

The Effect of Angular Momentum and Ostrogradsky-Gauss Theorem in the Equations of Mechanics

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Abstract: - There are many experimental facts that currently cannot be described theoretically. A possible reason is bad mathematical models and algorithms for calculation, despite the many works in this area of research. The aim of this work is to clarify the mathematical models of describing for rarefied gas and continuous mechanics and to study the errors that arise when we describe a rarefied gas through distribution function. Writing physical values conservation laws via delta functions, the same classical definition of physical values are obtained as in classical mechanics. Usually the derivation of conservation laws is based using the Ostrogradsky-Gauss theorem for a fixed volume without moving. The theorem is a consequence of the application of the integration in parts at the spatial case. In reality, in mechanics and physics gas and liquid move and not only along a forward path, but also rotate. Discarding the out of integral term means ignoring the velocity circulation over the surface of the selected volume. When taking into account the motion of a gas, this term is difficult to introduce into the differential equation. Therefore, to account for all components of the motion, it is proposed to use an integral formulation. Next question is the role of the discreteness of the description of the medium in the kinetic theory and the interaction of the discreteness and "continuity" of the media. The question of the relationship between the discreteness of a medium and its description with the help of continuum mechanics arises due to the fact that the distances between molecules in a rarefied gas are finite, the times between collisions are finite, but on definition under calculating derivatives on time and space we deal with infinitely small values. We investigate it.

Keywords: Ostrogradsky-Gauss theorem, Boltzmann Equations, Chapman-Enskog Method, discrete media

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1 Introduction

There are many experimental facts that currently cannot be described theoretically. A possible reason is bad mathematical models and algorithms for calculation, despite the many works in this area of research. The aim of this work is to clarify the mathematical models of describing for rarefied gas and continuous mechanics and to study the errors that arise when describing a rarefied gas by the framework of a continuous medium through the distribution function, that is solution of the Boltzmann equation. We also trace discuss some errors of numerical calculations. Now calculations are performed by three methods: by solving the Boltzmann equation: using various difference schemes, by the molecular dynamics

method and the Byrd method [1-9]. The question of the adequacy of the representation of the mathematical model and the apparatus used to solve the problem is a necessary stage in the work of the mathematician and programmer. There is an extensive literature on the calculations by each of the methods different problems of discrete mechanics [10-14]. It should be noted that for the kinetic theory (the Boltzmann equation) the law of conservation of angular momentum does not hold. The mechanic of a continuous environment is based on the laws of conservation of mass, momentum, and energy. The fundamental conservation laws, in addition, include the law of conservation of the angular momentum. Conservation laws are obtained by recording the balance ratios for an elementary volume

located in an infinite space. For each conservation law, its elementary volume is chosen. However, the law of conservation of angular momentum implies the existence of a specific frame of reference, a specific radius vector, going from the origin to the elementary volume, choosing the axis of rotation of the elementary volume. The role of the angular momentum is manifested in all processes associated with a non-uniform distribution of particles. The resulting effects can affect critical and near critical operating modes of aircraft, missiles, various devices, building structures, and also in some natural processes. The magnitude of the additional force is determined by the value of the gradient of physical quantities (density, velocity, momentum). Writing physical values conservation laws via delta functions, the same classical definition are obtained. In deriving the conservation laws of continuity mechanics, the Ostrogradsky-Gauss theorem is used for a fixed volume [15]. The theorem is a consequence of the application of the integration in parts for the spatial case. In reality, gas and liquid move are not only along a forward path, but also rotate. The out integral term is difficult to introduce into the differential equation. Therefore, to account for all components of the motion, it is proposed to use an integral formulation. In problems with discrete media, the question arises of approximating a discrete representation by a continuous distribution function. The method of solving the Boltzmann equation for the distribution function is based on variation methods and asymptotic analysis. In the construction of macro-functions, the same macroparameters are used for local equilibrium and for non-equilibrium distribution functions. This means that the distribution function that obtained by solving Euler's equation for a gas without friction and with solving Navie-Stokes equations need have equal value. This fact was noted by Hilbert without further use and correction [16-20]. It is proposed to take into account the role of the angular momentum in determining virial coefficients for moderately compressible gases. The role of the angular momentum is reduced to a change in the magnitude and direction of the velocities of the

molecules, which changes the pressure values. Besides we investigate order of influence of angular momentum in case large gradients. In accordance with the purpose of the work, the following sections are highlighted: analysis of the influence of the angular momentum contribution in continuum mechanics, a mathematical description of this influence and the role of the Ostrogradsky-Gauss theorem in the description, relaxation effects, the role of the moment in studying the processes of interaction of many particles.

2 Estimates of Angular Momentum Value Contribution

Let us investigate the order of magnitude of the angular momentum using the method of small order according to the version of work [21]. Let us choose as a zero approximation a value with a symmetric stress tensor. Let

$$\begin{aligned} \sigma_x, \tau_{yx}, \tau_{xy} &= \tau_{yx} + \Delta_x, \\ \tau_{zx}, \tau_{xz} &= \tau_{zx} + \Delta_z, \quad \sigma_y, \sigma_z, \tau_{zy}, \\ \tau_{yz} &= \tau_{zy} + \Delta_y. \end{aligned}$$

We use the equilibrium equations for the force and the moment of force in the classical version, taking into account the small value of the influence of the no symmetry of the tensor in the theory of elasticity. Force balance equation

$$\begin{aligned} \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} &= 0, \\ \frac{\partial (\tau_{yx} + \Delta_x)}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} &= 0, \\ \frac{\partial (\tau_{zx} + \Delta_z)}{\partial x} + \frac{\partial (\tau_{zy} + \Delta_y)}{\partial y} + \frac{\partial \sigma_z}{\partial z} &= 0. \\ \frac{\partial \Delta_x}{\partial x} &= \varepsilon f_1, \\ \frac{\partial \Delta_z}{\partial x} + \frac{\partial \Delta_y}{\partial y} &= \varepsilon f_2. \end{aligned}$$

The equilibrium equation of the angular momentum of force

$$\begin{aligned} y \left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z \left(\frac{\partial \sigma_{xy}}{\partial x} + \right. \\ \left. \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) + \sigma_{zy} - \sigma_{zy} = 0, \end{aligned}$$

$$\begin{aligned}
 & x \left(\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) - y \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \sigma_{yx} - \sigma_{xy} = 0, \\
 & x \left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \sigma_{zx} - \sigma_{xz} = 0, \\
 & y \left(\frac{\partial (\tau_{zx} + \Delta_x)}{\partial x} + \frac{\partial (\tau_{zy} + \Delta_y)}{\partial y} + \frac{\partial \sigma_z}{\partial z} \right) - \\
 & - z \left(\frac{\partial (\tau_{yx} + \Delta_x)}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + \sigma_{zy} - \\
 & - \sigma_{zy} = 0, \\
 & x \left(\frac{\partial (\tau_{yx} + \Delta_x)}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) - y \left(\frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) + \sigma_{yx} - \sigma_{xy} = 0, \\
 & x \left(\frac{\partial (\tau_{zx} + \Delta_x)}{\partial x} + \frac{\partial (\tau_{zy} + \Delta_y)}{\partial y} + \frac{\partial \sigma_z}{\partial z} \right) - \\
 & - z \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \sigma_{zx} - \sigma_{xz} = 0 \\
 & y \left(\frac{\partial \Delta_x}{\partial x} + \frac{\partial \Delta_y}{\partial y} \right) - z \frac{\partial \Delta_x}{\partial x} = \varepsilon f_1 \\
 & x \frac{\partial \Delta_x}{\partial x} = \varepsilon f_2, \quad \frac{\partial \Delta_x}{\partial x} = \frac{\varepsilon f_2}{x} \\
 & x \left(\frac{\partial \Delta_z}{\partial x} + \frac{\partial \Delta_y}{\partial y} \right) = \varepsilon f_3. \\
 & y \left(\frac{\varepsilon f_2}{x} + \frac{\partial \Delta_y}{\partial y} \right) - \frac{z}{x} \varepsilon f_2 = \varepsilon f_1,
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial \Delta_y}{\partial y} &= \frac{\varepsilon f_1}{y} + \frac{z}{xy} \varepsilon f_2 - \frac{1}{x} \varepsilon f_2, \\
 \frac{\partial \Delta_z}{\partial x} &= \frac{\varepsilon f_3}{x} - \left(\frac{\varepsilon f_1}{y} + \frac{z}{xy} \varepsilon f_2 - \frac{1}{x} \varepsilon f_2 \right).
 \end{aligned}$$

Consequently, in the presence of gradients in the vicinity of the origin of coordinates, the angular momentum about axis can play a significant role. Similarly, the role of the angular momentum will be reflected in the initial moment. The process will evolve both in the boundary layer for gas and liquid. An important effect is also the contribution of tangential velocities, arising due to the discrepancy between the strain rates and the direction of the axes. It is usually assumed that the velocity direction is normal and that the

velocity directions and the axis of the coordinates coincide. This is an additional addend in which elastic moduli work, creating dissipative effects. See Fig.1.

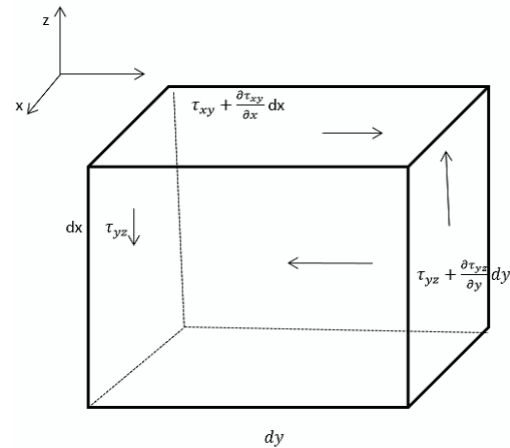


Fig1. Stress tensor components

3 General Theory

There is the Hilbert paradox [16,17]

$$\int \varphi(\xi) f^0 d\xi = \int \varphi(\xi) f d\xi = \beta,$$

here β -macroscopic parameter, $\varphi(\xi)$ -function.

$$n(t, \mathbf{x}) = \int f(t, \mathbf{x}, \xi) d\xi,$$

$$\mathbf{u}(t, \mathbf{x}) = \frac{1}{n} \int \xi f(t, \mathbf{x}, \xi) d\xi,$$

$$P_{ij} = m \int c_j c_i f(t, \mathbf{x}, \xi) d\xi,$$

$$\mathbf{q}_i = \int c^2 c_j f(t, \mathbf{x}, \xi) d\xi,$$

So for the equilibrium in collision integral we have

$$(c^2 = c_1^2 + c_2^2 + c_3^2) = (\xi - \mathbf{u})^2$$

$$f(t, \mathbf{x}, \xi) \equiv f^0(t, \mathbf{x}, \xi) = n \left\{ -\frac{m}{2kT} c^2 \right\}, \quad (1)$$

and for non-equilibrium distribution function

$$f = f^0 \left[1 + \frac{P_{ij} m}{2pkT} c_i c_j - \frac{q_i m}{pkT} c_i \left(1 - \frac{mc^2}{5kT} \right) \right]$$

we have the same macroparameters in f^0 .

There f is distribution function, n, \mathbf{u}, P_{ij}, T are macroparameters, t, \mathbf{x}, ξ coordinates.

Thus, we obtain an equilibrium function with macroparameters calculated by the zero approximation. Therefore, in order to agree on the approximation orders, it is necessary to perform an iterative procedure and substitute

the values obtained for the Navie-Stokes equation.

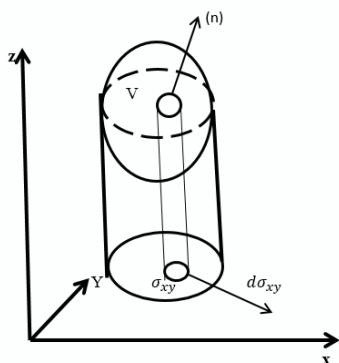


Fig 2. Elementary volume for Ostrogradsky-Gauss theorem

In the experiment they deal with material objects. Hence the original formulation of conservation laws is integral form. The change of the magnitude in the elementary volume is equal to the sum of the flows through the surface. When constructing a differential equation, the integral over the surface is replaced by an integral over the volume using the Ostrogradskogo- Gaussa theorem. However, the derivation of the formula assumes the absence of any circulation component. Volume can't twist. The Ostrogradsky-Gauss formula actually represents formula of integration in parts for the spatial case. By virtue of the approximation of the absence of a tangential component in mechanics, the extra-integral term is assumed to be zero. A visual representation gives the fig. 2.

When the volume is rotated, the extra-integral summand appears and must be taken into account. In practice, the non-integral summand, for example, when considering turbulent motion plays a significant role. As you know, when writing difference schemes, various options for writing differential operators are considered. As rule, conservative form and non-conservative are investigated. In experiments we measure averages over time and space. Actually, conservation laws are formulated in integral form for finite values of volume. The transition from integral to differential form is connected for a finite volume with the requirement of additional smoothness of the

function. The second method of transition is the contraction of the volume to zero and the construction of averages values. Consequently, the tangential component will also give the normal velocity component [22, 23].

As a result,

$$\frac{\partial \rho}{\partial t} + \frac{\partial [(\rho U) \cdot n + (\rho U) \cdot \tau]}{\partial x_i} = 0.$$

In addition, to obtain a differential equation, we take the integral in parts. After that, we discard the term that is out of integral, which in the case of n on symmetric motion will give circulation velocity. This is most clearly seen in the two-dimensional case.

$$\frac{\partial}{\partial t} \int_V \rho \delta \tau + \int_{\sigma} \rho U_n \delta \sigma = \int_V \dot{M} \delta \tau.$$

Recall the Ostrogradsky-Gauss formula

$$\iiint_{(V)} \left(\frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z} \right) dv =,$$

$$\int_{(0)} (P dx + Q dy + R dz) = \iint_{(s)} \left[\left(\frac{\partial R}{\partial y} - \frac{\partial Q}{\partial x} \right) \cos(n, x) + \left(\frac{\partial P}{\partial z} - \frac{\partial R}{\partial x} \right) \cos(n, y) + \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) \iint_s [P \cos(n, x) + Q \cos(n, y) + R \cos(n, z)] ds \cos(n, z) \right] ds.$$

Here ρ is the density, u is the velocity, n is the normal, τ is the ort of the tangent, τ is the elementary volume, P, Q, R are the flows through the corresponding sides, $\cos(n, x), \cos(n, y), \cos(n, z)$ – are the direction cosines of the angles, s is an element of the surface. Out i ntegral term will work well if the all volume rotates at a constant speed ω . An elementary volume is characterized by involvement in rotation with the environment. Therefore, the velocity circulation along the elementary volume has a v ariable value. ω is not a constant. Therefore, it is better to include the rotational velocity component as an additional term to the convective velocity.

$$U = u + 1/2 \omega \times r$$

How to proceed in this case to the differential form of the equation is not known.

$$\frac{d}{dt} (\delta r_1) = \frac{\partial U}{\partial x} \delta x, \quad \frac{d}{dt} (\delta r_2) = \frac{\partial U}{\partial y} \delta y,$$

$$\frac{d}{dt} (\delta r_3) = \frac{\partial U}{\partial z} \delta z.$$

Thus, the field representation (point representation of the elementary volume) does not allow for the rotation of the elementary volume. Consequently, the differential equation for the description of processes in an elementary volume does not allow us to take into account the possible rotation of an elementary volume. Hence the need to solve equations written in integral form. Therefore, difference schemes based on flow variables are preferred. Such schemes include the works by O.M. Belotserkovsky, A.V. Babakov, V.M. Goloviznin, M.A. Zaitsev, S.A. Karabasov, I.A. Korotkin [24, 25].

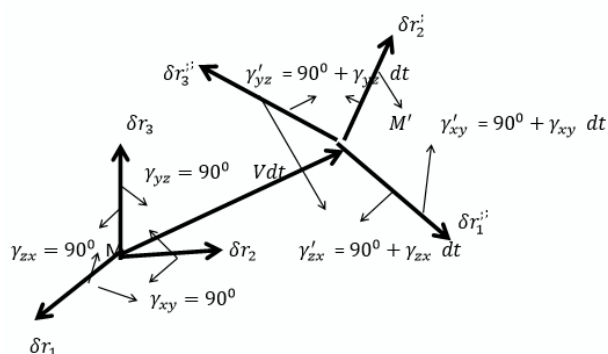


Fig 3. General picture of moving.

4 The Problem of Relaxation in a Rarefied Gas

The correspondence of a continuous description to a discrete one and back is a fundamental problem of modern science. The transition from continuous to discrete description has been studied in many works on computational mathematics [26,27], on inverse transformation is not given due attention, although it is important for studying phenomena associated with finite distances between molecules, particles in multiphase systems, etc. It is interesting to compare derivatives for discrete and continuous descriptions. First, we consider the relaxation process (in time) without flows through the boundaries. Let $f = f(t, r(t), \xi(t))$. Let the distribution function is represented as

$f = \frac{\sum_{i=1}^n \delta(r_i - r)}{\sum_{i=1}^N \delta(r_i - r)}$, that is $f = \frac{n}{N}$, where n is the number of molecules in an elementary volume, N is the number of molecules in a perturbed volume. Then

$$\frac{\partial f}{\partial t} |_{r=const} = \frac{\partial}{\partial t} \frac{\sum_{i=1}^n \delta(r_i - r)}{\sum_{i=1}^N \delta(r_i - r)}.$$

Consider the dependency $\delta(r_i - r)$ - from t just like $r_i(t) - r(t)$.

1. If there are no threads

$$\frac{F_1}{F_3} - \frac{F_2}{F_4} = \frac{\sum_{i=1}^n \delta(r_i - r) + \sum_i^n \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + \dots}{\sum_{i=1}^N \delta(r_i - r) + \sum_i^N \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + \dots} - \frac{\sum_{i=1}^n \delta(r_i - r)}{\sum_{i=1}^N \delta(r_i - r)} \approx$$

$$\approx \frac{\sum_{i=1}^n \delta(r_i - r) + \sum_i^n \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + \dots}{\sum_{i=1}^N \delta(r_i - r)}$$

$$\left(1 - \frac{\sum_i^n \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + \dots}{\sum_{i=1}^N \delta(r_i - r)} \right) - \frac{\sum_{i=1}^n \delta(r_i - r)}{\sum_{i=1}^N \delta(r_i - r)} \approx \frac{\sum_i^n \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + o((\Delta t)^2)}{\sum_{i=1}^N \delta(r_i - r)}$$

$\frac{\partial \delta(r_i - r)}{\partial t}$ - thus, for a rarefied gas, when solving the Boltzmann equation, we receive the time derivative is only depends from the macroparameters. This hypothesis is used in the theory of rarefied gas in constructing a solution to the Boltzmann equation by the Chapman-Enskog method.

2 When accounting for flows across the border, we will have

$$\frac{F_1}{F_3} - \frac{F_2}{F_4} =$$

$$= \frac{\sum_{i=1V}^n \delta(r_i - r) + \sum_{iV}^n \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + S}{\sum_{i=1V}^N \delta(r_i - r) + \sum_{iV}^N \Delta t \frac{\partial \delta(r_i - r)}{\partial t} + T}$$

$$S = \Delta t \sum_{j \in \Omega} \frac{p_j}{m} \delta(r_j - r) +$$

$$+ \sum_{j \in \Omega} \frac{p_j}{m} \Delta t^2 \frac{\partial \delta(r_j - r)}{\partial t} + \dots$$

$$T = \Delta t \sum_{j \in \Omega} \frac{p_j}{m} \delta(r_j - r) +$$

$$+ \sum_{j \in \Omega} \frac{p_j}{m} \Delta t^2 \frac{\partial \delta(r_j - r)}{\partial t} + \dots$$

Index V - refers to the volume, Ω - to the surface.

$\sum_{j \in \Omega} \frac{p_j}{m} \delta(r_j - r) = J_2 - J_1$ - flow of fast molecules from neighboring cells

Thus, the role of borders increases. The distribution function does not provide the correct parameter values. Here work only the molecular dynamics method with a very small on time step is correct.

5 Calculation of Space Derivative in Rarefied Gas

Let determine the differential in the usual way.

$$\begin{aligned} & \sum_1^n \delta(t, r_{i+1} - r) = \\ & = \sum_1^n \delta(t, r_i + \Delta r_{i+1} - r), \\ & n = \sum_1^n \delta(t, (r_i - r)), \end{aligned}$$

$$N = \sum_1^N \delta(t, (r_i - r)).$$

$$j(x) = \sum_j \frac{p_j}{m} \delta(r_j(t) - r(t)).$$

ξ_i is the velocity of the molecule, U is the velocity of the elementary volume, $p_i = \xi_i - u$ is the phase velocity of the molecule, r is the coordinate. In the definition of the Boltzmann equation and in the calculations for the models used, the velocity ξ_i of molecules enters as an independent variable. We believe that the number of molecules in the elemental volume is small compared with the number of molecules in the whole volume.

$$\frac{\partial f}{\partial t} \approx \frac{M_1}{Q_1} \frac{M}{N}, \quad n = n(t, r), \quad N = N(t, r). \quad \text{At the point } r + \Delta r,$$

$$\begin{aligned} M_1 = & \sum_{i=1}^n \delta(r_i - r) + \sum_{i=1}^n (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \dots + \sum_{j=n}^{n+\Delta n} \delta(r_j - r) + \\ & \sum_{j=n}^{n+\Delta n} (\Delta r_j - \Delta r) \frac{\partial \delta(r_j - r)}{\partial r} + \dots, \end{aligned}$$

$$\begin{aligned} N_1 = & \sum_{i=1}^N \delta(r_i - r) + \sum_{j=N}^{N+\Delta N} \delta(r_j - r) + \\ & + \sum_{j=N}^{N+\Delta N} (\Delta r_j - \Delta r) \frac{\partial \delta(r_j - r)}{\partial r} + \dots \end{aligned}$$

M_1 - the number of particles and the flux of particles entering the boundary of the elementary volume at time t .

N_1 - the number of particles and the flux of particles entering through the boundary at the time instant t of the perturbation region.

M_2 - for $t + \Delta t$, N_2 - for $t + \Delta t$.

$$\dot{r}_i = \xi_i, \quad \frac{p_i}{m} = \xi_i - u, \quad \frac{dr}{dt} = u.$$

If $r = r(t)$, then $\frac{dF}{dt} = \dot{r} \frac{\partial F}{\partial r}$, F - function.

In general, for slowly changing flows across the border

$$\frac{M|_{t=const}}{N|_{t=const}} = \frac{\sum_{i=1}^n \delta(r_i(t) - r(t))}{\sum_{i=1}^N \delta(r_i(t) - r(t))}$$

After decomposition in a row we get

$$\begin{aligned} F(t + \Delta t) = & \frac{\sum_{i=1}^n \delta(r_i(t) - r(t)) + H}{\sum_{i=1}^{N+\Delta N} \delta(r_i(t) - r(t)) + Q} \\ H = & \sum_{i=1}^n (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \\ & + \sum_{j=n}^{n+\Delta n} \delta(r_j - r) + \\ & + \sum_{i=N}^{N+\Delta N} (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \dots \\ Q = & \sum_{i=1}^N (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \\ & + \sum_{j=N}^{N+\Delta N} \delta(r_j - r) + \\ & + \sum_{i=N}^{N+\Delta N} (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \dots \end{aligned}$$

$$F(t) = \frac{\sum_{i=1}^n \delta(r_i(t) - r(t))}{\sum_{i=1}^N \delta(r_i(t) - r(t))}$$

$$Y = \sum_{i=1}^n (\Delta(r_i - r)) \frac{\partial \delta(r_i - r)}{\partial r} + \sum_{j=n}^{n+\Delta n} \delta(r_j - r) + \dots$$

$$W = \sum_{i=N}^{N+\Delta N} (\Delta(r_i - r)) \frac{\partial \delta(r_i - r)}{\partial r}$$

$$(F(t + \Delta t) - F(t)) / \Delta t \approx \left(\frac{\sum_{i=1}^n \delta(r_i(t) - r(t)) + Y}{\sum_{i=1}^N \delta(r_i(t) - r(t))} - \left(1 - \frac{\sum_{i=1}^n (\Delta(r_i - \Delta r)) \frac{\partial \delta(r_i - r)}{\partial r} + W}{\sum_{i=1}^N \delta(r_i(t) - r(t))} + \dots \right) - \frac{\sum_{i=1}^n \delta(r_i(t) - r(t))}{\sum_{i=1}^N \delta(r_i(t) - r(t))} \right) / \Delta t \approx$$

$$\frac{-\text{div}(\sum_{j=1}^{n_2} \frac{p_j \Delta t}{m} \delta(r_i - r) + \sum_{i=1}^n (\Delta(r_i - r)) \delta(r_i - r) + \dots)}{\sum_{i=1}^N \delta(r_i - r) + \sum_{j=1}^{N_1} \frac{p_j}{\Delta_k} \delta(r_j(t) - r)} / \Delta t$$

$$\frac{-\text{div}(\sum_{j=1}^{n_2} \frac{p_j}{m} \delta(r_i - r) + \sum_{i=1}^n \frac{p_j}{m} \delta(r_i - r) + \dots)}{(\sum_{i=1}^N \delta(r_i - r) + \sum_{j=1}^{N_1} \frac{p_j}{\Delta_k} \delta(r_j(t) - r) + \dots)}$$

$$\approx \frac{-\text{div}(\sum_{j=1}^{n_2} \frac{p_j}{m} \delta(r_i - r) + \sum_{i=1}^n \frac{p_j}{m} \delta(r_i - r) + \dots)}{(\sum_{i=1}^N \delta(r_i - r) + \sum_{j=1}^{N_1} \frac{p_j}{\Delta_k} \delta(r_j(t) - r) + \dots)}$$

$$\sum_{i=N}^{n+\Delta n} \delta(r_j - r) =$$

$$= -\text{div} \sum_{j=1}^{m_2} \frac{p_j}{m} \delta(r_j - r).$$

It can be seen from the formulas that in the case of coincidence of the velocities of molecules with an average speed, the time derivative in numerical calculation according to the difference scheme is just a flow of molecules along the sides of the elementary volume. When calculating by the molecular dynamics method, everything is functional. Accuracy is determined by the number of particles. In this case, the additional term defines self-diffusion. This is also the result of calculations for the equilibrium distribution function. For multi components gas one have

$$F_1 = \sum_p \sum_{j=1}^{n_2(p)} \frac{p_j}{m_j} \delta(r_j - r) + \sum_p \sum_{i=1}^{n(p)} (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \dots$$

$$F_2 = \sum_p \sum_{j=1}^{N(p)} \frac{p_j}{m_j} \delta(r_j - r) + \sum_p \sum_{i=1}^{N(p)} (\Delta r_i - \Delta r) \frac{\partial \delta(r_i - r)}{\partial r} + \dots$$

6 Effect of Moment for a Discrete Environment

Knowledge of virial coefficients is necessary in various practical problems [28, 29]. In previous works, the effect of angular momentum on physical parameters in the kinetic theory and continuum mechanics was discussed. It can be assumed that density fluctuations are associated with inhomogeneity of the velocity distribution at temperatures greater than zero Kelvin degrees, which in turn is associated with the movement of the inertia axis of elementary volumes. Here we consider the algorithm for calculating the additional force associated with the action of the moment in a discrete medium. The formula for determining the center of gravity of the system of material points.

$$r_c = \frac{\sum_{i=1}^k m_i r_i}{\sum_{i=1}^k m_i}.$$

The position of the center of inertia at different times

$$\frac{\sum_{i=1}^n m \delta(r_i - r_c) r_i}{Nm} = r_c$$

$$\frac{\sum_{i=1}^n m \delta(r_i + \Delta r_i - r_c + \Delta r_c) (r_i + \Delta r_i)}{(N + \Delta N) m} \approx \tilde{r}_c.$$

Angular momentum

$$\tilde{p}_i \times (r_i + \Delta r_i - \tilde{r}_c) - p_i \times r_i = L_i,$$

$$\frac{(p_i + \Delta p_i) \times (r_i + \Delta r_i - r_c - \Delta r_c) - p_i \times (r_i - r_c)}{\Delta t} = \frac{dL_i}{dt}.$$

$$\frac{dL}{dt} = M, \quad F = \frac{dM}{dr}.$$

$$\frac{dM_i}{dr} = \frac{d p_i (\Delta r_i - \Delta r_c)}{dr \Delta t} =$$

$$= \frac{d}{dr} p_i (\Delta p_i - \Delta p_c).$$

We can obtain additional force

$$\frac{\sum_{i=1}^n m \delta(r_i + \Delta r_i - r_c - \Delta r_c) (r_i + \Delta r_i)}{\left(N + \frac{\Delta N}{N}\right) m} -$$

$$- \frac{\sum_{i=1}^n m \delta(r_i - r_c) r_i}{Nm} =$$

$$\frac{\sum_{i=1}^n ((\Delta r_i - \Delta r_c) \frac{\partial \delta}{\partial r} r_i + \Delta r_i \delta(r_i - r_c)) + \dots}{N}$$

$$\cdot \left(1 + \frac{\Delta N}{N}\right) +$$

$$+ \frac{\sum_{i=1}^{n+\Delta n} ((\Delta r_i - \Delta r_c) \frac{\partial \delta}{\partial r} r_i + \Delta r_i \delta(r_i - r_c)) (r_i + \Delta r_i) + \dots}{N}$$

$$\approx \frac{\sum_{i=1}^n ((\Delta r_i - \Delta r_c) \frac{\partial \delta}{\partial r} r_i + \Delta r_i \delta(r_i - r_c) r_i)}{N}$$

In this way, we can obtain additional force acting upon the collective interaction of particles.

$$F_i^{ad} \approx \frac{\sum_{i=1}^n ((\Delta r_i - \Delta r_c) \frac{\partial \delta}{\partial r} r_i + \Delta r_i \delta(r_i - r_c) r_i)}{N}$$

$\Delta p_i^k = F_i^{ad} \Delta t$. p_k – the number of dimers.

$$p_i^{k2} \Delta t^2 + p_j^{k2} \Delta t^2 \leq (r + \sigma)_i^{k2} - (r + \sigma)_j^{k2}$$

The number of molecules that form dimer, number of decayed dimers

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The number of molecules that form dimer, number of decayed dimers

$$p_i^{k2} \Delta t^2 + p_k^{k2} \Delta t^2 \geq E.$$

Here p_j^k is the contribution of i components at time k . Therefore, we can determine the number of dimers in equilibrium conditions. Pressure P

$$\sum_{i=1}^n \frac{(p_i + \Delta p_i)^2}{m} + \sum_N^{n+\Delta n} \frac{p_i^2}{m} = P.$$

The first term is responsible for the usual thermodynamic pressure, taking into account the change in speed from the effect of the moment, the second term is responsible for the pressure caused by the dimers. This shows that the change in pressure is nonmonotonic.

7 Conclusion

The analysis of the assumptions underlying the classical models of a continuous medium and kinetic theory is performed. The possibility of describing discrete media within the framework of continuum mechanics is analyzed. The discarded physical effects resulting from the replacement of a discrete medium of a rarefied gas which has a finite mean free paths and a finite distance between molecules by the distribution function are analyzed. Based on the obtained estimates regarding the description of the dynamics of a rarefied gas, we can conclude that the calculations by the molecular dynamics method are preferable to using the distribution function. The range of applicability of the Ostrogradsky – Gauss theorem can be extended to the case of rotation of an elementary volume. The role of by using the Ostrogradsky-Gauss theorem for a fixed volume with ignoring of the velocity circulation over the surface of the selected volume is discussed for turbulent flows. A mechanism is proposed for taking into account the motion of the center of inertia of an elementary volume of gas or liquid, and the contributions of the center's motion to pressure are analyzed, which is important when calculating virial coefficients.

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