

Chapter 2

Elements of Kinetic Gas Theory

In this chapter, we present some aspects of kinetic theory. They will be used in deducing the quasi-gas-dynamic equations in Chap. 3, in constructing their generalizations (Chaps. 8 and 9), and in considering problems on the structure of a shock wave and the flow in microchannels (Appendices B and C). We present a schematic description of the kinetic DSMC algorithm,¹ which is widely used in numerical modelling of rarefied gas flows. Simulations within the framework of this approach were used for the verification of the QGD algorithm in modelling moderately rarefied flows. In the last section, we present a method for constructing kinetically consistent difference schemes whose differential analogs served as a basis for first variants of the QGD equations. The presentation in this chapter is based on [28, 51, 52, 54–56, 122, 127, 160, 184, 190].

2.1 Boltzmann Equation

In 1872, L. Boltzmann suggested the integro-differential kinetic equation, which became the classical model in rarefied monoatomic gas theory [27, 28, 118, 122, 141]. This equation has the form

$$f_t + (\xi \cdot \nabla_x) f + (F \cdot \nabla_\xi) f = \mathcal{I}(f, f) \quad (2.1)$$

and describes the evolution of the one-particle distribution function $f = f(x, \xi, t)$. Here, ξ is the velocity of a separate particle, which is considered as a spherical atom of mass m_0 , F is the exterior force acting on the particles relative to the mass unit, and ∇ is the Hamilton operator. The function f is normalized in such a way that the relation

$$m_0 dN = f(x, \xi, t) dx d\xi$$

defines a probable (or expected) number dN of particles in the volume element $dx d\xi$ near a point (x, ξ) of the phase space of coordinates and velocities at a fixed instant of time t .

¹ Direct simulation Monte Carlo algorithm.

The collision integral $\mathcal{I}(f, f)$ is a nonlinear functional determining the variation of the distribution function resulting from pair collisions. A concrete form of this integral can be found in [27, 28, 122, 141].

An important property of the collision integral, which we need in what follows, is its orthogonality to any of the so-called collision (or summator) invariants

$$h(\xi) = 1, \xi, \frac{\xi^2}{2}.$$

In other words, we can write

$$\int h(\xi) \mathcal{I}(f, f) d\xi = 0. \quad (2.2)$$

This relation expresses the conservation laws of mass, momentum, and energy of particles under their pair collision. Here and in what follows, the integration is performed over the whole three-dimensional velocity space of the particle.

If the distribution function f is known, we can define the gas-dynamic quantities—density ρ , velocity u , pressure p , temperature T , specific internal energy ε , viscosity stress tensor Π , and heat flux q —using the expressions

$$\begin{aligned} \rho &= \int f d\xi, \quad \rho u = \int \xi f d\xi, \quad p = \int \frac{c^2}{3} f d\xi, \\ \rho c_v T &= \rho \varepsilon = \int \frac{c^2}{2} f d\xi, \quad q = \int \frac{c^2}{2} c f d\xi, \\ \Pi &= \int \left[I \frac{c^2}{3} - c \otimes c \right] f d\xi. \end{aligned} \quad (2.3)$$

Here, $c = \xi - u$ is the velocity of the chaotic motion of a gas particle or thermal velocity, and $c_v = 3\mathcal{R}/2$ is the specific heat capacity at constant volume for monoatomic gases.

Integrating Eq. (2.1) with weights 1, ξ , and $\xi^2/2$ and using property (2.2), we obtain the following system of equations for the macroscopic parameters:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \rho u = 0, \quad (2.4)$$

$$\frac{\partial(\rho u)}{\partial t} + \operatorname{div}(\rho u \otimes u) + \nabla p = \rho F + \operatorname{div} \Pi, \quad (2.5)$$

$$\frac{\partial}{\partial t} \left[\rho \left(\frac{u^2}{2} + \varepsilon \right) \right] + \operatorname{div} \left[\rho u \left(\frac{u^2}{2} + \varepsilon + \frac{p}{\rho} \right) \right] + \operatorname{div} q = (\rho u \cdot F) + \operatorname{div}(\Pi \cdot u), \quad (2.6)$$

which, however, is not closed.

For positive solutions $f = f(x, \xi, t)$ of Eq. (2.1), under the assumptions that they exist, have a necessary smoothness, and tend to zero as $|\xi| \rightarrow \infty$, Boltzmann proved his famous H -theorem.

Assume that a monoatomic gas is in a bounded volume V_0 with interior wall that is mirror reflecting. Let the corresponding initial and boundary conditions for the particle distribution function be given in this volume. Then for the Boltzmann function

$$H(t) = \int_{V_0} dx \int f \ln f d\xi,$$

the following inequality holds for all $t \geq 0$:

$$\frac{dH(t)}{dt} \leq 0. \quad (2.7)$$

Therefore, the motion of the gas in the vessel considered is accompanied with the nonincrease of the quantity $H(t)$ in time, which indicates its nonreversible character.

2.2 Equilibrium Distribution Function and the Euler System

An exact solution of the Boltzmann equation is the distribution function called the locally Maxwell distribution function, which in dimensional quantities has the form

$$f^{(0)}(x, \xi, t) = \frac{\rho}{(2\pi\mathcal{R}T)^{3/2}} \exp\left(-\frac{(u - \xi)^2}{2\mathcal{R}T}\right). \quad (2.8)$$

For the function $f^{(0)}$, the relation $\mathcal{I}(f^{(0)}, f^{(0)}) = 0$ holds, and it is connected with f by the relations

$$\begin{aligned} \rho &= \int f d\xi = \int f^{(0)} d\xi, \\ \rho u &= \int \xi f d\xi = \int \xi f^{(0)} d\xi, \\ \rho c_v T &= \rho \varepsilon = \int \frac{c^2}{2} f d\xi = \int \frac{c^2}{2} f^{(0)} d\xi. \end{aligned} \quad (2.9)$$

By a direct substitution, we can verify that for the locally Maxwell distribution function, one has

$$q = \int \frac{c^2}{2} f^{(0)} d\xi = 0, \quad \Pi = \int \left[I \frac{c^2}{3} - c \otimes c \right] f^{(0)} d\xi = 0.$$

The function $f^{(0)}$ is also called the locally equilibrium distribution function.

The integration of the Boltzmann equation with weights 1, ξ , and $\xi^2/2$ in the zero approximation, i.e., when f is assumed to be equal to $f^{(0)}$, allows us to close system (2.4), (2.5), and (2.6) and obtain the Euler system.

2.3 Navier–Stokes Equations

In 1916–1917, S. Chapman and D. Enskog suggested an asymptotic method for solving the Boltzmann equation, which allows one to close system (2.4), (2.5), and (2.6) and obtain a system of equations in the first approximation for describing flows of a viscous heat-conducting gas, the Navier–Stokes system [28, 122, 141].

The essence of the method is that a solution of Eq. (2.1) reduced to a dimensionless form is sought for in the form of a formal asymptotic series in powers of a small positive parameter, the Knudsen number Kn , in the form

$$f = f^{(0)}(1 + \text{Kn} f^{(1)} + \text{Kn}^2 f^{(2)} + \dots),$$

where

$$\text{Kn} = \frac{\lambda}{L}, \quad (2.10)$$

λ is the mean free path of particles in the unperturbed flow and L is the characteristic size of the flow domain. As the zero approximation, the locally Maxwell function (2.8) is used.

In the first approximation by the number Kn , the calculations via the Chapman–Enskog method lead to the so-called Navier–Stokes distribution function

$$f_{\text{NS}} = f^{(0)} \left[1 - \frac{1}{p\mathcal{R}T} \left(1 - \frac{c^2}{5\mathcal{R}T} \right) (c \cdot q_{\text{NS}}) - \frac{1}{2p\mathcal{R}T} \Pi_{\text{NS}} : (c \otimes c) \right]. \quad (2.11)$$

The quantities Π_{NS} and q_{NS} were written earlier (see Eqs. (1.34) and (1.35)).

Sequentially integrating the Boltzmann equation with the summator invariants 1, ξ , and $\xi^2/2$, under the assumption that f coincides with f_{NS} , we obtain the Navier–Stokes system written above in Sect. 1.4. The Chapman–Enskog procedure allows us to perform an approximate calculation of the viscosity and heat conduction coefficients. For the hard-sphere gas, the approximate calculation of these coefficients leads to the expressions

$$\mu = \frac{5}{64} \frac{m_0}{r_0^2} \sqrt{\frac{\mathcal{R}T}{\pi}}, \quad \varkappa = \frac{c_p \mu}{\text{Pr}}, \quad (2.12)$$

where r_0 is the radius of the hard-sphere particle. The number Pr in Eq. (2.12) turns out to be equal to $2/3$, and the coefficients themselves depend only on the temperature, which is in concordance with the known experimental data.

Using the next approximation in the expansion of the distribution function with respect to the Knudsen number, we can obtain the Burnett equations. These

equations involve the third-order partial derivatives, which lead to essential difficulties in their numerical solution and in the substitution of the boundary conditions.

2.4 Bhatnagar–Gross–Krook Equation

In 1954, P. Bhatnagar, E. Gross, and M. Krook [25] suggested the approximate kinetic equation of the form

$$f_t + (\xi \cdot \nabla_x) f + (F \cdot \nabla_\xi) f = \frac{f^{(0)} - f}{\tau}, \quad (2.13)$$

i.e., Eq. (2.1) in which the collision integral $\mathcal{I}(f, f)$ was approximated by the expression

$$\mathcal{I}(f, f) = \frac{f^{(0)} - f}{\tau}. \quad (2.14)$$

At present, Eq. (2.13) is called the Bhatnagar–Gross–Krook model kinetic equation (BGK). Approximately at that time, Eqs. (2.13) and (2.14) were independently published by P. Velander [141]. The positive parameter τ in the right-hand side of relation (2.14) is interpreted as the characteristic time of relaxation of the function f to the locally Maxwell distribution $f^{(0)}$ function defined by formula (2.8) and is assumed to be a given function of the density and the temperature. The quantity τ has the order of the mean collision time of molecules in the gas and is called the Maxwell relaxation time. The macroscopic quantities entering the formula for calculating τ are also quadratures of f . An analog of the Boltzmann H -theorem holds for the BGK model.

The application of the Chapman–Enskog method to the BGK equation also leads to the Navier–Stokes system [28, 122, 141]. In this case, the dynamical viscosity coefficient μ and the heat conduction coefficient \varkappa are calculated by the formulas

$$\mu = p\tau, \quad \varkappa = c_p p\tau. \quad (2.15)$$

It follows from the presented formulas that in the BGK approximation, the Prandtl number is equal to unity.

At present, improved models of the BGK approximation type are elaborated. In particular, the Shakhov S-model has been suggested; it allows one to consider the real value of the Prandtl number. Moreover, instead of the equilibrium distribution function, in the collision integral (2.14), one chooses the distribution function of the form

$$f_S = f_0(1 + (1 - \text{Pr})\psi(c, \rho, T, u)),$$

where ψ is a certain function [176].

There are generalizations of the BGK approximation to the case where the characteristic time of relaxations depends on the velocity of the particles $\tau = \tau(\xi)$. A variant of the relaxation equation that takes into account the nonequilibrium character with respect to internal degrees of freedom of the particles [28] is used in Chap. 8 for the construction of the gas-dynamic equations. A variant of the BGK approximation for a gas mixture and its use for constructing the moment equations is discussed in Chap. 9.

2.5 Mean Collision Quantities of the Particle Motion

Let us present the definitions of the basic quantities characterizing the chaotic motion of particles in a gas with distribution function f . The expressions obtained are used in the sequel.

The *mean thermal velocity* of particles is calculated as follows:

$$\langle \bar{c} \rangle = \frac{1}{\rho} \int \bar{c} f dc, \quad \text{where} \quad \bar{c} = \sqrt{c_x^2 + c_y^2 + c_z^2}. \quad (2.16)$$

The *mean relative velocity* of particles is defined in the form

$$\langle \bar{c}_r \rangle = \frac{1}{\rho^2} \iint \bar{c}_r f_1 f_2 dc_1 dc_2, \quad (2.17)$$

where $c_r = \xi_1 - \xi_2$ is the relative velocity of two colliding molecules,

$$\bar{c}_r = [(c_{x1} - c_{x2})^2 + (c_{y1} - c_{y2})^2 + (c_{z1} - c_{z2})^2]^{1/2},$$

and f_1 and f_2 are the corresponding one-particle distribution functions.

In the case of the equilibrium distribution function $f = f^{(0)}$ defined according to Eq. (2.8), integrals (2.16) and (2.17) can be calculated analytically, and the values of the corresponding means are defined as follows:

$$\langle \bar{c} \rangle = \sqrt{\frac{8}{\pi} \mathcal{R}T}, \quad \langle \bar{c}_r \rangle = 4\sqrt{\frac{\mathcal{R}T}{\pi}}. \quad (2.18)$$

The *most probable velocity* of particles is determined by the “width” of the distribution function, and in the equilibrium case (2.8), it is

$$c_m = \sqrt{2\mathcal{R}T}.$$

The mean frequency of collisions (the mean collision rate) ν is given by

$$\nu = \frac{\rho}{m_0} \langle \sigma c_r \rangle, \quad (2.19)$$

where σ is the collision cross-section and

$$\langle \sigma c_r \rangle = \frac{1}{\rho^2} \iint \sigma \bar{c}_r f_1 f_2 dc_1 dc_2$$

is the scattering cross-section.

For gases with the Maxwell distribution function $f_1 = f_1^{(0)}$, $f_2 = f_2^{(0)}$ in the VHS approximation [28], we have

$$\langle \sigma c_r \rangle = 4\sigma_{\text{ref}} \sqrt{\frac{\mathcal{R}T_{\text{ref}}}{\pi}} \left(\frac{T}{T_{\text{ref}}} \right)^{1-\omega}, \quad (2.20)$$

where σ_{ref} is the value of the collision cross-section at the temperature T_{ref} . For the hard-sphere gas ($\sigma = \sigma_0$, $\omega = 0.5$), expression (2.20) takes the form

$$\langle \sigma c_r \rangle = \sigma_0 \langle c_r \rangle = 4\sigma_0 \sqrt{\frac{\mathcal{R}T}{\pi}}. \quad (2.21)$$

The mean collision time is the inverse of the frequency of collisions:

$$\tau_c = \frac{1}{\nu}. \quad (2.22)$$

For the hard-sphere gas,

$$\tau_c = \frac{\sqrt{\pi} m_0}{4\rho\sigma_0\sqrt{\mathcal{R}T}}. \quad (2.23)$$

In the VHS approximation the Maxwell relaxation time is connected with the mean collision time (see [28]):

$$\tau = \frac{\mu}{p} = \Omega(\omega)\tau_c, \quad \text{where} \quad \Omega(\omega) = \frac{30}{(7-\omega)(5-\omega)}. \quad (2.24)$$

For the hard-sphere gas, $\Omega(\omega = 1/2) = 5/4$.

The mean free path λ of particles is determined by the mean collision time τ_c and the mean thermal velocity (2.16):

$$\lambda = \tau_c \langle \bar{c} \rangle. \quad (2.25)$$

For the hard-sphere gas with Maxwell distribution function, the substitution of relations (2.18) and (2.23) leads to the expression

$$\lambda = \frac{m_0}{\sqrt{2}\rho\sigma_0}. \quad (2.26)$$

Let us present certain estimates for the characteristic parameters of air. At atmospheric pressure at sea level, the number of particles is $n = 2.4 \times 10^{25} \text{ m}^{-3}$, the mean distance between particles is $r_* = n^{-1/3} = 3 \times 10^{-7} \text{ m}$, the mean free path is $\lambda = 10^{-7} \text{ m}$, the mean collision time $\tau_c = 2.5 \times 10^{-10} \text{ s}$, the mean thermal velocity is $\langle \bar{c} \rangle = 300 \text{ m/s}$, and the collision cross-section is $\sigma = 10^{-18} \text{ m}^2$.

At a height of 300 km from the Earth's surface the concentration of particles is $n = \rho/m_0 \approx 10^{15} \text{ m}^{-3}$, the mean distance between molecules is $r_* \approx 3 \times 10^{-5} \text{ m}$, the mean free path is $\lambda \approx 10^3 \text{ m}$, and the mean collision time is $\tau_c \approx 1 \text{ s}$.

The estimates presented show clearly that the mean values in gases vary strongly when the density of the particles varies. In particular, this refers to the relation between the mean free path and the mean distance between molecules. This explains the fact that the scales of the spatial average V and the time average Δt introduced in Sect. 1.1 can substantially change depending on the concrete problem considered.

2.6 Transport Coefficients in Equilibrium Gases

The chaotic motion of particles considered on the microscopic level is accompanied by the redistribution of their number and also by the transport of the momentum and energy by each particle. Thus, on the macroscopic level, the description of the motion of molecules generates three interconnected transport processes: diffusion or self-diffusion, viscosity, and heat conduction.

These three transport processes are closely related to each other. In all three cases, the fluxes are proportional to the gradients of the corresponding quantities. According to [160], these processes can be uniformly described by using basic concepts of kinetic theory, namely, in terms of the mean thermal velocity of particles and the mean free path.

Indeed, let the mean free path λ be much less than the characteristic size of the problem, which is related to the gradients of the macroscopic quantities, the density, the velocity, and the pressure. Consider the transport of a certain scalar quantity A through a unit area, which is perpendicular to the axis z , for a unit time. Then the normal component of the flow Γ_A through this small area due to the chaotic motion of particles at a unit time is defined as follows:

$$\Gamma_A = -\frac{1}{3}(n\bar{v}\lambda)\frac{dA}{dz}, \quad (2.27)$$

where n is the density of particles, \bar{v} is the mean velocity of chaotic motion, and λ is the mean free path. The coefficient $1/3$ is chosen from the assumption that all three coordinate directions are equally probable in the chaotic motion.

If the quantity A is the concentration, $A = n_1/n$, then we find the diffusion flux through the unit area:

$$\Gamma_n = j_\rho = -\frac{1}{3}(n\bar{v}\lambda)\frac{dn_1/n}{dz} = -\frac{1}{3}(\bar{v}\lambda)\frac{dn_1}{dz}. \quad (2.28)$$

This yields the expression for the diffusion coefficient in the form

$$D = \frac{1}{3}\bar{v}\lambda. \quad (2.29)$$

To calculate the momentum transport through the unit small area, we take $A = m_0 u$, where u is the macroscopic velocity of the gas flow along the small area. Then the flow of the quantity A transported in the random walk corresponds to the component of the viscous stress tensor:

$$\Gamma_A = \Pi = -\frac{1}{3}(n\bar{v}\lambda)\frac{m_0 du}{dz} = -\frac{1}{3}(\rho\bar{v}\lambda)\frac{du}{dz}. \quad (2.30)$$

Therefore, we obtain the kinetic estimate for the coefficient of viscosity, the Maxwell formula

$$\mu = \frac{1}{3}\rho\bar{v}\lambda. \quad (2.31)$$

If A is the heat energy of a particle, $A = m_0\bar{v}^2/2$. Replacing \bar{v}^2 by the most probable velocity $\bar{v}^2 = c_m^2 = 2\mathcal{R}T$, we obtain the following expression for the heat flux through the unit area:

$$\Gamma_A = q_z = -\frac{1}{3 \cdot 2}(n\bar{v}\lambda)\frac{d}{dz}m_0 2\mathcal{R}T = -\frac{1}{3}(n\bar{v}\lambda)k_B \frac{dT}{dz}. \quad (2.32)$$

In other words, the heat conduction coefficient has the form

$$\kappa = \frac{1}{3}n\bar{v}\lambda k_B = \frac{1}{9}\rho\bar{v}\lambda c_v, \quad (2.33)$$

where $c_v = 3k_B/m_0$ is the specific heat capacity at constant volume for the monoatomic gas.

The values of coefficients of diffusion, viscosity, and heat conduction obtained on the basis of simple kinetic estimates turn out to be connected with each other and are proportional to the mean free path λ and the mean velocity \bar{v} of chaotic motion of particles. Defining again \bar{v} as the mean thermal velocity (2.18) or the most probable velocity, we obtain the well-known expressions for these three transport coefficients for $\text{Sc} = 1$ and $\text{Pr} = 1$ and also the connection of the mean free path with the coefficient of viscosity, which differs from the Chapman formula (see Sect. 3.4) by a numerical coefficient of unit order.

Therefore, the simplified consideration of the transport processes in an equilibrium gas allows us to obtain qualitatively correct expressions for the coefficients of diffusion, viscosity, and heat conduction. These transport processes have equal rights and explicitly participate in the QGD/QHD equations. The Navier–Stokes system contains only two of them, the momentum and heat energy transports related to the coefficients of viscosity and heat conduction.

2.7 Numerical Simulation of Flows of Rarefied Gases

2.7.1 General Remarks

A simple characteristic of the rarefaction degree of a gas-dynamic flow is the Knudsen number $\text{Kn} = \lambda/L$, which is the quotient of the mean free path λ of molecules and the characteristic size L of the problem considered. As usual, a gas is assumed to be dense if $\text{Kn} \rightarrow 0$ (in practice, $\text{Kn} < 0.01$). The conditions under which

$Kn \rightarrow \infty$ (in practice, $Kn > 10$) are characteristic for free molecule flows when collisions between particles are practically absent. For intermediate values of Kn , the gas is considered to be rarefied.

The methods of simulation of free molecule regimes are sufficiently well elaborated at present. For these problems, we can neglect collisions of particles between each other and take into account only the interaction of particles with walls. We can assume that the velocity distribution of particles is known with large accuracy, for example, we can assume that it is in equilibrium with the distribution function $f^{(0)}$. In this case, the main problem is the description of the interaction of particles with walls. This process can be approximately described by using the accommodation coefficient σ . The simplest models are the complete accommodation of particles on the wall, or the so-called diffusion reflection, which corresponds to $\sigma = 1$, and the model of mirror reflection, in which $\sigma = 0$.

By a moderately rarefied flow of a gas one means flows for which the Knudsen number lies in the interval between 0.01 and 0.1, depending on the problem considered. The flows of moderately rarefied gases present a domain lying on the limits of applicability of the kinetic approach and the approach related to the solution of the moment equations. The simulation of such flows by methods of kinetic theory requires unwarranted large computational resources, which is stipulated by a high density of the gas. At the same time, the Navier–Stokes equations obtained in the approximation $Kn \rightarrow 0$ lose their accuracy in analyzing the regimes discussed.

To calculate flows of moderately rarefied gases in the framework of the moment equations, there arises a necessity to take into account the deviation from the continuous flow regimes, first of all, near the flowing around a surface. For this purpose, one uses special boundary conditions.

For all Knudsen numbers, whatever small, in the boundary near the wall, there exists a gas layer whose thickness is of order of the mean free path of molecules, the so-called Knudsen layer. To take into account the influence of this layer on the flow field in the framework of the macroscopic equations, one introduces the boundary conditions being slip conditions for the velocity and jump conditions for the temperature.

The first variant of such conditions was written by Maxwell under the assumption of the diffusion reflection of molecules from the wall [148]. At present, in the literature, there are different variants of such conditions (see, e.g., [28, 122, 142]). They have a similar structure and differ from each other only by numerical coefficients of order 1. Here, we present the condition in the Smoluchowski form in which, as compared with the classical Maxwell conditions, the value of accommodation coefficients for the velocity σ_u and the energy σ_e , which can be different, are taken into account, and the influence of the gradient of temperature along the wall (temperature crip) is also taken into account:

$$u_s = \frac{2 - \sigma_u}{\sigma_u} \lambda \left(\frac{\partial u_n}{\partial n} \right)_s + \frac{4}{3} \left(\frac{\mu}{\rho T} \frac{\partial T}{\partial s} \right)_s,$$

$$T_s - T_w = \frac{2 - \sigma_e}{2\sigma_e} \frac{2\gamma}{\gamma + 1} \frac{\lambda}{\text{Pr}} \left(\frac{\partial T}{\partial n} \right)_s,$$

where u_n and u_s are the normal component of the gas velocity near the wall and the slip velocity along the wall, respectively, n and s , respectively, are the coordinates along the exterior normal to the wall and along the wall itself, T_s is the temperature of the gas near the wall, and T_w is the temperature of the wall.

For most materials, under the supersonic flowing around, the velocity and energy accommodation coefficients can be assumed to be equal and close to the unit. In the formula for the slip velocity, the second term plays an appreciable role only for Knudsen numbers approaching the unit (see [99]).

Flows of gases in the range 0.1–10 of the Knudsen numbers are substantially difficult for the analytical study and the numerical simulation since in this range, it is impossible to introduce a small parameter with respect to Knudsen number of the type Kn or $1/\text{Kn}$. In this range, methods of kinetic theory are applied. The numerical analysis of flows is performed either by the direct solution of the Boltzmann equation or its simplified variants, or by using methods of direct numerical simulation, the Monte Carlo methods or DSMC methods (see [27, 28]).

The difficulty in using these approaches is related to large expenditures of computer time in modelling the particle collisions and a large dimension of the problem as a whole, which is considered in the space of seven dimensions (x, ξ, t) . An additional difficulty is stipulated by the necessity of the computation of averaged characteristics in order to obtain the gas-dynamic quantities being measured: the velocity, the density, and the pressure. In the framework of DSMC approaches, additional difficulties are the computations of nonstationary flows and flows with small (i.e., subsonic) velocities since such computations are accompanied with considerable fluctuations of average quantities.

2.7.2 Monte Carlo Method

In a wide sense, the Monte Carlo methods are methods based on random variables. Monte Carlo methods are successfully used for the solution of various problems of statistical physics, computational mathematics, game theory, mathematical economics, etc. (see [93]).

The direct-simulation method for computation of flows of a rarefied gas (the direct simulation Monte Carlo, DSMC) was first elaborated by G. A. Bird in the 1960s and was then improved and developed (see [27, 28]).

In gas dynamics, a version of the Monte Carlo method is applied; it is based on modelling a real gas flow by using a relatively small number of molecules. In other words, a numerical experiment is performed in which the history of a bounded number of particles is traced; each of them is representative of a large number W of real molecules. The quantity W is called the weighting factor.

For each molecule, its coordinates, velocity, and energy are stored. According to these quantities, by averaging, the gas-dynamic parameters of the flow are found.

For stationary problems, the computation starts from prescribing an arbitrary distribution in the computational domain, which develops to its equilibrium state with time. Now we list the main steps of the DSMC method.

2.7.2.1 Discretization and Modelling of the Particle Motion

The flow domain is partitioned into spatial cells such that the change of gas-dynamic parameters in each of the cells is small. For the efficiency of simulation, the number of particles in each cell must not be very different and is of order equal to several tens.

Modelling the physical motion of molecules is performed by discrete steps in time Δt , which are small as compared with the mean free path time, $\Delta t < \tau_c$. The motion of molecules and molecule collisions on the interval of time are sequentially modelled. At each time step Δt , the motion of particles is partitioned into two steps and is described in the framework of the kinetic model, which is a cyclically repeating process of free collision scattering and subsequent collisions that are considered as instantaneous. This model corresponds to two steps of computation.

2.7.2.2 Movement

At the first step, all molecules move by a distance determined by their velocities $\xi \Delta t$. The intersection of molecules and rigid bodies, lines, symmetry planes, and boundaries of the flow is taken into account. If there is a flow inside the domain, new molecules are generated. If a molecule leaves the computational domain, then it disappears.

2.7.2.3 Collisions

At the second step, the number of collisions between molecules are computed resulting in a change in their velocities. The choice of the colliding pair of particles is performed in the same cell randomly, taking into account that the probability of a pair of molecules to collide is proportional to σc_r .

An important part of the direct modelling method is the computation of a correct number of collisions (collision rate). The frequency of collisions ν is determined by properties of the real gas, for which the problem is solved, and precisely this quantity determines the dissipative characteristics of the flow, the coefficients of viscosity μ and heat conduction κ of the gas modelled.

2.7.2.4 Computation of Macroscopic Characteristics

When the computation is completed, a number of quantities (Σc , Σc^2 , etc.) are accumulated to obtain the macroscopic parameters of a gas (ρ , u , p , and T). The longer the cumulation process, the smaller the statistical fluctuations of macroscopic parameters.

2.8 Difference Approximation of the Boltzmann Equation and Kinetically Consistent Difference Schemes

The numerical solution of the Boltzmann equation (2.1) is severely limited by computational requirements, due to the large number of independent variables and problems of approximation and calculation of the collision integral. Corresponding numerical algorithms are presented, e.g., in [11, 12].

The left-hand side of Eq. (2.1) has the form of the transport equation for the function f with velocity ξ , and it can be approximated by a first-order finite-difference scheme with up-wind differences, the Courant–Isaacson–Rees (CIR) scheme. For a consistent choice of steps in time and space, $h = |\xi|\Delta t$, this finite-difference scheme describes the transport of a given perturbation of the function f without distortion (see [163, 167]).

Let us present the form of the corresponding finite-difference scheme for a one-dimensional spatial flow without exterior forces on a uniform spatial grid with space step $h = x_{i+1} - x_i$ and time step $\Delta t = t^{j+1} - t^j$:

$$\begin{aligned} \frac{f_i^{j+1} - f_i^j}{\Delta t} + \xi_x \frac{f_i - f_{i-1}}{h} &= \mathcal{I}(f, f)_{h,i}, & \xi_k > 0, \\ \frac{f_i^{j+1} - f_i^j}{\Delta t} + \xi_x \frac{f_{i+1} - f_i}{h} &= \mathcal{I}(f, f)_{h,i}, & \xi_k < 0. \end{aligned} \quad (2.34)$$

Here ξ_k is a component of the particle velocity, $f = f^j = f(x_i, \xi, t^j)$, and $\mathcal{I}(f, f)_{h,i}$ is the difference analog of the collision integral.

The finite-difference scheme (2.34) can be identically transformed to the equivalent form

$$\frac{f_i^{j+1} - f_i^j}{\Delta t} + \xi_k \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h}{2|\xi_k|} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} = \mathcal{I}(f, f)_{h,i}. \quad (2.35)$$

For the finite-difference analog of the collision integral $\mathcal{I}(f, f)_{h,i}$, let the orthogonality conditions with summator invariants $h(\xi)$ hold. The finite-difference scheme (2.35) can be averaged in the velocity space assuming that $f = f^{(0)}$. In this case, all the integrals can be analytically calculated, and it is possible to construct immediately the finite-difference scheme for the gas-dynamic quantities—density ρ , velocity u , and energy E (see [40, 41, 51, 55, 184]).

The scheme obtained is rather cumbersome since it involves error integrals arising in averaging the modules of the velocities ξ_k . However, this scheme turned out to be very efficient for solving the Euler equations, and it was used in performing simulations of one-dimensional, as well as some two-dimensional, supersonic gas-dynamic flows. Later on, finite-difference equations having a close structure were obtained in [48].

In the finite-difference scheme (2.35), let us replace the coefficient of the last term by setting $|\xi| \sim c$, where c is the sound speed. Taking into consideration a

time $\tau = h/2c$ characterizing the time to cross a computational cell by a particle, we obtain

$$\frac{h}{2} |\xi_k| = \frac{h \xi_k^2}{2 |\xi_k|} \sim \frac{h}{2c} \xi_k^2 = \tau \xi_k^2. \quad (2.36)$$

Then scheme (2.35) takes the form

$$\frac{f_i^{j+1} - f_i^j}{\Delta t} + \xi_k \frac{f_{i+1} - f_{i-1}}{2h} - \tau \xi_k^2 \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} = \mathcal{I}(f, f)_{h,i}. \quad (2.37)$$

Expression (2.37) in the case $f = f^{(0)}$ also admits an analytical averaging with the summator invariants $h(\xi)$ and leads to constructing a more elegant, as compared with the previous case, system of finite-difference equations for describing the macroscopic quantities in the gas. The schemes thus obtained are called kinetically consistent difference schemes.

Using the notation for central difference derivatives of the first and second order in space accepted in [170], we rewrite the difference scheme (2.37) in the form

$$\frac{f_i^{j+1} - f_i^j}{\Delta t} + (f \xi_k)_x^\circ - \tau (f \xi_k \xi_k)_{\bar{x}x} = \mathcal{I}(f, f)_{h,i}. \quad (2.38)$$

Here, $f_x^\circ = (f_{i+1} - f_{i-1})/h$ is the first-order central difference derivative, $f_x = (f_{i+1} - f_i)/h$ and $f_{\bar{x}} = (f_i - f_{i-1})/h$ are the left and right difference derivatives, respectively, and $f_{\bar{x}x} = (f_x - f_{\bar{x}})/h$ is the second-order central difference derivative.

Using the notation introduced, we write the kinetically consistent difference schemes for the case of a plane one-dimensional flow in the form

$$\begin{aligned} \frac{\rho_i^{j+1} - \rho_i^j}{\Delta t} + (\rho u)_x^\circ &= \tau (\rho u^2 + p)_{\bar{x}x}, \\ \frac{(\rho u)_i^{j+1} - (\rho u)_i^j}{\Delta t} + (\rho u^2 + p)_x^\circ &= \tau (\rho u^3 + 3pu)_{\bar{x}x}, \\ \frac{E_i^{j+1} - E_i^j}{\Delta t} + (u(E + p))_x^\circ &= \tau (u^2(E + 2p))_{\bar{x}x} + \tau \left(\frac{p}{\rho} (E + p) \right)_{\bar{x}x}. \end{aligned} \quad (2.39)$$

The schemes of type (2.39) modified later turned out to be very efficient in modelling a wide range of gas-dynamic flows [8–10, 40, 41, 51, 52, 54–56, 104, 105].

Differential analogs of these schemes served as a base of the first variant of the QGD equations.

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