

0. Introduction

0.1 The General Scheme of Monte Carlo Methods

The first publication on the use of Monte Carlo methods was made by Hall¹ in 1873 while organizing the stochastic process of experimental determination of π number by means of throwing of needle on the sheet of lined paper. The bright example of the application of Monte Carlo methods consists in the use of idea by J. von Neumann realized in 1940s of the past century, by the modeling of the neutron's trajectories in Los Alamos laboratory. In spite of the fact that Monte Carlo methods are connected with a large amount of computations, the lack of electronical computational technique did not embarrass investigators in neither case during their application of the methods of statistical modeling, because in both cases, the study was concerned with realization of accidental processes. And these methods acquired their romantic title by the name of enclave of Monaco, which is famous due to its gambling houses, where the principal object is roulette — the most perfect instrument for obtaining the accidental numbers. And the first publication with a systematic exposition of that matter was made in 1949 by Metropolis and Ulam,² where Monte Carlo method was applied to a solution of linear integral equations. And in that publication was implicitly revealed the problem of the passing of neutrons through the substance. When speaking of Russia, the publications on Monte Carlo methods began to appear actively after the International Conference in Geneva devoted to the peaceful applications of nuclear energy. As one of the first one could mention the work by Vladimirov and Sobol.³ Beginning with the earliest 1970s, side by side with the regular methods those of Monte Carlo obtained their proper place in computational mathematics (Marchuk, Samarskii, Popov, Belotserkovskii, Bakhvalov, Ermakov, Mikhailov, Sobol, Bird, Haviland, Kogan, Perepukhov, and Janitskii).

The general scheme of Monte Carlo method is based on the central limiting theorem of the theory of probability, which states that the accidental quantity $Y = \sum_{i=1}^n X_i$ which is equal to a sum of the large amount N of arbitrary accidental numbers X_i having identical mathematical expectations m and dispersions σ^2 , is

always distributed according to a normal law with mathematical expectation $N \cdot m$ and dispersion $N \cdot \sigma^2$.

Let us assume that we wish to find a solution of some equation or a result of some process I . If the accidental quantity ξ with a probability density p is built up in such a way that the mathematical expectation for this quantity would be equal to the solution we are looking for, $M(\xi) = I$, then that would give the simple way of estimation of both the solution and the error,

$$I = M(\xi) \approx \frac{1}{N} \sum_{i=1}^N \xi_i \pm \frac{3\sigma}{\sqrt{N}}.$$

Following from above are the general properties of the methods:

- the absolute convergence to a solution as $1/N$;
- the strong dependence of the error ε on the number of trials, as $\varepsilon \approx \frac{1}{\sqrt{N}}$ (that is, for the diminishment of the error on one order it is necessary to increase the number of trials on two orders);
- the main way of the error's diminishment consists in the maximal diminishment of dispersion or, in the other words, it is necessary to draw as near as possible the probability density $p(x)$ of the accidental quantity ξ to the mathematical formulation of the problem or to the physics of a phenomenon modeled;
- the error does not react on the problem's dimensionality (by the use of finite-difference methods the transition from the one-dimensional problem to the three-dimensional one the number of computations would be increased on two orders, while in Monte Carlo methods the number of computations remains on the same order);
- the simple structure of computational algorithm (number N of the single-type computations by the realization of accidental quantity);
- moreover, the construction of accidental quantity ξ might be based on the physical nature of process only, and would not demand, as it is in the regular methods, the compulsory formulation of the equation; such a quality becomes more and more actual for modern problems.

The main properties of Monte Carlo methods, as well as the conditions at which they yield or surpass the traditional finite-difference approaches, might be demonstrated by the application to some simple problem, for example, to the problem of the computation of an integral

$$I = \int_a^b f(x)dx,$$

where \mathbf{x} , \mathbf{a} , and \mathbf{b} are vectors in a n -dimensional Euclidian space. Let us build up the accidental quantity ξ with density $p(x)$ in such a way that the mathematical expectation

$$M(\xi) = \int_{-\infty}^{\infty} \xi \cdot p(x) dx,$$

would occur to be equal to our integral I . Then, if within the proper limits one would choose $\xi = f(x)/p(x)$, then the central limiting theorem would give

$$I = \frac{1}{N} \sum_{i=1}^N \xi_i \pm \frac{3\varepsilon}{\sqrt{N}}.$$

Thus, we have as *the first*: The computation of the integral I might be interpreted, from one side, as a solution of mathematically formulated problem, and, from the other side, as a direct modeling of determination of a volume found under the function $f(x)$.

The second: The computation of the one-dimensional integral I_1 by the Monte Carlo method corresponds to the integral's computation by the method of rectangles with a step $\Delta x \approx 1/N$ and an error $O(\Delta x)$. In principle, by the sufficiently good function $f(x)$ in one-dimensional case the integral I_1 might be calculated with accuracy $O(\Delta x^2)$ with trapezoids, with accuracy $O(\Delta x^3)$ with parabola's, and, generally speaking, with any predicted accuracy. In multi-dimensional case, the difficulties of use of the high-order schemes become to acquire such an essential character that by the computation of n -dimensional integrals I_n with $n \geq 3$ the high-order schemes are used just very rarely.

Let us build up the correspondence in effectiveness between regular methods and statistical ones. Let it be that n is the problem's dimensionality, Y — the number of knots at the axis, $R = Y^n$ — the total number of knots for regular methods, q — the order of accuracy of the scheme, N — the number of statistical trials, ν — the number of operations for a treatment of a single knot, $\varepsilon_L = Y^{-q}$ — the error of computations for regular methods, $\varepsilon_K = N^{-1/2}$ — the error of computations for Monte Carlo, $L(\varepsilon) = \nu \cdot R = \nu \cdot \varepsilon^{-n/q}$ — the number of operations by the problem's solution with regular methods, $K(\varepsilon) = \nu \cdot N = \nu \cdot \varepsilon^{-2}$ — the number of operations by the use of Monte Carlo method. For the case of one and the same number of operations by the computation of solution by one or another method one would obtain the relation $n = 2q$. This means that with $n \geq 3$, when mainly the first-order schemes are used, the Monte Carlo methods occur to be preferable.

0.2 Special Position of Monte Carlo Methods in Computational Aerodynamics

Dynamics of the rarefied gases is treated by means of well-known integro-differential equation — *Boltzmann* equation:

$$\frac{\partial f}{\partial t} + \vec{\xi} \nabla f = \int (f' \cdot f'_1 - f \cdot f_1) \cdot \vec{g} \cdot b \cdot db \cdot d\varepsilon \cdot d\vec{\xi}_1, \quad (0.2.1)$$

where $f = f(t, x, y, z, \xi_x, \xi_y, \xi_z)$ is the function of molecule's distribution in respect of time, coordinates, and velocities, f', f'_1 — distribution functions corresponding to the molecule's velocities after collision, $\vec{\xi}', \vec{\xi}'_1, \vec{g}$ — relative velocities of molecules by collisions in pairs, $\vec{g} = \vec{\xi} - \vec{\xi}_1 = \vec{\xi}' - \vec{\xi}'_1$, b , and ε — aiming distance and azimuthal angle by the collisions of particles. The complicated nonlinear structure of the integral of collisions and large number of variables (in the general case — 7) do create the essential difficulties for the analysis, including the numerical one, and, practically, lead to the exclusion of the finite-differential approach from the process of the solution of serious problems. At the same time, the multi-dimensionality and probabilistical nature of kinetic processes create the natural ground for the application of Monte Carlo methods.

Historically, the application of Monte Carlo methods to the computational aerodynamics was initiated in TSAGI by the pioneering works by M.N. Kogan and V.A. Perepukhov devoted to the modeling of free-molecular flows about space objects, in the part of trajectory of their orbital flight. Such a modeling is just the simplest form of rarefied gas dynamics. The further development of the statistical computational methods was realized in the following three directions:



Professor M.N. Kogan. 1965.

- use of the Monte Carlo methods for the calculation of collision integrals found in the regular finite-difference schemes designed for the solution of kinetic equations;
- direct statistical modeling of the physical phenomenon which is splitted in two approaches: modeling of the trajectories of “trial particles” according to Haviland⁴ and modeling of the evolution of “ensemble of particles” according to Bird⁵;
- construction of the accidental process of the type of a procedure by Ulam and Neumann described in Ref. 6 and corresponding to a solution either of linearized kinetic equation,⁸ or of Master Equation by Kac.⁷

The probabilistical nature of the aerodynamics of rarefied gases, which is so important for application and development of the numerical schemes of Monte Carlo, follows quite naturally from the general principles of kinetic theory and statistical physics.



Laureate of State prize
V.A. Perepukhov. 1965

The reasoning cited below might be, quite perfectly, looked at as the levels of completeness of description of a large molecular system. Further on, these levels will be needed for a construction of the effective methods of statistical modeling. The most detailed level of description is presented by a dynamical system. To describe such a system which comprises of a large number of elements N (note that molecular gas is just such a system with $N \approx 10^{23}$ molecules), it is necessary to

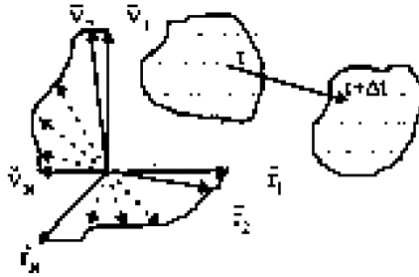


Fig. 0.1 Evolution of the dynamical system in $6N$ -dimensional space.

set the initial coordinates and velocities of each molecule (\vec{r}_j, \vec{v}_j) and the equations of evolution of this system:

$$m \frac{d^2 \vec{r}_j}{dt^2} = \sum_{i \neq j}^N R_{ij}. \quad (0.2.2)$$

Solution of such a system appears to be quite unreal problem, even for a strongly rarefied gas — at the height of 400–600 km (the most popular orbits of satellites) one cubic centimeter contains 10^9 molecules. For this reason one comes to the less complete, that is, statistical description of the behavior of the system. In accordance to a Gibbs formalism one considers not a single system, but the ensemble of them in $6N$ -dimensional Γ -space (Fig. 0.1), with system's distributed according to the N -particle distribution function $F(t, \vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}_N) = F_N$, of which the sense is that of a probability for a system to be in the time moment t at the point $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, \vec{v}_1, \vec{v}_2, \dots, \vec{v}_N$, in vicinity of $d\vec{r}_1, \dots, d\vec{r}_N d\vec{v}_1, \dots, d\vec{v}_N$ we have

$$dW = F_N d\vec{r}_1, \dots, d\vec{r}_N d\vec{v}_1, \dots, d\vec{v}_N.$$

Such an ensemble is described by the famous *Liouville* equation:

$$\frac{\partial F_N}{\partial t} + \sum_{i=1}^N v_i \frac{\partial F_N}{\partial r_i} + \sum_{i \neq j}^N \sum_{i=1}^N \frac{R_{ij} \partial F_N}{m \partial v_i} = 0. \quad (0.2.3)$$

And beginning with that moment the *Liouville* equation and all other kinetic equations following from the *Bogoljubov's* chain, including the last link — *Boltzmann* equation — possess the probabilistical nature. And in spite of the fact that Eq. (0.2.3) is simpler than system (0.2.2), it takes into consideration the N -particle collisions of molecules and also remains to be extremely complicated for a practical analysis. The transition to a less detailed level of description is connected with the further coarsening of system's description with the help of s -particle distribution functions $F_s = \int F_N d\vec{r}_{s+1} \dots d\vec{r}_N d\vec{v}_{s+1} \dots d\vec{v}_N$, which determine the probability of

the simultaneous revelation of s particles independently of the state of the remaining $N - s$ particles. Following the ideas of *Bogoljubov* one obtains the chain of interconnected equations:

$$\frac{\partial F_s}{\partial t} + \sum_{i=1}^s v_i \frac{\partial F_s}{\partial r_i} + \sum_{0=1}^s \sum_{j \neq i}^s \frac{R_{ij} \partial F_s}{m \partial v_i} = - \sum_{i=1}^s (N-s) \frac{\partial}{\partial v_i} \int \frac{R_{i,s+1}}{m} F_{s+1} dr_{s+1} dv_{s+1}, \quad (0.2.4)$$

up to the one-particle distribution function $F_1 = f(t, \vec{r}, \vec{\xi})$ for the Boltzmann's gas, taking into account only by-pair collisions:

$$\frac{\partial f}{\partial t} + \vec{\xi} \frac{\partial f}{\partial \vec{r}} + \frac{R_{12} \partial f}{m \partial \vec{\xi}} = - \frac{\partial}{\partial \vec{\xi}} \int \frac{R_{12}}{m} F_2 d\vec{r}_1 d\vec{\xi}_1.$$

Following Boltzmann we shall consider the molecules to be spherically symmetrical and, adopting the hypothesis of a molecular chaos, $F_2(t, \vec{r}, \vec{v}_1, \vec{v}) = F_1(t, \vec{r}, \vec{v}_1) F_1(t, \vec{r}, \vec{v}_2)$, one obtains Eq. (0.2.1).

As rather interesting one might consider the particular case of Liouville's equation (0.2.3) and Bogoljubov's chain (0.2.4) for the spatially uniform gas consisting of the limited number of particles. At the terminal link this case leads to obtaining the famous equation by *Kac* — "Master Equation"⁷:

$$\frac{\partial \phi_1(t, \vec{\xi}_1)}{\partial t} = \frac{N-1}{N} \int [\phi_2(t, \vec{\xi}'_1, \vec{\xi}'_2) = \phi_2(t, \vec{\xi}_1, \vec{\xi}_2)] \cdot g_{12} d\sigma_{12} d\vec{\xi}, \quad (0.2.5)$$

where ϕ_1 and ϕ_2 are one- and two-particle distribution functions. Unlike the Boltzmann's equation, Eq. (0.2.5) is linear, and this fact will be used by the construction and estimation of the effective computational schemes of direct statistical modeling. When coming back to the Boltzmann equation, from the determination of the function f it would be easy to obtain all the macroscopic parameters. Thus, the number n of molecules within the unit volume of gas is equal to

$$n(t, x) = \int f(t, x, \xi) d\xi.$$

Similarly to that, the mean velocity of molecules, stress tensor and vector of the flow of energy are defined by the relations

$$u(t, x) = (1/n) \int \xi f(t, x, \xi) d\xi,$$

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

$$q_i = (m/2) \int c^2 c_i f(t, x, \xi) d\xi,$$

where $c = \xi - u$ is thermal velocity of molecules. The mean energy of the thermal motion of molecules is usually characterized by temperature

$$\frac{3}{2}kT = \frac{1}{n} \int \frac{mc^2}{2} f(t, x, \xi) d\xi.$$

By way of application to the Boltzmann equation procedure of Enskog and Chapman one obtains the hydrodynamical level of description. Thus, on that level the description corresponds to Navier–Stokes equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0, \\ \left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} \right) u_i &= \frac{1}{\rho} \frac{\partial P_{ij}}{\partial x_j} + \frac{X}{m}, \\ \frac{3}{2} R \rho \left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} \right) T &= -\frac{\partial q_j}{\partial x_j} - P_{ij} \frac{\partial u_j}{\partial x_j}, \\ P_{ij} &= p_{ij} + \rho_{ij} p, \quad p = \rho RT, \\ p_{ij} &= \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_r}{\partial x_r} \right), \\ q_i &= -\lambda \frac{\partial T}{\partial x_i} \end{aligned} \tag{0.2.6}$$

and Euler's equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0, \\ \left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} \right) u_i &= -\frac{1}{\rho} \text{grad} \cdot p, \\ \frac{3}{2} R \rho \left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} \right) T &= -p \cdot \text{div} u, \\ p &= \rho RT. \end{aligned} \tag{0.2.7}$$

Following the general logic of the present exposition one might assume that dynamics of continuum, as a particular case of kinetical approach to the treatment of motion of a gas, possesses the features of statistical nature and permits the realization of statistical modeling, just what will be demonstrated below.

0.3 The Position of Monte Carlo Methods in Modern Mathematics

The singular features of Monte Carlo methods cited in the preceding section just lead to the necessity of marking the position of methods of the statistical modeling in modern mathematics. Undoubtedly, at the present moment

the priority is firmly kept by the traditional theoretical approaches (see works by Sadovnichij,^{258,259} Matrosov,²⁷⁰ Zhuravlev, Fljorov,²⁸⁵ and others) and finite-differential approaches (see Marchuk,²³⁶ Bakhvalov,^{235,247} Kholodov, Magomedov,²⁴⁹ Popov, Samarskii,^{252,254} Rudakov,²⁶⁴ Rusanov,^{265,282} Kostomarov, Tikhonov,^{260,262,271} Konovalov,²⁷⁴ and others) to the solution of equations of mathematical physics. But permanently in larger and larger degree are beginning to come true the prophetic words of academician Vladimirov spoken out by him more than half a century ago: "... will come the time when along the development of the computational technique the Monte Carlo methods will the more and more successfully compete with the traditional ones". And this time has already come in reality. The Monte Carlo methods have safely obtained their place in the list of traditional methods of theoretical and applied mathematics (see Vladimirov,³ Marchuk, Ermakov, Mikhailov, Sobol,^{6,33-40,236,237} Bird, Haviland,^{4,5} Kogan, Perepukhov,^{8,51} Belotserkovskii, Yanitskii⁹). It is likely that this tendency of expansion of Monte Carlo methods into the realm of modern mathematics will steadily last. Just at the present time there exists the whole number of regimes of the gaseous flows, which cannot be properly analyzed with the help of network algorithms. That is the class of problems connected with the simulation of flows in high-altitude hypersonic aerodynamics and with solution of the Boltzmann equation. Moreover, one can indicate certain cases, as, for example, the flow of rarefied gas about thin cold bodies, where Monte Carlo methods prove to be the only source of information on the aerodynamical characteristics of such bodies. It is impossible to simulate flows of such a type in the wind tunnels presently existing.

The modern stage of development of the computational technique, of the computational methods and of the programming is, first of all, connected with perfection of the parallel computations (see Evtushenko,²⁵⁶ Koroljov,^{271,273} Voevodin, Voevodin,²⁴ Ivannikov,^{239,248} Zabrodin,²³⁹ Pavlovskii²⁶⁸). The powers of modern computers reach the figures of hundreds of teraflops. The most powerful in the world is the platform BLUEGENE/L, created by the IBM company and projected for 596 teraflop. Accepted for realization in USA is the 5-year project uniting the efforts of the companies SANDIA, OAK RIDGE, Ministry of Energetics and the number of other ministries, aimed to a creation of the computational complex with the power of one exaflop (one million of teraflops). In this connection, the singular features of Monte Carlo methods indicated above acquire quite a new tincture. For this reason the present book cannot avoid the consideration of the prospect of parallelization of the algorithms of statistical modeling.

Nonuniform and anisotropical turbulent flows of fluid and gas represent the most frequently met in nature forms of the motion of matter. Such flows are met in micro-, macro- and megaworld. The laws of turbulent motions call

forth the processes in nanotechnologies, the dynamics of flight of flying apparatuses, influence the geophysical processes, the climatic changes, the evolution of stellar accumulations (see works by Velikhov, Popov, Belotserkovskii, Berdyshev, Vasin, Dymnikov, Iljin, Kholodov, Gushchin, Zhuravlev, Zhizhchenko, Chechetkin^{241–246,249–253,278,279,283}). The hope of using for the description of complicated unsteady flows the permanently increasing powers of the modern computers was not justified — just as it was warned 40 years ago by Anatilii Alexeevich Dorodnicyn. The absence of the adequate physical models for description of complicated flows of the fluid and gas cannot be substituted by teraflops of the modern processors. Therefore, in this book much attention is given to the methods of formation of the physical models of turbulence. Extremely useful proves to be the experience of formation of the models based on the general principles in various areas of physics, climatology, geophysics, navigation, turbulence (works by Velikhov, Popov, Dymnikov, Zhizhchenko, Petrov, Krasnoshchekov, Kostomarov, Pavlovskii, Savin, Vasin, Berdyshev, Malinetskii, Alexeev^{234,252–255,261,268,275–279,283,286}). Presented in this book are the original models of turbulence, such as kinetical molecular and fluidical models and the model of three-wave resonance.

The volume of this book does not permit to make a comparison of the methods of statistical modeling with such an important section of mathematical science as optimization problems which are closely connected with a solution of large systems of the algebraic equations (see Zhuravlev, Iljin, Moiseev, Evtushenko, Matrosov, Arutjunov, Eremin, Tyrtysnikov^{245,246,250,251,257,263,266–269,287}). These questions were considered in the preceding books of the present authors (see Khlopkov, Gorelov^{288,289}), which, unfortunately, became at the present moment the bibliographical rarity. Therefore, it is planned to come back to the questions of solution of the linear and nonlinear problems of algebra and of mathematical physics, to the optimizational and extremal problems, and it is planned to devote to these areas of science some special editions.

0.4 Short Survey of Monte Carlo Methods in Computational Aerodynamics

The great scientific and applied importance possessed presently by the dynamics of rarefied gases (DRG) is explained by the practical importance of the vast area of problems connected with the modern stage of mastering the space, with the development of vacuum technology, of laser technique, and with the other branches of scientific and technical progress. The methods developed in rarefied gas dynamics are widely applied to the solution of problems not connected with the rarefaction

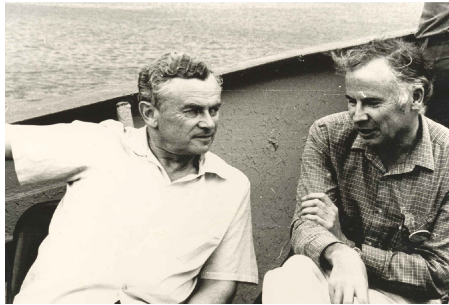
of matter — the theory of homogeneous and heterogeneous processes, the theory of evaporational and adsorptional processes, of the nonequilibrium flows, of the prescription and setting of the boundary conditions and coefficients of transfer in mechanics of continuum. The necessity of qualitative and numerical analysis of the phenomena in rarefied gas dynamics, the complexity, and multi-dimensionality of the equations which are to be dealt with, stimulated the development of effective and original numerical methods. The special features of physical phenomena which are met in DRG and of equations describing these phenomena (those are, mainly, equations of Boltzmann and of Navier–Stokes) lead to the imposition of the multitude of demands on the methods under development:

- Justification of the computational procedure and accuracy of the solution resulted, aimed at the use of that procedure as model one.
- The possibility of the effective modeling of complicated flows, such as three-dimensional flow about bodies in all the ranges of transitional regime, beginning with the free-molecular one and finishing with one for continuum, as well as taking into account physical and chemical properties of gases.

In accordance with the main demands the methods existing might be united into groups, determined by the degrees of their justification and by their connection with kinetical equations, as well as by degree of possibility of modeling the complicated phenomena. For inclusion into *the first group* one might mention, first of all, the regular methods — classical finite-difference approaches; semiregular methods with the use of Monte Carlo procedures for computation of collision integrals; and, finally, statistical procedures of the type of Ulam–Neumann, aimed at the solution of the kinetic equations. For inclusion into *the second group* might be singled out the methods of direct statistical modeling of the real flows. It is necessary to note that such a subdivision of methods occurs to be rather conditional, and between many of these methods is established an interconnection. According to our opinion, the main point in classification is, after all, the effectivity of solution of the complicated problems.

The concise retrospective of the development of methods might be presented in the following way. In the monograph by *Kogan*⁸ are presented the main computational methods of rarefied gas dynamics developed up to the mid-1960s. The analysis of methods developed somewhat later was given in the survey paper by Belotserkovskii,⁹ while the detailed description of the main approaches of statistical modeling is presented in the collection of papers and in monographs by Bird and Belotserkovskii.^{10,11,12} The description of regular and semiregular methods was given by *Ryzhov*.¹³ As it was already noted, speaking of the degree of justification of computational procedure one should mention, first of all, the regular

methods. Generally speaking, the essence of these methods consists in approximation of the distribution function by its values in the points of phase space and in subsequent solution of the difference equations. In addition to the natural demand of the ability of conservation of the large volume of information and of operation with that volume, the serious difficulties arise in connection with finite-differential approximation of the collision integrals. Just for that reason the natural stage of the development of methods was in many cases reduced to the use of Monte Carlo procedures for the computation of collision integrals. By application of these methods to Boltzmann equation a number of model solutions was obtained, mainly for spatially uniform and one-dimensional flows, as for example, by *Ender M., Ender A., Tcheremissin*,^{14,15} and for two-dimensional problems by *Tcheremissin, Shcherbak*.^{6,17} By the solution of modified kinetic equations the possibilities of methods are essentially amplified — see *Krook, Holway, Shakhov, Larina, Rykov, Limar, Huang*.^{18–26} The substitution of the collision integral by some simplified expression does in many cases permit to build up the computational procedure for collision integral at the level of macroparameters, and in such a way the effectiveness of the methods applied is considerably increased — see *Krook, Holway, Shakhov*.^{18–20}



J. Bird and O. Belotserkovskii. XIII International Symposium on dynamics of rarefied gas. Novosibirsk, 1983.

The complicated multi-dimensional structure of kinetic equations, on one hand, and the abundance of information brought by the distribution function, on the other hand, stimulated the application and development of statistical procedures for the solution of problems in rarefied gas dynamics. The first application of statistical methods was connected with direct modeling of gaseous flows — see *Haviland, Bird*.^{27–32} It should be immediately noted that the methods of direct statistical modeling proved to be the most effective in rarefied gas dynamics. In addition to reasons mentioned earlier, this property might be explained by the statistical nature

of kinetic equations. Among the methods of direct statistical modeling one is able to single out two approaches: the method of stationary direct statistical modeling by *Haviland*^{27–29} and the method of nonstationary direct statistical modeling by *Bird*.^{30–32} Since this work is devoted, mainly, to the statistical methods, let us briefly describe the essence of approaches mentioned above.

By the use of either of these methods, within the area of flow is chosen a certain volume, on the boundaries of which is by the usual way prescribed the form of distribution function and the law of interaction of gas with a surface. The area of computation is divided in cells, within each of which the distribution function is modeled by some quantity of particles. The sizes of cells are chosen on the basis of condition of constancy of distribution function over the cell's volume. The evolution of particles is divided in time in small intervals of the length Δt chosen from a condition $\bar{\xi}\Delta t \ll \bar{\lambda}$, where $\bar{\xi}$ and $\bar{\lambda}$ are characteristic values of velocity and mean free path of molecules. The main distinctive feature of the procedures under consideration consists in the fact that in the case of nonstationary modeling is realized the simultaneous watching at the whole ensemble of particles. This behavior permits to construct the particle's trajectories taking into account the varying in time frequency of collisions and leads to some stabilization process. In the case of stationary modeling, the watching is realized for singular, so called trial, particles, which in fact leads to a necessity of knowing the distribution function for field particles, and, correspondingly, to some iterational process. Both approaches admit the number of modifications of the principal character, which are essentially increasing their effectiveness and lead to their successful use for three-dimensional problems. Generally speaking, the direct modeling of gaseous flows proves to be the universal tool of studies not only in the area of rarefied gas, but also, as it is shown in the present book, in mechanics of continuum. However, one of the positive qualities of direct modeling — solution of the problems without addressing to the equations — proves sometimes to be also its main negative property. The lack of a direct connection with the equation describing the process evokes the certain mistrust to the results obtained and leads to certain difficulties in systematic approach to the increase of method's effectiveness. For this reason, the works on justification and settlement of correlation between statistical procedures controlling equation. The well-known statistical procedure by Ulam — Neumann for the solution of integral equations and widely applied in the theory of radiation (see *Marchuk, Ermakov, Mikhailov, Sobol*^{33–35}) might be directly applied to kinetic equations only in the case of linearized kinetical equation (see *Khlopkov*³⁶). In nonlinear case (see *Ermakov, Nephedov*^{37,38}) the modification of procedure by Ulam–Neumann was proposed on the basis of theory of branching processes. However, the practical realization of this method was connected with large amount of

computations and proved to be rather difficult. The construction of standard procedure by Ulam and Neumann for nonlinear equation demands to carry out the artificial linearization, and this leads to an iterative process, to keep in memory the information on preceding iteration, and, correspondingly, to a division of phase space in cells, which leads to appearance of an additional source of errors and does not enter as necessary part into methods by *Khlopkov, Ivanov* and *Grigorjev*.^{39,40} The procedure, constructed in such a way, corresponds to the method of stationary statistical modeling and this fact was used for the formation and justification of the methods by *Khlopkov* and *Ivanov*.^{39,40} A somewhat more complicated situation arises in connection with justification of the method of nonstationary modeling. Devoted to the determination of its connection with a solution of kinetic equations are the works by *Belotserkovskii* and *Yanitskii*.^{9,12} After all, in the practical realization the preference is rendered to the methods of direct statistical modeling. Just with the help of these methods were solved the most of extremely complicated problems of practical importance. The modernization of the methods of stationary statistical modeling was realized, mainly, by way of cutting down the operative memory of a computer. Thus, in the papers by *Vlasov*^{41,42} proposed is the procedure of construction of trajectories which does not demand conservation in memory of the distribution function. The corresponding idea is based on the fact that density of probability of the velocity of a field molecule is equal to the distribution function we are looking for, which is normalized over unity. As the other direction of increase of the method's effectiveness appears the approximation of the distribution function of field particles with the help of a certain number of moments. The vast possibilities for the improvement of the methods of stationary modeling are found by means of use of the model kinetic equations (see *Khlopkov, Ivanov*^{39,40}). In this case, the realization of the procedure of computation of collisions does not demand a knowledge of the distribution function of the field particles, because after collision the trial particle acquires the velocity corresponding to the distribution function in equilibrium.

As the central point in the method of nonstationary statistical modeling appears the procedure of calculation of collisions. The pair of particles is chosen for collision in the correspondence to the frequency of molecular collisions, but independently of the distance between particles within the cell considered. The velocities of particles after collision are chosen in correspondence with the laws of molecular interaction. In spite of the fact that method's effectiveness depends on comparatively numerous amount of the parameters of calculation scheme (stabilization, splitting in time, achievement of the steady regime, step in time, step of the spatial net, and so on), the main works on the method's improvement are devoted to the perfection of a collisional procedure and to the diminishment of a statistical error

of the scheme as a principal factor permitting to diminish a number of particles in cells, and thus to diminish the operative memory of a computer. For example, in the paper by *Eropheev* and *Perepukhov*⁴³ was proposed a modification of collisional procedure for Maxwellian molecules, by the use of which the computational results are, practically, independent of the number of particles in cell when this number varies between 40 and 6 (in the traditional computations the number of particles in cell is of the order of 30). In the papers by *Belotserkovskii* and *Yanitskii*^{44–49} proposed was the method, in which at the stage of collisions the subsystem of model particles is considered as the N -particle model of Kac. The modeling of collision is reduced to a statistical realization of the evolution of Kac's model during the period of time Δt . The time of collision in Kac's model is calculated in correspondence with statistics of collision in perfect gas. This scheme permits to use essentially smaller number of particles in cell and smaller step of computational network. The analysis of results of the calculations has shown that these results are practically independent on the number of particles in cell up to the value of 2. As it was already noted, in the practical realization for the problems of rarefied gas dynamics the statistical methods proved to be more effective in comparison with regular methods and semiregular ones. For the problems of flow about objects, which are the most essential in aerodynamics, these methods were, first of all, successfully applied by *Perepukhov*^{51,52} for the obtainment of aerodynamical characteristics of various, including complicated, bodies in the free-molecular flow, and in the flow, close to free-molecular one. In this direction, with the help of statistical methods based on stationary and nonstationary approaches, one was able by the solution of problems of flow about objects to advance to the *Knudsen* numbers up to the order of 0.001 in the planar and axisymmetrical cases (see *Khlopkov*, *Eropheev*, *Perepukhov*, *Ivanov*, *Vlasov*, *Gorelov*^{39,40,53–69}), as well as in three-dimensional cases (see *Eropheev*, *Kravchuk*, *Serov*, *Khlopkov*, *Ivanov*^{70–76,100}). According to all the evidences, the application of statistical modeling in its traditional form with the aim of penetration in the area of the mechanics of continuum proves to be ineffective with the contemporary computational background. And since the contemporary stage of development of the aerocosmic technique demands, nevertheless, to obtain the information within the whole range of transitional regime, then the flows of slightly rarefied gases demand, for their treatment, that some special methods of solution would be developed. Thus, of a certain interest are the methods which use the information on distribution function obtained on the basis of the physical considerations connected with continuum character of the matter. One of such directions is reduced to a solution of the equations for moments, of which the order is higher than that of Euler and Navier–Stokes equations. Up to the present moment, however, stays to be open the question whether the obtained improvement of accuracy

would overpower the considerable complication of the corresponding macroscopic equations and difficulties in setting the boundary conditions.



Participants of the International Symposium on dynamics of rarefied gas in Novosibirsk, 1983. At center — V. Yaniyskiy, Yu. Khlopkov, M. Ivanov.

The other direction of investigation is connected with a simultaneous solution at the subsequently posed elementary intervals of time of both kinetic and continuum equations, thus obtaining the results leading to mutual complementations and improvements of accuracy. However, following in this direction one sees that to the difficulties of solution of the kinetic equations are, certainly, added the difficulties of solution of the Navier–Stokes equations, and just for that reason this method is applied only to one-dimensional problems. It seems to be more effective to single out within the bulk of a flow the certain areas with different physical properties, governed by the equations of different types, which are knitted together at the boundaries of these areas. Such a trick is widely used in mechanics of continuum (see *Sychev*⁵⁰), but presently was not yet extensively spread in computational dynamics of rarefied gas and is presented only by some isolated works, like that by *Khlopkov*.⁷⁰ Furthermore, it seems to be extremely interesting and deserving of the further development that the computational methodologies developed in rarefied gas dynamics would be extended to such nontraditional areas of application as viscous and nonviscous flows of continuous matter. In particular, such a way of action permits to develop a unique computational procedure which would be independent of the degree of rarefaction of the matter.

In this connection of certain interest are the methods based on modeling the continuous matter by the ensemble of particles (see *Belotserkovskii*, *Harlow*, *Khlopkov*,

Kravchuk^{12,70,71,74,77,79–82}), which would possess the proper peculiarities and the aggregate of which would characterize the matter under consideration. Thus, in methods by *Harlow*, *Gentry* and *Belotserkovskii*^{12,79,80} the particles are representing the Lagrangian form of description of the flow of perfect gas, while in the papers by *Pullin*, *Khlopkov* and *Kravchuk*^{74,81} the continuum is modeled by the molecular distribution function. Generally speaking, the use of statistical approach in the description of a continuous matter with the help of the particles ensemble permits, on the one hand, to use the experience obtained in computational dynamics of rarefied gas, and, on the other hand, to develop a unified procedure of computation for all the regimes of flow (see *Kogan*, *Khlopkov*^{82,83}). Finally, it is impossible not to note the practically important direction of the development of computational methods based on the hypothesis of locality (see *Barantsev*, *Galkin*, *Eropheev*, *Tolstykh*, *Bunimovich*, *Bass*, *Khlopkov*^{84–96}). These methods appear as approximate and semi-empirical ones, permitting the effective obtainment of the integral aerodynamical characteristics of the apparatuses at all the regimes of flow.



J. Bird and Yu. Khlopkov. XXV International Symposium on dynamics of rarefied gas. Saint Petersburg, 2007.

0.5 Construction of the Effective Methods of Statistical Modeling

It is clear that at the present time the central place in studies on rarefied gas dynamics belongs, quite certainly, to the methods of direct statistical modeling. The main portion of each of these methods consists in modeling such a procedure of molecular collisions which would be able to increase just in several orders the computational speed and to diminish the volume of operative memory of the computer, when the comparison is made with its initial version. However, by the consideration

and substantiation of the application of these methods it is impossible, practically, to avoid the survey of that kinetic equation which describes the phenomenon to be modeled. The formalization of connection between statistical procedure and solution of the kinetic equation is inevitable due to a number of reasons. First, it is needed for a solution to be trusted, and for the results obtained to be used as a sample ones, since the solutions of numerous typical problems were obtained initially just by the methods of direct modeling, and up to the present moment were not repeated with the help of other methods. Second, the determination of the interrelation between modeling and solution of the equation leads to a possibility of using the well-developed apparatus of the numerical, both regular and statistical, methods of solution of the equations of mathematical physics for the analysis of the methods and improvement of their effectiveness. And, third, such a way of action permits to formulate a certain general approach to the construction of methods and firmly excludes any false modifications of these.

It is to be stressed that on the way of development of the effective numerical algorithms the complexity of the practical problems of high-altitude aerodynamics demands, inevitably, to bring home the whole arsenal of the analytical, experimental, and numerical means of investigation of the flows of rarefied gases. In this connection, acquires the special value the analysis of kinetic equation and study of various models of it. Frequently used are the approximate representations of the collisional integral and of the distribution function. The most widespread approximate forms of kinetic equations are:

— The model equation by *Krook*¹⁸:

$$\frac{df}{dt} = \nu(f_0 - f), \quad (0.5.1)$$

where ν is the frequency of collisions,

$f_0 = n \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-m/(2kT)(\vec{\xi}-\vec{v})^2}$ is the equilibrium distribution function.

— The ellipsoidal model by *Holway*¹⁹:

$$\frac{df}{dt} = \nu(f_e - f), \quad (0.5.2)$$

f_e — the ellipsoidal distribution function.

— The approximational model by *Shakhov*,²⁰ which, unlike the preceding models, gives the correct Prandtl number Pr :

$$\frac{df}{dt} = \nu(f^+ - f), \quad (0.5.3)$$

$f^+ = f_0 \left[1 + \frac{4}{5} (1 - Pr) s_\alpha c_\alpha (c^2 - \frac{5}{2}) \right]$, $s_i = \frac{1}{n} \int c_i c^2 f d\vec{\xi}$, c is dimensionless molecular thermal velocity.

Just at the same point it is necessary to mention the linearized Boltzmann equation, which is rigorously deduced from the complete Boltzmann equation under the condition that distribution function is only slightly different from equilibrium one — see *Kogan*⁸:

$$\frac{d\phi}{dt} = k(\vec{\xi})\phi + \int L(\vec{\xi}, \vec{\xi}_1)\phi_1 d\vec{\xi}_1, \quad (0.5.4)$$

where $f = f_0(1 + \varphi)$, $\varphi \ll 1$; $k(\vec{\xi})$ and $L(\vec{\xi}, \vec{\xi}_1)$ are some known functions of molecular velocities, dependent on the kind of particles.

In distinction of the linearized equation the model ones do not rigorously follow from the Boltzmann equation. Moreover, the model equations are found to be significantly more nonlinear than initial one, but in practical realization by the numerical modeling these equations might prove to be simpler. Naturally, by their practical realization the methods of direct statistical modeling based on approaches by Bird and Haviland proved to be more effective, and their modifications with alternating success realized their victorious train in computational aerodynamics. At the present moment, the unconditional priority belongs to the Bird's method. Due to the works of Russian scientists *O. Belotserkovskii*, *V. Yanitskii*, *M. Ivanov*, *V. Perepukhov* and *A. Eropheev*,^{12,10–20} the modifications of Bird's method permitted to increase the effectiveness of that method, actually in several orders of value. The main feature of the method consists in the assumption that system's evolution at the small interval of time Δt is splitted in two quite obvious physical processes:

(1) relaxation in accordance to the collisional operator in kinetic equation:

$$\frac{\partial f}{\partial t} = J(f),$$

(2) free-molecular transfer,

(3)

$$\frac{\partial f}{\partial t} = -\vec{\xi} \nabla f.$$

This is well-known scheme of the first-order splitting in Δt for any arbitrary operator equation, but in the present case the advantage of scheme consists in the fact that it is splitting the dynamics of extremely complicated kinetical system in two obvious physical processes. The distribution function is modeled with the help of N particles, which at the first stage collide between themselves within each cell and in accordance with collisional frequency, during the time interval Δt , while at the second stage they fly during Δt , covering the distance $\vec{\xi}_0 \Delta t$.

The central point in the method of nonstationary statistical modeling lies in procedure of calculation of the collisions. The pair of particles for collision is selected in accordance with frequency of molecular collisions and independently of the distance between these molecules within the cell chosen. The velocities of particles after the collision are selected in accordance with the laws of interaction between molecules. In spite of the fact that method's effectiveness depends on comparatively large number of parameters of the computational scheme (steadification, splitting in time, taking out to the steady regime, time-step, type of the spatial network, and so on) the main body of work on the method's perfection was devoted to the improvement of collisional procedure and to the diminishment of a statistical error of the scheme as a main factor, which would permit to diminish the number of particles within the cells and, correspondingly, to diminish the operative memory of a computer and to minimize the computational time. Thus, proposed in Ref. 18 was the modification of collisions for one particular case — Maxwellian molecules. By that modification the computational results do not, practically, depend on the number of particles within the cell, if that number varies between 40 and 6 (by the computations with the help of ordinary methods this number is of the order of 30). Proposed in Refs. 11–16 is the general method, independent of the kind of molecules, in which at the stage of collisions the subsystem of particles within each cell is considered as the N -particle model by Kac⁶:

$$\frac{\partial \phi_1(t, \vec{\xi}_1)}{\partial t} = \frac{N-1}{N} \int [\phi_2(t, \vec{\xi}'_1, \vec{\xi}'_2) - \phi_2(t, \vec{\xi}_1, \vec{\xi}_2)] \cdot g_{12} d\sigma_{12} d\vec{\xi}_2.$$

Modeling of a collision is reduced to the statistical realization of evolution of the equation, however not of the Boltzmann's one (0.2.1), but of the Kac's model (0.2.5), during the interval Δt . The duration of collision in Kac's model is calculated in accordance with statistics of collisions in ideal gas consistent with the scheme of Bernoulli. This scheme permits to use essentially diminished number of particles within the cell and smaller size of step in the computational network. As it was shown by the analysis of results of the calculation, these results do not, practically, depend on the number of particles within the cell, up to the number of 2. The reason of that follows from the fact that Boltzmann equation demands, imperatively, the assumption of the molecular chaos to be fulfilled. However, with such a number of particles in cell, as is accessible in nowadays computers, the assumption of chaos is fulfilled only with a systematical error, whereas Eq. (0.2.5) is free of such a demand and, therefore, the stage of collision is computed as a purely Markovian process. From the other side, however, by $N \rightarrow \infty$ exists the complete equivalence between Kac's model and spatially uniform equation by Boltzmann.

Thus it might be said that the approach developed by Belotserkovskii and Yanitskii:

- (1) Opens the way to a construction of the effective computational schemes, which would provide the possibility of solution of the three-dimensional problems of aerodynamical flow about objects.
- (2) Permits to solve the most important methodological problem of the equivalence of a numerical method to a solution of the kinetic equation.

There exists a tremendous number of works on the traditional use of statistical modeling and, therefore, we shall limit ourselves, mainly, by the problems of aerodynamics. As it was already noted, in a practical realization of solution of the problems in rarefied gas dynamics the statistical methods proved to be more effective than regular ones and semiregular ones. For the problems of a flow about objects, which are the most essential in aerodynamics, these methods were, for the first time, successively applied to the obtainment of aerodynamical characteristics of various bodies, including complicated ones, in a free-molecular or nearly free-molecular flow. The corresponding methodics, developed more than 20 years ago, is presently brought to the state of standard programs and is widely used in the pertinent project and design institutions. The advance to lesser numbers Kn is connected with a sharp increase of computational difficulties due to a lesser free path of molecules and, consequently, to lesser steps in time and in space, and, in the case of direct modeling, due to an increased number of the particles modeling the distribution function.

As it was noted previously, at the present moment the indisputable priority belongs to the modern methods based on the Bird's approach to the modeling of dynamics of "molecular ensemble". But such a situation was not invariable. There was a period when the priority belonged to the method of "trial particles" based on the approach by Haviland. Probably, in the future will appear the effective scheme by this author, as it was already earlier, which would overpower those effective schemes by Bird's approach, which were mentioned above. Moreover, might appear, also, some new class of problems for which these schemes will prove to be preferable. But just at the present time one might single out some problems of physical chemistry for which the preference is given up to the method of trial particles. Certainly, there exists also a class of linear problems which happened to be, actually, the origin of this method.² And there is one obvious additional advantage of this method, consisting in the fact that, in distinction to the Bird's method, for it is not very important to obtain a complete identity of its solution and that of a kinetic equation. As concerns the computational aerodynamics, this method is based on the linearized Boltzmann's equation (0.5.4).

The conversion of computations into action on parallel lines with the help of high-performance supercomputer systems stays as one of the main directions in development of the modern computational mathematics (see *Voevodin, Voevodin, Ivannikov, Zabrodin, Kraïko*^{226,231,238,239,240,248}). The supercomputer systems are permanently more and more widely used for a solution of fundamental and applied problems in the fields of nuclear physics, climatology, economics, pharmacology, modeling of the training devices and of virtual reality, computational aerodynamics. Due to the special qualities of Monte Carlo methods, in all the areas cited above the statistical modeling begins to play the ever-growing and outstanding part.