

Monte Carlo method in problems of atmospheric optics

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A concise retrospective analysis of works reflecting the history of the Monte Carlo method development in Siberian Branch of RAS is presented. The theoretical school founded in the middle of 70s of the last century by Academician G.I. Marchuk mainly contributed in producing and promoting of new efficient methods and algorithms of statistic modeling. Many-year cooperation of physicians of the Institute of Atmospheric Optics and the Institute of Computation Mathematics and Mathematical Geophysics SB RAS allowed a solution of many problems of the atmospheric optics and hydrooptics, quantitative justification of potentialities of optical-location systems, and a forecast of a series of new physical effects.

Introduction

The appearance of the statistical simulation methods was historically caused by extreme circumstances related with the necessity of fast estimation of critical parameters of the first nuclear reactor. This problem implied numerical solution of integrodifferential transfer equation under complicated boundary conditions. The methods for solving the transfer equation available to that time (1944, the height of the World War II) were inconsistent. A group of excellent mathematicians, J. von Neiman, S. Ulam, and N. Metropolis proposed principally new approach in the framework of the closed state project "Monte Carlo," based on the idea that the complicated process of multiple scattering of a neutron is virtually splitted into a sequence of independent random events admitting elementary probability description. The Markovian chain of random motion of an individual neutron stops in the case of its absorption or flying beyond the limits of an active medium. Thus, the model trajectory of the neutron was associated with a sequence of random events. Multiple numerical realization of the model trajectories made it possible to obtain a mean statistical estimate of the sought functionals with a known error.

Obviously, the closeness of such numerical experimental results to the natural analogue is determined by the quality of random numbers representing real physical events, which form the process of neutron (or other particles) diffusion. Obtaining the sought estimates with admissible variance requires multiple repetition of the sequence of relatively simple arithmetic operations, i.e., an essential calculative resource. Two these problems predetermined the further history of development of the Monte Carlo method.

The name of the method came into practice of mathematical physics after the appearance of the first open paper by Metropolis and Ulam.¹ During

following 10–15 post-war years, the Monte Carlo method has acquired an unusual popularity, especially in the field of nuclear power engineering,^{2–5} vast bibliography of early researches is presented in Ref. 3. However, the method was ahead of its time, and its effective use for solving complicated multi-dimension problems has been retarded many years because of limited capabilities of the available calculative technique. Now there is some renaissance of the Monte Carlo method. The avalanche-like amount of papers in different fields of science and technique, economics, calculative mathematics, ecology, medical tomography, and so on is the evidence of this fact.

In this paper we consider only retrospective analysis of the work carried out in Siberian Branch of Russian Academy of Sciences in the field of applications of the Monte Carlo method to the problems of atmospheric optics.

1. Main definitions; calculation of brightness of the twilight aureole of the Earth

The system of algorithms and programs for calculating the brightness field of the scattered solar radiation in the Earth atmosphere^{6–9} was developed under the direction of G.I. Marchuk in Computing Center of Siberian Branch of the Academy of Sciences of USSR (now Institute of Computational Mathematics and Mathematical Geophysics SB RAS). The possibility of application of the Monte Carlo method to the problems of atmospheric optics was theoretically justified. Further these investigations were generalized in a series of monographs [Refs. 30, 33, 49, 51, 55, 56, 58, 65, 72, 98].

Specific peculiarities of the radiative interaction of the short-wave optical radiation with a medium put the requirements to the technique for statistical simulation. General physical statement of the

problem is the following^{8,33,51} The process of radiation transfer from some source in the atmosphere is under consideration. Radiation sources can be both external (solar radiation) and internal (local or distributed over the volume). Optical radiation inside the atmosphere is absorbed, scattered or reemitted due to elastic and inelastic interaction with aerosol and gaseous components of the atmosphere and the underlying surface. As a result, there appears a transformation of spatial-angular distribution of radiation, as well as a change of the state of polarization and redistribution of the light energy over the frequency spectrum. In case of sources of non-stationary radiation of high intensity (lasers), a necessity appears of additional accounting of the whole class of non-linear optical phenomena.

In the simplest case of stationary transfer of monochromatic radiation, its intensity at any point of the scattering medium satisfies the 3D-integro-differential transfer equation $\mathbf{r} = \mathbf{r}(x, y, z)$

$$\omega \nabla I(\mathbf{r}, \omega) = -\sigma(\mathbf{r})I(\mathbf{r}, \omega) + \frac{1}{4\pi} \int_{2\pi} I(\mathbf{r}', \omega') G(\mathbf{r}, \omega', \omega) d\omega' + I_0(\mathbf{r}, \omega), \quad (1)$$

where $I(\mathbf{r}, \omega)$ is the intensity of radiation at the wavelength λ at the point \mathbf{r} in the direction $\omega(a, b, c)$; $a^2 + b^2 + c^2 = 1$; $I_0(\mathbf{r}, \omega)$ is the source function, $G(\mathbf{r}, \omega', \omega)$ is the volume coefficient of the elastic monochromatic scattering in the direction $\vartheta = \omega' \cdot \omega$; $\sigma(\mathbf{r}) = \sigma_a(\mathbf{r}) + \sigma_s(\mathbf{r})$ is the extinction coefficient, σ_a , and σ_s are the absorption and scattering coefficients, respectively.

Generally speaking, realization of the Monte Carlo method is not connected with solution of the integro-differential equation (1), however, general principles of enhancement of the efficiency of specific simulation algorithms are based on the analysis of this equation, preferably, in the integral form.^{30,33,34} The transfer equation just in the integral form takes the probability character representing the ideology of the Monte Carlo method. Really, from the probability standpoint, the process of photon diffusion can be interpreted as the homogeneous Markovian chain, the successive states of which are the "positions" of the photon ($\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N$) in the given phase space X ; \mathbf{x}_N is the state just before emission of the photon from the medium or absorption. The process is completely defined provided that the density of initial collisions $\psi(\mathbf{x})$, the density of transition $k(\mathbf{x}', \mathbf{x})$ from the point \mathbf{x}' to the point \mathbf{x} , and the probability of absorption $p(\mathbf{x})$ at the point \mathbf{x} are known. These functions should satisfy the following conditions:

$$\psi(\mathbf{x}) \geq 0, \quad k(\mathbf{x}', \mathbf{x}) \geq 0, \quad \int_X \psi(\mathbf{x}) d\mathbf{x} = 1, \\ \int_X k(\mathbf{x}', \mathbf{x}) d\mathbf{x} = 1 - p(\mathbf{x}') \leq 1 \text{ for all } \mathbf{x}' \in X.$$

The density of transition for such chain has the form^{33,65}:

$$k(\mathbf{x}', \mathbf{x}) = \Lambda(\mathbf{r}') \frac{e^{-\tau(\mathbf{r}', \mathbf{r})} \sigma(\mathbf{r}) g(\mu)}{2\pi |\mathbf{r}' - \mathbf{r}|^2} \delta(\omega - s_0), \quad (2)$$

where $\tau(\mathbf{r}', \mathbf{r})$ is the optical length of the fragment $[\mathbf{r}', \mathbf{r}]$; $g(\mu)$ is the scattering phase function, $\mu = s_0 \omega'$; $s_0 = (\mathbf{r} - \mathbf{r}') / |\mathbf{r} - \mathbf{r}'|$; $\Lambda = \sigma_s / \sigma$ is the single scattering albedo. Then the integral transfer equation corresponding to Eq. (1) written for the density of collisions $f(\mathbf{x})$ has the form

$$f(\mathbf{x}) = \int_X k(\mathbf{x}', \mathbf{x}) f(\mathbf{x}') d\mathbf{x}' + \psi(\mathbf{x}). \quad (3)$$

The density of collisions $f(\mathbf{x})$ is connected with the radiation intensity (or the flux density) $I(\mathbf{x})$ by the relationship $f(\mathbf{x}) = \sigma(\mathbf{r})I(\mathbf{x})$.

Equation (3) is often used in the operator form

$$f = Kf + \psi, \quad (4)$$

where K is the integral operator with the kernel $k(\mathbf{x}', \mathbf{x})$.

According to the known principle of compressing images, fulfillment of the condition $\|K^n\| < 1$, where n is a natural number, is sufficient for the existence, uniqueness, and continuity of solution of Eq. (4). The operator K^n is defined by the formula

$$[K^n f] = \int_x \dots \int_x \Psi(\mathbf{x}_0) k(\mathbf{x}_0, \mathbf{x}_1) \dots k(\mathbf{x}_{n-1}, \mathbf{x}) d\mathbf{x}_0 \dots \mathbf{x}_{n-1}. \quad (5)$$

In the space L_1 of the integrated functions

$$\|K\|_{L_1} \leq \sup_r \Lambda(\mathbf{r}'). \quad (6)$$

Hence, at $\Lambda(\mathbf{r}') \leq \Lambda_0 < 1$ $\|K\|_{L_1} < 1$. The source of initial collisions in the problems of the theory of optical radiation transfer often has a generalized density, so it is expedient to consider Eq. (3) with the kernel (2) in the wider space N_1 of the generalized densities of the limited variation measures. Obviously, for a limited medium $\|K^2\|_{L_1} < 1$ and $\|K^2\|_{N_1} < 1$, are always true, even at $\Lambda(\mathbf{r}') \equiv 1$. All real scattering media are limited in space, and, hence, a solution of the transfer equation exists in such media: it is single and continuous. Thus, at fulfillment of the condition (6), it is rational to search for the integral equation (3) solution in the form of the finite Neuman series:

$$f = \sum_{n=0}^{\infty} K^n \psi, \quad K^0 \psi = \psi. \quad (7)$$

Different integral parameters of the transfer process can be represented, as a rule,^{33,65} in the form of linear functionals of the solution (7):

$$I_{\varphi^*} = (f, \varphi^*) = \int_{\tilde{X}} f(\mathbf{x}) \varphi^*(\mathbf{x}) d\mathbf{x} = \sum_{n=0}^{\infty} (K^n \psi, \varphi^*), \quad (8)$$

where the function $\varphi^*(\mathbf{x}) \geq 0$ is determined by the character of the calculated functionals.

It directly follows from Eq. (8) that for estimation of the sought functionals it is necessary to calculate the mathematical expectation

$$I_{\varphi^*} = M\xi, \quad \xi = \sum_{n=0}^N \varphi^*(x_n). \quad (9)$$

However, as it was shown in practice, such simulation scheme called direct or analogue, is acceptable for solving very simple model problems, for example, for estimation of the integral flux of diffusely reflected or transmitted radiation by a layer of a scattering medium. So called "weight" methods were used even in early papers⁶⁻⁸ for solving more serious problems, where the Markovian chain was simulated, being more rational from the standpoint of the variance of the estimate, but, generally speaking, not reflecting the physics of the process. Unbiasedness of the sought estimate is reached here by the use of special weights Q_n :

$$\xi = \sum_{n=0}^N Q_n \varphi^*(x_n). \quad (10)$$

Corresponding member of RAS G.A. Mikhailov with colleagues made the determining contribution^{9,10,13,17,18,24,30,40,43,44,55,70,82,98} in further development of the "weight" methods.

First realistic estimates of the spectral brightness of twilight aureole of the Earth in the range 0.45–0.8 μm were obtained by the Monte Carlo method^{7,8,37} using the weight algorithms of the type (10) for boundary conditions representing the scheme of the real experiment on remote optical sensing of the atmosphere from the spaceship "Vostok-6." The results of calculations are in good qualitative agreement with the data of field measurements.

2. Solution of non-stationary problems of the optical radiation transfer theory

The efficiency of the new statistic approach to solving the complex problems of atmospheric optics demonstrated in Refs. 6–8 stimulated an extension of the range of optical-physical applications of the Monte Carlo method. Researches were started at the Institute of Atmospheric Optics, related with applications of the Monte Carlo methods to solving the problems of the pulse laser radiation propagation in the atmosphere. The special class of problems

requiring the quantitative estimates of high accuracy was connected with invention of promising systems for laser sensing of atmospheric parameters. Physical specificity of optical radar researches required essential modification of the traditional Monte Carlo algorithms and development of new approaches. In particular, following Eqs. (9) and (10), the sought functional I_{φ^*} estimates the number of collisions in the range of detector $D^* \subset X$, if

$$\varphi^*(x) = \begin{cases} 1, & x \in D^*, \\ 0, & x \notin D^*. \end{cases} \quad (11)$$

In actual problems, the detector phase volume in the space of coordinates and directions is, as a rule, small, therefore, rare collisions in this space cause a great statistical error in the analogue methods of the form (9). One of the effective weight methods enabling one to overcome the appearing difficulties is the method of the flux local estimation.

Assume that for each state of the chain of photon wandering $\{x_n\}$, one of the events can give the effective value $\varphi(x)$, where $x \in D^*$, before the character of the event is revealed. In this case the corresponding estimate⁵ of \hat{I}_{φ} can be obtained, if the contribution from each collision, determined by the photon statistic "weight," to multiply by the probability density of the required event and to summarize over all states of the chain, i.e.,

$$\hat{I}_{\varphi} = \frac{1}{N_i} \sum_{i=1}^{N_i} \sum_{n=1}^N \omega_n \tilde{k}(x_n \rightarrow x^*). \quad (12)$$

It is shown^{10,11} that the transfer kernel for non-stationary atmospheric optical problems takes the form

$$\tilde{k}(x \rightarrow x^*) = \frac{\Lambda(\mathbf{r}) \exp[-\tau(\mathbf{r}, \mathbf{r}^*)] g(\mu^*)}{2\pi |\mathbf{r} - \mathbf{r}^*|^2} \times \\ \times \delta(\omega^* - \frac{\mathbf{r}^* - \mathbf{r}}{|\mathbf{r}^* - \mathbf{r}|}) \delta \left[t^* - \left(t + \frac{|\mathbf{r}^* - \mathbf{r}|}{c} \right) \right]. \quad (13)$$

The presence of the factor $1/|\mathbf{r} - \mathbf{r}^*|^2$ leads to infinite variance of the estimate (12) if the detector is placed within the limits of the scattering medium. To overcome this difficulty, special techniques were developed^{11,12,24,33,49} for selection of the points $\mathbf{x}^*(\mathbf{r}^*, \omega^*, t^*)$ in the volume of the detector D^* . In a certain class of the problems of laser sensing of atmospheric aerosol, the compensation of the factor $1/|\mathbf{r} - \mathbf{r}^*|^2$ is reached by instrumental correction of the estimated functional.²⁶ The value of the probability $\tilde{k}(x \rightarrow x^*)$ is essentially determined by the range of variations of the angular scattering function. This range for coarse atmospheric hydrometeors (cumulus clouds, rain, hail) reaches a few orders of magnitude.

When estimating the temporal configurations of the optical signal, this leads to noticeable statistical fluctuations. To smooth them, many millions of realizations are required.

Calculational economy is increased by application of another weight method – “simulation by value.”^{17,18,30,33,49,55} In the scattering regimes close to deep, the asymptotic solution of the Miln problem^{18,49} can be used as a value function. The weight estimate^{32,72} gives good results in the range of active optical thickness $\tau = 1.0 - 10.0$.

In statistical imitation of the laser ranging systems, especially in the case, when the receiver and transmitter are spatially remote, such states of the chain $\{\mathbf{x}_n\}$ are possible, when none of the possible random $\{\mathbf{x}_n\}$ extension leads to non-zero estimate, i.e., $\tilde{k}(x_n \rightarrow x^*) = 0$. Under such boundary conditions it is expedient to extend the estimate to two forward collisions by selection of an intermediate point within the limits of angular size of the detector \mathbf{V}^* , i.e., using the value $\tilde{k}(x_n \rightarrow x')\tilde{k}(x' \rightarrow x^*)$, instead of $\tilde{k}(x_n \rightarrow x^*)$, where $x' = (\mathbf{r}', \omega', t')$ and $\omega' \in \mathbf{V}^*$.

The idea of realization of such algorithm was proposed in Ref. 14, caused by a physical necessity of more effective taking into account intermediate collisions of the photons in the area of reflector of finite size. The applicability of the algorithm under different boundary conditions is justified more completely in the monograph.³³ The transfer equation (4) can be written in the following equivalent form:

$$f = K^2 f + K\Psi + \Psi. \quad (14)$$

Let Ψ be the density of fictitious collisions equivalent to the particle flux incident on the medium. Then the density of collisions $K\Psi$ corresponds to non-scattered flux in the medium. Therefore, the double local estimate of the radiation intensity at the given point of the phase space is determined by the formula

$$I(x^*) = \int_X \frac{\tilde{k}_1(x \rightarrow x^*)}{\sigma(x^*)} f(x) dx, \quad (15)$$

where

$$k_1(x \rightarrow x^*) = \int_X k(x \rightarrow x')k(x' \rightarrow x^*) dx'.$$

The methodology of statistical simulation developed for the problems of pulse laser radiation transfer^{10,12,14,25} was used in solving the specific scientific-technical problems. In particular, the interrelation between the envelope shape of the reflected pulse and the optical-geometric conditions of the laser sensing was comprehensively studied first in Refs. 16, 20, 23, 26; the potentialities of optical radar systems were quantitatively justified in Refs. 27, 52, 76, 77. A validity of the obtained statistical estimates was confirmed many times by comparison with the data of field experiments.^{15,50,51,58,72}

3. Solution of the vector transfer equation

To solve with greater accuracy the problems of the theory of optical radiation transfer in disperse media, equation (1) should be considered in generalized form with accounting for transformation of the radiation polarization parameters. Among numerous ways of description of the light polarization properties, the most convenient for corpuscular theory of transfer is the Stokes formalism proposed in 1852. The author introduced four parameters: I, Q, U, and V, having the dimension of intensity and determining the intensity, degree of polarization, plane of polarization, and the degree of radiation ellipticity.

Note that independent use of these parameters essentially extends the information content of direct and inverse problems of radiative physics. In the transfer theory they are usually considered as components of the Stokes vector-parameter $\mathbf{F}(I, Q, U, V)$ in a four-dimension functional space. The non-stationary transfer equation in the vector form can be written as follows^{33,36,86}:

$$\begin{aligned} & \frac{1}{c} \frac{\partial \mathbf{F}(\mathbf{r}, \omega, t)}{\partial t} + \omega \nabla \mathbf{F}(\mathbf{r}, \omega, t) = \\ & = -\mathbf{A}(\mathbf{r})\mathbf{F}(\mathbf{r}, \omega, t) + \frac{1}{4\pi} \int_{4\pi} d\omega' \mathbf{S}(\omega', \omega, \mathbf{r})\mathbf{F}(\mathbf{r}, \omega', t), \quad (16) \end{aligned}$$

where $\mathbf{A}(\mathbf{r})$ is the extinction matrix normalized to σ , $\mathbf{S}(\omega', \omega, \mathbf{r})$ is the scattering matrix 4×4 .

The extinction and scattering matrices most completely represent microphysical characteristics of scattering media. This is connected with the fact that the number of non-zero elements in the matrices, their values and properties of symmetry essentially depend on the medium phase composition, shape and orientation of suspended particles, and their optical activity. In particular, in the absence of the latter, the extinction matrix is degenerated to the scalar extinction coefficient $A_{ij} = \sigma \delta_{ij}$, where δ_{ij} is the Kronecker symbol; $i, j = 1, 2, 3, 4$. The solution of the stationary transfer equation taking into account polarization for simple models was considered by many authors. The full bibliography of these papers is presented in Ref. 65.

For justified use of the weight modifications of the Monte Carlo method, it is necessary to consider Eq. (16) in the integral form. In the papers of Siberian scientists,^{19,33,43} the existence of such equation was first strictly shown, the conditions of its solution convergence in the form of the Neuman series were indicated, and some problems of finiteness and possibility of minimization of the vector algorithms were studied. Actually, if to introduce the vector function of the density of collisions $\mathbf{f}(\mathbf{r}, \omega, t) = \mathbf{F}(\mathbf{r}, \omega, t) \times \sigma(\mathbf{r})$ and the vector function of the distribution density of the source $\Psi(\mathbf{r}, \omega, t)$, then the vector transfer equation (16) after known³³

transformations gains a standard form of the Fredholm equation of the second type.

The matrix of transition ($\mathbf{x}' \rightarrow \mathbf{x}$) takes here the form

$$\mathbf{K}(\mathbf{x}' \rightarrow \mathbf{x}) = \frac{\Lambda(\mathbf{r}') \exp[-\tau(\mathbf{r}', \mathbf{r})] \mathbf{P}(\boldsymbol{\mu}, \mathbf{r})}{2\pi |\mathbf{r}' - \mathbf{r}^*|^2} \times \\ \times \sigma(\mathbf{r}) \delta(\boldsymbol{\omega} - \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|}) \delta \left[t' - \left(t + \frac{|\mathbf{r}' - \mathbf{r}|}{c} \right) \right], \quad (16a)$$

where $\mathbf{P}(\boldsymbol{\mu}, \mathbf{r})$ is the phase matrix 4×4 connected with the scattering matrix by the relationship

$$\mathbf{P}(\boldsymbol{\mu}, \mathbf{r}) = \mathbf{L}(\pi - i_2) \mathbf{S}(\boldsymbol{\mu}, \mathbf{r}) \mathbf{L}(\pi - i_1);$$

\mathbf{L} is the known in optics^{4,33,65} matrix rotation operator.

Program realization of the mathematical formalism determined by the basis relationships (16) and (16a) allowed the statement and solution of the class of new problems of passive^{33,37,65} and active^{35,47,50,51} sensing of the atmosphere. In particular, the detailed algorithm and the results of solution of the non-stationary transfer equation under boundary conditions representing the scheme of real experiment on polarized lidar sensing of homogeneous liquid-droplet cloudiness were presented first in Ref. 35. Further development of this work was connected with the study of polarization characteristics of crystal clouds,^{47,51,92} including the scheme of spaceborne laser sensing.^{59,63,77}

4. Accounting for absorption by atmospheric gases

When estimating the efficiency of atmospheric optical IR channels, the processes of continual and spectral absorption by the atmosphere molecular component and scattering become of importance. Calculation of the radiative characteristics of aerosol formations in the near and middle IR ranges, rich in absorption bands of water vapor and different gases, is one of the traditional and most difficult problems of atmospheric optics. Absorption properties of the medium are characterized by the transmission function $P_{\Delta\nu}(l)$, where l is the geometric path length of the photon, $\Delta\nu$ is the frequency interval. The technique for statistical simulation was proposed in Refs. 21 and 22, which allows one to obtain the spatial-angular distribution of upward and downward spectral radiation fluxes in cloudy atmosphere as the integral with respect to photon path lengths:

$$\Phi_{\Delta\nu} \uparrow (l) = \int_0^{\infty} \tilde{P}_{\Delta\nu}(l) J(l) dl, \quad (17)$$

where $\tilde{P}_{\Delta\nu}(l)$ is the effective transmission function of the gas mixture, which was estimated from empirical

data on the spectral absorption by atmospheric gases, $J(l)$ is the photon distribution function over the path lengths in the reflected and transmitted light.

However, the use of the tables of empirical constants decreases operative flexibility of the Monte Carlo method. The modified method for taking into account molecular absorption (method of k -distribution) was proposed in subsequent papers.^{79,80} It was based on expansion of the effective transmission function into series of exponents. Briefly, the essence of the k -distribution method is as follows. Return to formal solution of integral equation (3). When integrating the radiation intensity over frequency (7), taking into account the formula for the integral operator (5), we can select the transmission function stipulated by molecular absorption. In this case, it is necessary to select such a width of the spectral interval $\Delta\nu$, within the limits of which optical characteristics of elastic scattering can be meant constant. Then all multipliers, which do not contain the molecular scattering parameters, can be factored outside the integral sign. The effective function of molecular transmission remains in explicit integral form:

$$P_j = \frac{1}{\Delta\nu} \int_{\Delta\nu} \exp\{-\tau_j(\nu)\} d\nu, \quad (18)$$

where $\tau_j(\nu)$ is the optical thickness of the j -th term of the series (7).

For the path fragment with constant molecular absorption coefficient $\beta_{\text{mol}}(\nu)$, $\tau_j = \beta_{\text{mol}}(\nu) L_j$, where L_j is the total path length. Exponential dependence of transmission on the path length makes it possible to pass to the space of cumulative wave numbers g using the Laplace transform. The transmission function there takes the form

$$P_j = \frac{1}{\Delta\nu} \int_0^1 \exp\{-\beta_{\text{mol}}(g) L_j\} dg, \quad (19)$$

where $\beta_{\text{mol}}(g)$ is monotonically increasing function of g , rather than quickly oscillating $\beta_{\text{mol}}(\nu)$. Applying quadrature formulas to Eq. (19), it is easy to obtain a short (5–10 terms) series of exponents. As test estimates have shown, the error of the method does not exceed 1%.

The generalization to the case of inhomogeneous paths is given in Refs. 79 and 80.

5. Simulation of radiation transfer in stochastically inhomogeneous cloudiness

Essential factor decreasing reliability of the forecasted estimates in real atmospheric optical radar channels is the stochastic nature of practically all atmospheric parameters: refractive index, concentration of aerosol and cloud particles, particle

size distribution, etc. Fluctuations of the detected optical signals are especially noticeable in the case of the stochastic inhomogeneous cloudiness. This fact was noted already in the first Monte Carlo calculations^{28,36,48} for quite simple statistical models. Analytical justification of the algorithm of statistical estimation of multi-point moments of the radiation intensity, in general, of any order, for a medium with continuous random inhomogeneous field of microphysical and, hence, optical characteristics, is presented in Ref. 28 in the framework of the theory of disturbances. Low efficiency of computers in the beginning of 80th, when that work was performing, did not allow the complete realization of the algorithm possibilities. The known assumption about Gaussian character of fluctuations of the field of cloud particle concentration enabled the authors³⁶ to essentially simplify the weight relationships and to obtain reliable estimates for two first moments of the backscattering intensity, depending on the cloudiness model and observation geometry. Another approach connected with the use of the algorithm of optical splitting of the trajectories in a homogeneous stochastic layer was developed by B.A. Kargin [Refs. 48 and 49]. These laborious investigations did not received further development.

The number of papers devoted to light fields in local-inhomogeneous stochastic cloudiness is much greater. Vast bibliography is presented in Ref. 71. Practical urgency of these investigations is obvious. This is related with the fact that broken cloudiness dominates on the planet megascale. To date, three approaches to simulation of the random field of cloudiness and radiation conventionally exist.

The historically first model approach³¹ based on the Monte Carlo method included a countable set of sphere-like clouds of the finite radius r ; centers $(x_j, y_j, z_j) = 1, 2, \dots$, homogeneously distributed in the layer $z_j \in [-H, H]$; the points (x_j, y_j) distributed on the XY plane according to the Poisson law, i.e., i points located on the area s with the probability

$$P_i(s) = e^{-vs} (vs)^i / i!,$$

where $v = |\ln(1-p)|/\pi r^2$, p is the cloud amount. The spheres can overlap and form a more complicated configuration of cloud elements close to actual. Optical parameters within the limits of cloud elements are considered as constant.

The closed system of equations for mean intensity was then obtained for statistically homogeneous cloud fields, as well the effective Monte Carlo algorithms were developed.^{53,54,71,78,81} A number of practically important problems were solved,^{64,71,78} for example, the efficiency of orbital systems for optical sensing under conditions of broken cloudiness was estimated.⁵⁷ A generalization of the Poisson model to the case of multi-layer model of inhomogeneous broken cloudiness was presented in Refs. 78, 83, 84.

In the last years, a number of serious investigations are devoted to development and application of so-called "Gaussian" models of broken cloudiness.^{69,71,73,96,97} It is assumed in this model that the plane $z = H_0$ is the bottom boundary of the cloudiness, and the top boundary $z = w(x, y)$ is described by the formula

$$w(x, y) = H_0 + \max(\sigma_0[v(x, y) - d], 0),$$

where $d \in (-\infty, +\infty)$; $\sigma_0 > 0$; $v(x, y)$ is the homogeneous Gaussian field with zero mean. The input data of the model [d , $K(x, y)$, and $\sigma_0 = K(0, 0)$] can be related with experimentally determined parameters: the cloud fraction p , the mean vertical and horizontal size of clouds. The increase of the method efficiency is connected with the spectrum randomization^{40,44,55,96} and selection of more realistic models of the correlation function $K(x, y)$.

The quest for taking into account extremely inhomogeneous configuration of actual clouds has led to appearance of the fractal model of cloudiness. Specialists of Siberian Branch of the Russian Academy of Sciences^{71,96} made essential contribution into its development. However, cumbersome algorithms of both cascade and multiplicative fractal versions of simulation⁹⁶ do not allow the wide use of them. Nevertheless, as forecasting estimates obtained by G.A. Titov in his last paper⁷⁸ show, these methods, undoubtedly, are promising and important, because they make it possible to construct clouds of the given fractal dimension, the estimates of which can be obtained based on the data of spaceborne optical sensing.

6. Statistical simulation of non-linear and trans-spectral processes induced by laser radiation in the atmosphere

Propagation of laser radiation, especially of high intensity, in the atmosphere as multi-component disperse medium is accompanied by a wide spectrum of non-linear and trans-spectral processes. Nonlinear processes lead to spatial and temporal transformation of the optical signal and to dynamic transformation of the medium optical properties due to effects of optical breakdown, evaporation and burning of the aerosol particles, etc. As a result, the Markovian character of the radiation transfer processes becomes fully broken, which is the criterion of the Monte Carlo method applicability. The transfer equation becomes nonlinear. The trans-spectral processes, first of all, such as Raman scattering, Mandelshtam–Brilluin scattering, and laser induced fluorescence lead to redistribution of the scattered radiation intensity over frequency, that, from the point of view of the transfer theory causes the transition to multi-rate and, in some cases, to nonlinear transfer equation. The invention of the technique of

generation of ultra-short pulses and the phenomenon of supercontinuum⁸⁵ significantly increased the significance of the above processes. A subsequent accounting for the aforementioned optical effects, on the one hand, makes the algorithm of statistical simulation more complicated, and on the other hand, opens a vast field for validation of the developed algorithms and for statement of new problems of laser spectroscopy.

First attempts of using the Monte Carlo method for solving the nonlinear transfer equation under conditions of self-induced transparency of the high-power laser radiation channel were undertaken in Ref. 29. In the regime of pre-explosion evaporation of liquid-droplet aerosol, the particle radius $r(I, t)$ is a monotonically decreasing function of the radiation intensity and the time of impact. This fact makes it possible to optimally digitize the processes in coordinates of time and space, and, using a combination of the method of discrete ordinates and the Monte Carlo method, to effectively solve the linear problem. Further this technique turned to be useful for numerical solution of the transfer equation, non-stationarity of kernel of which is caused by the resonance interaction of the femtosecond laser pulse with cloud droplets, the size of which is comparable with the pulse duration.⁹⁹ General methodology of solution of nonlinear integral equations by the Monte Carlo method is successively developed by G.A. Mikhailov.^{55,70,82}

Trans-spectral processes in the atmosphere at their proper recording and interpretation essentially extend the laser sensing capabilities. Recording the spatially resolved backscattering signal at frequencies of vibration-rotational Raman spectrum of water vapor, ozone, nitrogen, and other atmospheric gases makes it possible to obtain the pattern of vertical distribution of the aforementioned components.^{88,94} This information is adequate, if the signal satisfies the lidar sensing equation,⁵¹ i.e., is caused by single scattering. In the actual atmosphere, especially in the presence of cloudiness, there appears a necessity to estimate the noise, first of all, of the multiple scattering.

During the last decade, the algorithms for statistical simulation of trans-spectral phenomena in the field of hydrooptics and medical tomography are actively developing. The first attempts to estimate the distortions of Raman signal in cloudy atmosphere by the Monte Carlo method have led to obvious underestimation of the multiple scattering contribution. Using the principles of value simulation^{32,55,72} in the selection of the Raman scattering angle, we succeeded^{88,91} in elimination of the aforementioned displacement and obtained the results comparable with estimates obtained by other methods. The developed algorithm⁸⁸ for solving the multi-rate transfer equation was then successfully used for solving the practical problems.^{93,94} It was shown⁸⁹ that extension of the algorithm to the case of vector form of the transfer equation does not pose great difficulties.

A variety of trans-spectral transformations accompanying the phenomena of spontaneous and multi-photon fluorescence induced by laser radiation in biogenic and organic aerosol, opens a vast field for application of the Monte Carlo method for estimation of the fluorescent signals in complicated atmospheric conditions and in vegetation. These investigations in atmospheric optics are now at the initial stage. The closed system of non-stationary integro-differential equations regulating the transfer of wide-band radiation of laser-induced fluorescence in scattering medium is formulated, as well as the algorithm for its solution is proposed in Ref. 100. The obtained model estimates of the spatially resolved fluorescence spectra of plant secondary metabolites are in good qualitative agreement with the results of the field experiment.¹⁰⁰ The system of transfer equations¹⁰⁰ ignores the effect of reabsorption and resonance energy exchange (FRET-effect). These assumptions require additional investigations. The peculiarities of formation of the two-photon and multi-photon fluorescence spectra induced by femtosecond radiation are also of interest.

7. Solution of inverse problems

From the very beginning, the Monte Carlo method application to solution of classic problems of radiation transfer is accompanied by attempts of statement and solution of inverse problems, i.e., attempts of reconstruction of initial optical or microphysical parameters. Formally, the theory of inverse problems in optics of disperse media is connected with the search for methods for inverting the Fredholm integral equation of the first type, for example, in the form^{38,39}

$$\beta_s(\lambda) = \int_R K_s(r, \lambda) \pi r^2 n(r) dr, \quad (20)$$

where $K_s(r, \lambda)$ is the scattering efficiency factor, $n(r)$ is the particle size spectrum to be revealed. Estimation of the $\beta_s(\lambda)$ spectral values based on lidar or spectrophotometric measurements is always connected with errors, which make the problem of analytical inversion of Eq. (20) ill-posed. Application of the Monte Carlo method to solving the inverse problems of optical sensing is realized in the papers of Siberian scientists in two directions. The approach developed in Refs. 8, 33, 37, 56, 65 is based on estimation of derivatives from the measured functional in the framework of the theory of disturbances.

For example, let a series of measured functionals be available:

$$\tilde{I}_k(\sigma_1, \sigma_2, \dots, \sigma_n) = (f, \varphi_k), \quad k = 1, 2, \dots, n_0,$$

where f is the solution of the transfer equation (3); and it is required to find $(\sigma_1, \sigma_2, \dots, \sigma_n)$. If $(\sigma_1^{(0)}, \sigma_2^{(0)}, \dots, \sigma_n^{(0)})$ are some forecasted values of

these parameters, then, applying the theory of disturbances, we come to the system of equations

$$\sum_{i=1}^n a_{ik} \delta \sigma_i = \tilde{I}_k - I_k^{(0)} \quad (21)$$

providing the linear dependence of L on σ_i ; here $I_k^{(0)} = I_k(\sigma_1^{(0)}, \sigma_2^{(0)}, \dots, \sigma_n^{(0)})$. If the noted dependence is nonlinear, the problem can be solved by the method of successive approximations using the formulas of small disturbances, then the coefficients a_{ik} are actually the partial derivatives:

$$a_{ik} = \frac{\partial I_k}{\partial \sigma_i}, \quad k = 1, 2, \dots, n_0, \quad i = 1, 2, \dots, n. \quad (22)$$

Calculation of derivatives by the Monte Carlo method is described, for example, in Refs. 33 and 65.

The idea of the closed numerical experiment was proposed and realized in Refs. 27, 38, 39, 85, 101. The direct problem was simulated by the Monte Carlo method, the problem of reconstruction of the initial microphysical parameters, taking into account the distorting effect of the multiple scattering noise, was solved by one of the traditional methods: the method of optimal parameterization^{38,39} or Tikhonov's method of regularization.⁸⁵ The genetic algorithm of the method of artificial neuron networks has also well showed itself.¹⁰¹

Conclusions

As it was mentioned above, the development of the Monte Carlo methods for atmospheric optics was based on the papers in the field of neutron physics. In turn, new algorithms and methods obtained in solving the problems of optical sensing of the atmosphere favored effective solving of new class of problems in close fields of physical optics. Combination of the algorithms for simulation of non-stationary transfer of short-wave radiation with the results of the theory of linear systems has led to appearance of statistical linearly-system approach to imitation of the optical channels of vision in turbid media.^{41,42,67,68,72} A strict in the framework of the Monte Carlo method, accounting for the effect of multiple scattering, made it possible to reveal a number of basic regularities in formation of images of 2D-objects in the "atmosphere—underlying surface" system. In particular, in Refs. 45 and 46, a forecast was proposed and geometric conditions were determined of extreme smoothing of the image of spatially limited self-radiating objects; the criteria of spatial resolution for aerospace vision systems were revealed in Refs. 63 and 72.

The universal character of the algorithms for simulation of regularly inhomogeneous and stochastic cloud fields in the atmosphere made it possible to realize⁶⁶ the effective algorithm for simulation of inhomogeneous boundary between the media in the "atmosphere—ocean" system and to perform a number

of important applied investigations.^{74,75,90,95} The algorithms for local estimations are useful in solving some problems of atmospheric acoustics.^{60,61}

A limited volume of the paper does not allow us to present an exhaustive analysis of all data obtained in long-term and complementary scientific cooperation of physicists of the Institute of Atmospheric Optics and mathematicians of the Institute of Computational Mathematics and Mathematical Geophysics SB RAS. It is obvious that possibilities of such fruitful cooperation are not limited, because the capabilities of the Monte Carlo method are inexhaustible.

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