' \mid \mathbf{v}) = \frac{1}{M_1} \iint\limits_{z_y < \cot\theta_1} dz_x dz_y \mathrm{V}_0(\mathbf{v} \mid \mathbf{v}_1, \mathbf{n}) \cdot [1 - (z_x \cos\psi_1 + z_y \sin\psi_1)\tan\theta_1] \cdot \\ \cdot \int_{-\infty}^{\infty} g(z, z_x, z_y) \Pi^{(1)}(\theta_1, \sigma_1, z, z_x, z_y) dz, \quad (3)$$

where $g(z, z_x, z_y)$ is probability density of z, z_x, z_y, M_1 is normalizing factor, and θ_1, ψ_1 are spherical coordinates of incident gas atoms velocity $\mathbf{v}_1$. The function g controls the position of the point of collision and the direction of the local normal vector **n**.

The computation of the conditional probability $\Pi^{(1)}$ requires the evaluation of an integral in a functional space (the so-called continuum integral). Hence, $\Pi^{(1)}$ must be approximated by integrals of high dimension (up to 200), and its calculation is difficult.

We develop a new method to calculate the velocity **v** of reflected gas atoms, based on the analytical expression of the distribution of the reflected gas atoms for given velocity $\mathbf{v}_1$. The equations (1)-(3) allow us to find the parameters of this distribution.

In practice, we only need to compute the mean values and the standard deviations of the velocity components v_x, v_y, v_z. Note that the mean value of v_x is usually equal to zero due to the symmetry of the distribution, which leaves us with only five parameters to estimate. In our computations, we used the ray-diffuse scattering model (which is a generalization of diffuse-specular scattering) and the Cercignani-Lampis model. However, this condition (the number of distribution parameters $m \le 5$) is valid for many other distributions used in practice.

To compute these parameters on rough surface we apply equations (1)-(3). Normalized mean values $\overline{v}_x$, $\overline{v}_y$, $\overline{v}_z$ are uniquely defined by the momentum exchange coefficients (or by the momentum accomodation coefficients). However, normalized variances D_{v_x}, D_{v_y}, D_{v_z} are not uniquely defined by the energy exchange coefficients. We

express the values of $\bar{v}_x$, $\bar{v}_y$, $\bar{v}_z$, D_{v_x}, D_{v_y}, D_{v_z} as continuum integrals by applying the roughness operator to velocity components v_x, v_y, v_z and its squares v_x^2, v_y^2, v_z^2 and taking into account (1)-(3). Thus two types of continuum integrals are obtained (similar continuum integrals appear in local methods [11]):

$$K_k^x(\theta) = \hat{S}^{(1)}(\cos^k \theta_n), \; k = 1, 2, 3, \tag{4}$$

$$K_k^y(\theta) = \hat{S}^{(1)}\left(\frac{\cos^k \theta_n}{\sin\theta}\left(\frac{1}{\sqrt{1+z_x^2+z_y^2}} - \cos\theta\cos\theta_n\right)\right), \; k = 1, 2, 3. \tag{5}$$

To compute the function space integrals $\Pi^{(1)}$, K_k^x and K_k^y we use the Rice series

$$\Pi^{(1)} = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} N_m . \tag{6}$$

Here, N_m denotes the factorial moment of m-th order of the number of crossings of random field $z(x,y)$ with the trajectory of a gas atom. The values of N_m can be expressed as $2m$-fold integrals of the joint probability density of $z(x,y)$ and its derivatives ξ_i (i=1,2,…m). To the best of our knowledge, Rice series were not used in aerodynamic computations so far, the reason being the singularities in the integrals for N_m. We use a novel technique to eliminate these singularities by rewriting the roughness-simulating random process as an integral of a Wiener process.

DIRECT SIMULATION – MONTE CARLO METHOD

Continuum integrals K_k^x and K_k^y depending only on the angles θ_1, ψ_1 and on roughness parameter σ_1, but not on the physical parameters of the flow, can be computed from (2)-(6). Hence, the values K_k^x and K_k^y could be represented as the functions $K_k^x(\theta_1, \psi_1, \sigma_1)$ and $K_k^y(\theta_1, \psi_1, \sigma_1)$ and consequently could pre-computed in a preliminary step as tables. This representation is important advantage of the described method, since it allows sparing a lot of computing time.

There is no need to simulate the shape of the rough surface in the DSMC calculations because it is taken into account by the roughness operator $\hat{S}$. Moreover, we do not need to compute the scattering function of gas-surface interaction anymore. Hence, the computation time at the stage of atoms scattering simulation from rough surface is very small.

The algorithm to simulate the reflection of gas atoms from rough surface has three steps.

1. **Computation of continuum integrals**. This step should be performed prior to the simulation of gas atom trajectories in the channel. However it is the most difficult and time-consuming step. The statistical description of the surface roughness (i.e., the basic roughness parameter σ_1 and the normalized correlation function $\rho(r)$) is the only information needed at this step. As a result of this pre-computation, we have either tables or approximating functions of the function-space integrals K_k^x and K_k^y.

2. **Simulation of gas-surface interaction based on the chosen analytical model for the scattering function**. This step also has to be performed prior to the simulation of the atom trajectories. It is possible to use, for example, the diffuse-specular model (or, more generally, the ray-diffuse model), as well as the Cercignani-Lampis-Lord scattering model. Other scattering functions can be used as well; the only restriction in our framework is that it must have five or less parameters to describe the physical and chemical features of the gas and the surface. The parameters should be related one-to-one to the normalized mean values and standard deviations of v_x, v_y and v_z. Then, we compute the parameters of the distribution of the scattered gas atoms. Knowing the analytical scattering model for the smooth surface without roughness, the estimated parameters can be transformed according to the integrals K_k^x and K_k^y, computed at the first step. From equations (1) and (3)-(5), it follows that the parameters for the rough surface are linear combinations of the parameters on the smooth surface; the coefficients of the linear expansion depend on K_k^x and K_k^y. As a result of this step, we obtain the parameters of the distribution for the rough surface.

3. **Computation of the velocity V of scattered gas atoms**. First, we compute the parameters of the distribution of the scattered gas atoms. From the second step, we know the analytical scattering model for the smooth surface without roughness. The estimated parameters are transformed according to the integrals K_k^x and K_k^y, computed at the first step. From equations (1) and (3)-(5), it follows that the parameters for the rough surface are linear combinations of the parameters on the smooth surface; the coefficients of the linear expansion depend on K_k^x and K_k^y. As a result of this step, we obtain the velocities of the gas atoms that are scattered from the rough surface.

In terms of computational speed, our algorithm outperforms the methods that use geometrical models to simulate the shape of the rough surface, such as polygonal-line or conical-hole based models. This is achieved by eliminating the need for the geometrical-shape simulation in the Monte-Carlo method; all shape information is accounted for at the preliminary steps.

In Figs. 2-3, we show typical graphs of the computed continuum integrals K_k^x and K_k^y for different values of σ_1 and of the incidence angle (in degrees; k = 2, 3). We observe the significant influence of roughness on the main statistical parameters of the reflected gas atoms.

The precision is satisfactory if σ_1 is less than 0,5 and θ does not exceed 70° (sliding angles $\theta \approx 90°$ require accounting second reflections [12]).

Once the five parameters of the flow are estimated, the velocity **v** of reflected gas atoms could be simulated through a DSMC computation.

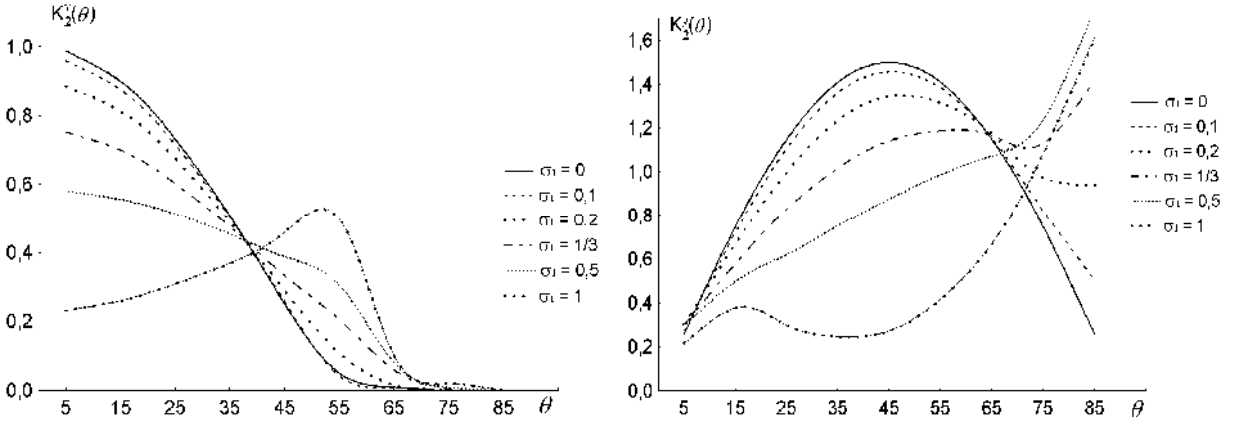

FIGURE 2. Typical graphs of continuum (functional space) integrals K_2^x and K_2^y for different values of σ_1.

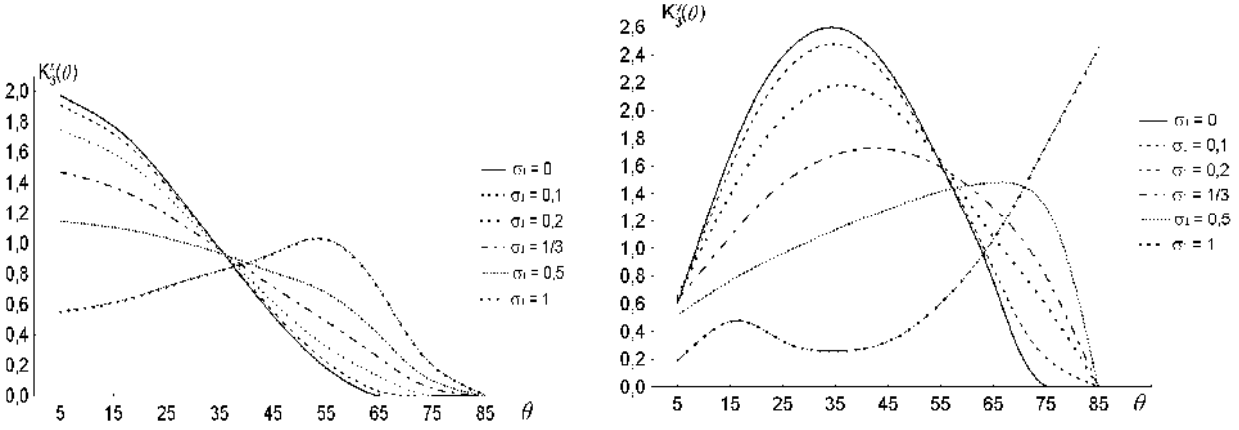

FIGURE 3. Typical graphs of continuum (functional space) integrals K_3^x and K_3^y for different values of σ_1.

CONCLUSION

Efficient approach associated with the Direct Simulation – Monte Carlo (DSMC) method to studying the influence of surface roughness on rarefied gas flow in a channel is developed. Based on statistical model of rough surface approach indicate appreciable effect of surface roughness.

The comparison of different models of roughness shows that statistical approach requires more difficult calculation, including the computation of continuum (functional space) integrals. For example, if we use fractal model to calculate statistical parameters of velocity distribution of reflected atoms, we must compute the integrals of dimension 5. Applying statistical model we calculate integrals of dimension 11 for the same precision (five terms of Rice series). Moreover, by using statistical approach it is necessary to eliminate the singularities.

The computation of the velocity distribution and of the flux of gas in channels shows similar results for both models. Surface roughness has more influence on aerodynamic resistance of a channel than on aerodynamic lift and drag coefficients in external flows. The flux decreases by 20-30% for $\sigma_1 = 0.5$. The dependence of the flux on surface roughness has a maximum by the length of the channel about 5—10 (relative to the width).

The comparison of statistical and deterministic models shows following results. Statistical model of a roughness has better performance in terms of computational speed if the integrals K_k^x and K_k^y are pre-computed in a preliminary step. Deterministic model of a roughness has an advantage if the surface is simulated during the calculations.

However, using special technique of calculations, we obtain computing time economy for statistical model. The most difficult and time-consuming step of computation of continuum integrals can be performed in preliminary step prior to the simulation of gas atom trajectories in the channel. Following this procedure we obtain computing time for statistical model much less than computing time for fractal model as well as for standard deterministic models.

Additional advantage of statistical approach is that Gaussian random fields build a wider class of surface models than other models used in practice; hence, this model can simulate real rough surfaces in details.

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