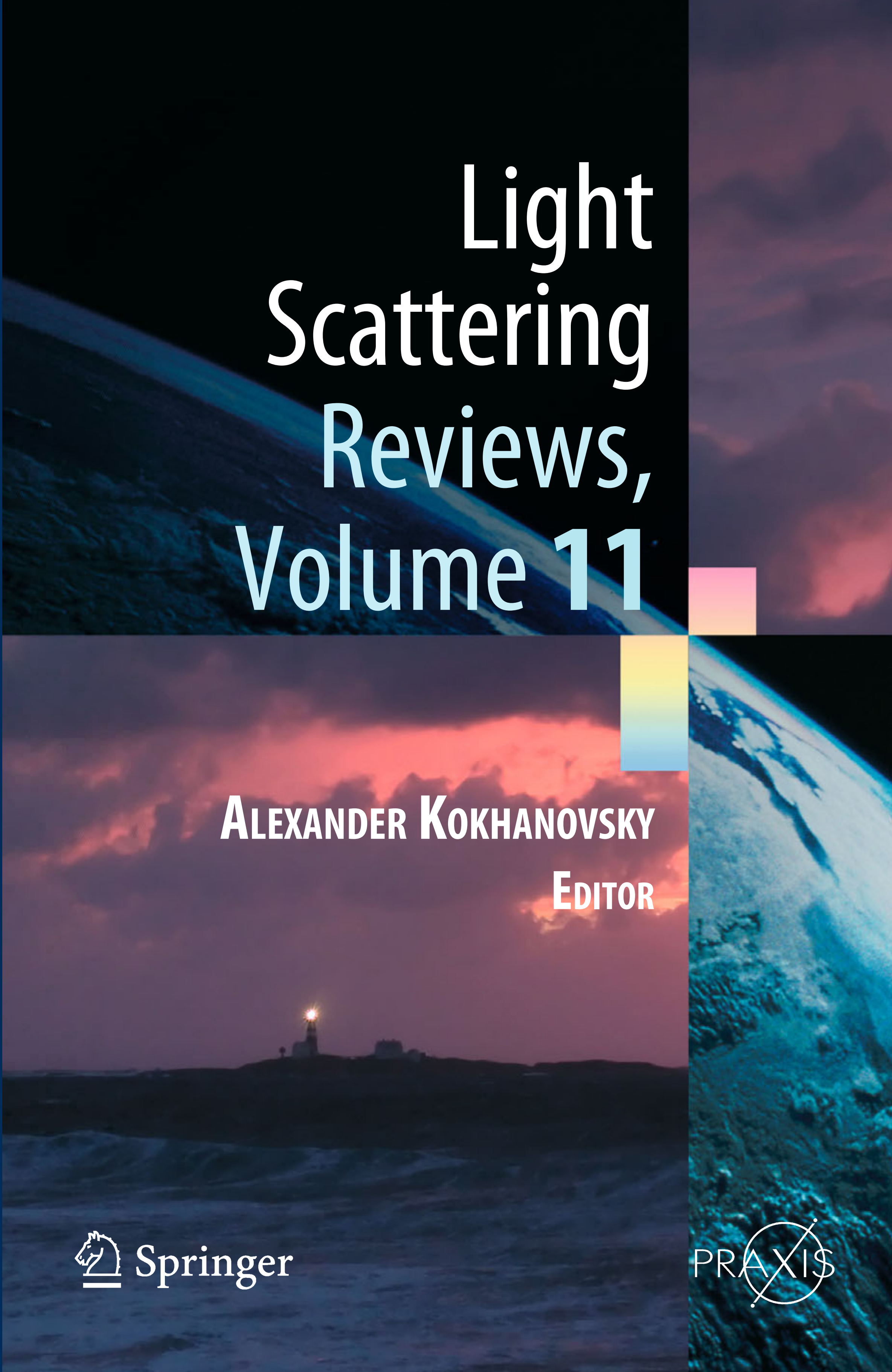
Light Scattering Reviews, Volume 11

Alexander Kokhanovsky
Editor



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Light Scattering Reviews, Volume 11

Light Scattering and Radiative Transfer

Springer

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Published in association with Praxis Publishing, Chichester, UK

Springer Praxis Books
ISBN 978-3-662-49536-0 ISBN 978-3-662-49538-4 (eBook)
DOI 10.1007/978-3-662-49538-4

Library of Congress Control Number: 2016933799

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer-Verlag GmbH Berlin Heidelberg

Preface

This volume of *Light Scattering Reviews* is aimed at the presentation of recent advances in radiative transfer, light scattering, and polarimetry and consists of nine chapters prepared by leading experts in respective research areas. A state-of-the-art discrete-ordinate algorithm for the transfer of monochromatic unpolarized radiation in non-isothermal, vertically inhomogeneous media, as implemented in the computer code discrete-ordinate-method radiative transfer, DISORT, is reviewed by Laszlo et al. in chapter "The Discrete Ordinate Algorithm, DISORT for Radiative Transfer". Both the theoretical background and its algorithmic implementation are covered in detail. These include features common to solutions of many radiative transfer methods, including the discrete-ordinate method, and those specific to DISORT. The common features include expansions of the phase function and the intensity into a series of Legendre polynomials and Fourier series, respectively, which transform the radiative transfer equation into a set of equations that depend only on the optical depth and the zenith angle, and the transformation of the integro-differential equations into a set of ordinary differential equations by approximating the integral in the source function by a quadrature sum. The features specific to DISORT include the reduction of the order of the standard algebraic eigenvalue problem to increase efficiency in both homogenous and particular solutions of the system of coupled ordinary differential equations, application of the scaling transformation to make the solution unconditionally stable for arbitrary large values of optical depth, application of the δ-M method to handle highly anisotropic scattering, the correction of intensities by the Nakajima–Tanaka method, and the implementation of a realistic bidirectional bottom boundary condition as realized in version 3 of DISORT. Numerical considerations that make the implementation robust and efficient are also discussed. Examples of setting up DISORT runs are shown by using test cases with increasing complexity. Brief summaries of the versions released to date are provided as well. Chapter "Community Radiative Transfer Model for Air Quality Studies" prepared by Liu and Lu presents the latest community radiative transfer model (CRTM), which is applicable for passive optical, microwave, and infrared sensors. The CRTM has been used in operational radiance assimilations in supporting of weather forecasting and in the generation of satellite products. In this chapter, CRTM applications to assimilate aerosol optical depths derived from satellite measurements are discussed. In particular, the assimilation improves the analysis of aerosol mass concentrations. A retrieval algorithm and a retrieval product of carbon monoxide by using satellite measurements are introduced. Wei and Xu has presented the analytical solution of the time-dependent scalar and vector RTE in an infinite uniform medium with an arbitrary light scattering phase function using cumulant expansion in chapter "Analytical Solution of Radiative Transfer Using Cumulant Expansion". Analytical expressions for the exact distribution in angle and the spatial cumulants at any angle, exact up to an arbitrary high order, *n,* of photons are derived. By a cutoff at the second cumulant order, a Gaussian analytical approximate expressions of the scalar and vector photon spatial distribution is obtained as a function of the direction of light propagation and time, whose center position and half-width are always exact at arbitrary time. The center of this distribution advances and the half-width grows in time, depicting the evolution of the particle migration from near ballistic, through snake-like, and into the final diffusive regime. Contrary to what occurs in other approximation techniques, truncation of the cumulant expansion at order *n* is exact at that order and cumulants up to and including order *n* remain unchanged when contributions from higher orders are added. Various strategies to incorporate the boundary conditions in the cumulant solution are presented. The performance of the cumulant solution in an infinite and a semi-infinite medium is verified by exact numerical solutions with Monte Carlo simulations. At the end, the particular applications of the cumulant solution to RTE in biophotonics for optical imaging and in remote sensing for cloud ranging are discussed. Kolesov and Korpacheva have reviewed the radiative transfer theory in turbid media of different shapes in chapter "Radiative Transfer in Spherically and Cylindrically Symmetric Media". In particular, the authors have presented the research of radiative transfer in spherically and cylindrically symmetric media with anisotropic scattering of light. The problems of radiation transfer in an infinite homogeneous absorbing and anisotropically scattering media illuminated by a planar or point sources are considered. The relationship between the characteristics of the radiation fields in these two problems is obtained. Also an overview of the problems of radiation transfer in an infinite medium with arbitrary spherically symmetric distribution of sources is presented. The authors also discuss the structure of the radiation field in a sphere of a finite optical thickness and a spherical shell. The asymptotic expressions in the theory of radiation transfer in atmospheres with spherical symmetry are presented as well. The authors discuss the applications of the methods developed in the theory of radiative transfer in spherically symmetric media to the case of media with a cylindrical symmetry. They provide an overview of studies on the nonstationary radiative transfer in plane-parallel, spherical, and cylindrical media. Lock and Laven describe the Debye series for scattering by a sphere, a coated sphere, a multi-layer sphere, a tilted cylinder, and a prolate spheroid in chapter "The Debye Series and Its Use in Time-Domain Scattering". In electromagnetic scattering of an incident beam by a single particle possessing a reasonably high degree of symmetry, the Debye series decomposes the partial wave scattering and interior amplitudes into the contributions of a number of intuitive physical processes. The authors comment on the meaning of the various Debye series terms, and briefly recount the method by which the formulas of ray scattering can be derived from them. They also consider time-domain scattering of a short pulse by a spherical particle and describe the way in which the time-domain scattering signature naturally separates out the various Debye series terms. Lastly, the authors show how time-domain scattering further separates a number of cooperating sub-processes present in the individual Debye series terms. Kahnert et al. discuss the models of inhomogeneous particles used in light scattering computations in chapter "Morphological Models Forinhomogeneous Particles: Light Scattering by Aerosols, Cometary Dust, and Livingcells". Light scattering by chemically heterogeneous particles with inhomogeneous internal structure is an important field of study in such diverse disciplines as atmospheric science, astronomy, and biomedical optics. Accordingly, there is a large variety of particle morphologies, chemical compositions, and dielectric contrasts that have been considered in computational light scattering studies. Depending on the intended applications, physical particle properties, and computational constraints, one can find inhomogeneous particle models ranging from simple core-shell geometries to realistic quasi-replicas of natural particles. The authors review various approaches for representing the geometry of encapsulated light-absorbing carbon aerosols, mineral dust, volcanic ash, cometary dust, and biological particles. The effects of particle inhomogeneity on radiometric properties are discussed. The authors also consider effective medium approximations, i.e., approaches that aim at avoiding the computational difficulties related to particle inhomogeneity altogether by representing such particles by a homogeneous material with an effective refractive index. Chapter "Some Wave-Theoretic Problems in Radially in Homogeneous Media" prepared by Noontaplook et al. is aimed at consideration of wave-theoretic problems in radially inhomogeneous media. The wave-theoretic aspects are based on the solution of Maxwell's equations for scattering of plane electromagnetic waves from a dielectric (or "transparent") sphere in terms of the related Helmholtz equation. There is a connection with the time-independent Schrödinger equation in the following sense: the time-independent Schrödinger equation is identical in form to the wave equation for the scalar radiation potential for TE-polarized electromagnetic waves. In regions where the refractive index is constant, it is also identical to the scalar radiation potential for TM-polarized electromagnetic waves, but with different boundary conditions than for the TE case. The authors examine scattering of the TE mode from a piecewise-uniform radial inhomogeneity embedded in an external medium (as opposed to an off-axis inclusion). The corresponding theory for the TM mode is also developed, and the well-known connection with morphology-dependent resonances (MDRs) in these contexts is noted. Kimura et al. focus on numerical approaches to deducing the light scattering and thermal emission properties of primitive dust particles in planetary systems from astronomical observations in chapter "Light Scattering and Thermal Emission by Primitive Dust Particles in Planetary systems". The particles are agglomerates of small grains with sizes comparable to visible wavelength and compositions being mainly magnesium-rich silicates, iron-bearing metals, and organic refractory materials in pristine phases. These unique characteristics of primitive dust particles reflect their formation and evolution around main-sequence stars of essentially solar composition. The development of light scattering theories has been offering powerful tools to make a thorough investigation of light scattering and thermal emission by primitive dust agglomerates in such a circumstellar environment. In particular, the discrete dipole approximation, the T-matrix method, and effective medium approximations are the most popular techniques for practical use in astronomy. Numerical simulations of light scattering and thermal emission by dust agglomerates of submicrometer-sized constituent grains have a great potential to provide new state-of-the-art knowledge of primitive dust particles in planetary systems. What is essential to this end is to combine the simulations with comprehensive collections of relevant results from not only astronomical observations, but also in situ data analyses, laboratory sample analyses, laboratory analogue experiments, and theoretical studies on the origin and evolution of the particles. The concluding chapter "Polarimetry of Man-Made Objects" prepared by S. Savenkov is aimed at applications of environmental polarimetry. Polarimetry has already been an active area of research for about fifty years. A primary motivation for research in scatter polarimetry is to understand the interaction of polarized radiation with natural scenes and to search for useful discriminants to classify targets at a distance. In order to study the polarization response of various targets, the matrix models (i.e., 2 x 2 coherent Jones and Sinclair and 4 x 4 average power density Mueller (Stokes) and Kennaugh matrices etc.) and coherent and incoherent target decomposition techniques has been used. This comes to be the standard tools for targets characterization. Polarimetric decomposition methods allow a physical interpretation of the different scattering mechanisms inside a resolution cell. Thanks to such decompositions, it is possible to extract information related to the intrinsic physical and geometrical properties of the studied targets. This type of information is inestimable if intensity is measured only. The goal of this chapter is to explain the basics of polarimetric theory, outline its current state of the art, and review some of important applications to study the scattering behavior of various man-made and urban targets like buildings (tall and short), ships, oil rigs and spills, mines, bridges, etc. The author considers both optical range and radar polarimetry.

Darmstadt, Germany Alexander Kokhanovsky
October 2015

Contents

Editor and Contributors

About the Editor

Alexander Kokhanovsky graduated from the Department of Physics at the Belarusian State University, Minsk, Belarus, in 1983. He has received his Ph.D. in Optical Sciences from the B. I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus, in 1991. The Ph.D. work was on the study on light scattering properties of aerosol media and foams. His habilitation work (Main Geophysical Observatory, St. Petersburg, Russia, 2011) was devoted to the development of advanced cloud and snow remote sensing techniques based on spaceborne observations. Dr. Kokhanovsky has worked at the Atmospheric Optics group in the Laboratory of Light Scattering Media Optics at Institute of Physics in Minsk (1983–2004) and he has belonged to the SCIAMACHY/ENVISAT algorithm development team (Institute of Environmental Physics, University of Bremen, 2001–2013). He is currently working on aerosol and cloud remote sensing algorithms for the imaging polarimeter (3MI) to be launched in 2021 on board EUMETSAT Polar System-Second Generation (EPS-SG). His research interests include studies on light propagation and scattering in terrestrial atmosphere. Dr. Kokhanovsky is the author of books *Light Scattering Media Optics: Problems and Solutions* (Chichester: Springer-Praxis, 1999, 2001, 2004), *Polarization Optics of Random Media* (Berlin: Springer-Praxis, 2003), Cloud Optics (Amsterdam: Elsevier, 2006), and *Aerosol Optics* (Berlin: Springer-Praxis, 2008). He has published more than 300 papers in the field of environmental optics, radiative transfer, and light scattering.

About the Contributors

John Adam is Professor of Mathematics at the Department of Computational and Applied Mathematics (Old Dominion University, USA) and have had varied research interests, from astrophysical MHD and the related singular differential equations, to modeling tumor growth and wound healing. His current area of research is in theoretical meteorological optics, specifically ray and wave propagation in radially inhomogeneous media, with potential applications to the study of certain types of metamaterials. He has written several books published by Princeton University Press (see http://www.odu.edu/~jadam for details), including *Mathematics in Nature: Modeling Patterns in the Natural World.*

Wei Cai is a Senior Scientist at the Institute of the Ultrafast Laser and Spectroscopies, City College of City University of New York. He received his Bachelor degree in Physics at Quinghua University, Beijing, China and later a Ph.D. degree in Physics at University of Houston in 1985. He has published a total of 63 papers in Physical Review Letters, Physical Review, and other peer-referred journals. Dr. Cai hold six U.S. patents and is the co-author of the book titled "Random Processes in Physics and Finance" (2006, Oxford Press).

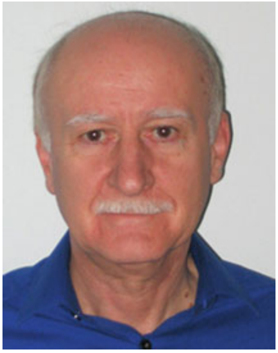
Michael Kahnert is a Senior Scientist at the Research Department of the Swedish Meteorological and Hydrological Institute, and an Adjunct Professor at the Department of Earth and Space Sciences of Chalmers University of Technology in Gothenburg. His research interests cover fundamental questions and numerical methods in electromagnetic scattering theory, applications to aerosols, ice clouds, and cosmic dust, radiative transfer in planetary atmospheres, as well as inverse modeling, remote sensing, chemical data assimilation, air pollution modeling, and aerosol-cloud coupling. He received his Ph.D. in 1998 at the University of Alaska Fairbanks (USA), and his Habilitation/senior Lecturer Expertise in 2010 at Chalmers University of Technology (Sweden).

Hiroshi Kimura is currently a Research Fellow at the Graduate School of Science of Kobe University in Japan. His research interest lies in the life cycle of cosmic dust in order to answer the question as to whether cosmic dust is the origin of life in the universe. He has conducted research on physical and chemical processes of dust occurring in interplanetary space, cometary comae and tails, the surfaces of airless bodies, debris disks, protoplanetary disks, and the interstellar medium. He has been leading the Scientific Organization Committee (SOC) and the Local Organizing Committee (LOC) of a series of the international meeting on Cosmic Dust, since he established the SOC and the LOC in 2006.

Alexander Kolesov is a Professor of the Department of General Mathematics and Informatics of the St. Petersburg State University. Kolesov is one of the representatives of the scientific school of theoretical astrophysics, established in St. Petersburg (Leningrad) University, by the academician Ambartsumian and headed by academician Sobolev. His research interests relate to the theory of multiple scattering of light in anisotropic scattering media with flat, cylindrical, or spherical symmetry. In 1988 he was awarded the degree of Doctor of Physical and Mathematical Sciences for the development of the theory of radiation transport in a spherically symmetric media. In recent years he studies the nonstationary radiation fields generated by a momentary point source.

Ludmilla Kolokolova is a Senior Research Scientist at the Astronomy Department of the University of Maryland, College Park. Her main scientific interest is remote sensing of dust in Solar system and beyond using photopolarimetric techniques. Her research is focused on laboratory and computer modeling of light scattering by complex particles and regolith surfaces and interpretation of ground-based and space mission observations. She is also the manager of the NASA Planetary Data System Small Bodies Node and is responsible for long-term preservation and archiving of the data collected by space missions to small bodies (comets, asteroids, TNOs, satellites of planets).

Natalia Kropacheva is an Associate Professor of the Department of General Mathematics and Informatics of the St. Petersburg State University, Candidate of Physical and Mathematical Sciences, specialist in the field of modeling complex systems. In recent years the range of her scientific interests included the study of nonstationary processes of radiation transfer in spherical and cylindrical symmetric media, illuminated by a momentary point source.



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Aigen Li is a Professor of Astrophysics at the University of Missouri in the USA. Since he started his graduate study in 1994 under the supervision of J. Mayo Greenberg at Leiden University in The Netherlands, he has been studying the physics and chemistry of the interstellar medium and interstellar dust, comets, planet-forming dust disks, dust-making evolved stars, and dust in external galaxies, active galactic nuclei, and gamma-ray bursts.

Quanhua Liu is a Physical Scientist at the NOAA/NESDIS and is leading the soundings team at NOAA/STAR. The sounding system utilized satellite-based microwave observations and infrared hyper-spectral measurements to acquire vertical profiles of atmospheric temperature, water vapor, ozone, CO, CH_4, CO_2, and others chemical species. Quanhua Liu studied the infrared hyper-spectral sensor and the community radiative transfer model (CRTM). The CRTM has been operationally supporting satellite radiance assimilation for weather forecasting. The CRTM also supports JPSS/NPP and GOES-R missions for instrument calibration, validation, long-term trend monitoring, and satellite retrieved products. He received a B.S. from Nanjing University of Information Science and Technology (former Nanjing Institute of Meteorology), China, a Master's Degree in Physics from the Chinese Academy of Science, and a Ph.D. in Meteorology and Remote Sensing from the University of Kiel, Germany.

James Lock received his Ph.D. in Theoretical Physics in 1974 from Case Western Reserve University in Cleveland OH, USA. Following a 40-year teaching career first in the physics department of CWRU and then in the Physics Department of Cleveland State University, he is currently Professor Emeritus at CSU. His main research interest is single-scattering of a plane wave or a shaped beam from a particle having a relatively high degree of symmetry. He is especially interested in the wide variety of beautiful phenomena that dominate scattering in the short-wavelength limit.

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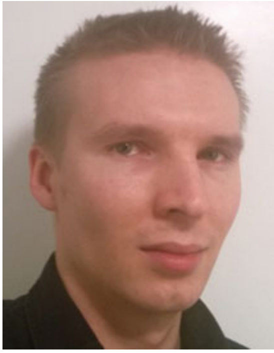


Johannes Markkanen received his D.Sc. (Tech.) degree in electromagnetics from the Aalto University, Finland, in 2013. Currently he is a Postdoctoral Researcher at the Department of Physics, University of Helsinki, Finland. He works with the planetary science research group and his research interests include computational methods in electromagnetics (particularly integral equation methods, regularization techniques, and fast algorithms), multiple-scattering theory, and electromagnetic modeling of natural and artificial materials.

Timo Nousiainen has studied the single-scattering modeling of various types of nonspherical, atmospheric particles for over 20 years, during which he has authored or co-authored over 60 peer-reviewed original research papers and three reviews. He has contributed particularly to research on mineral dust particles, with secondary emphasis on tropospheric ice crystals. For the last 2 years, he has mainly written proposals on various topics and managed weather-radar-related service development. He is currently working in the Radar and Space Technology group at the Finnish Meteorological Institute.

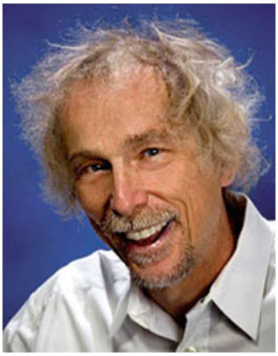
Umaporn Nuntaplook received her Ph.D. in Computational and Applied Mathematics from Old Dominion University, USA, in 2013. Currently she is a Lecturer at the Department of Mathematics, Mahidol University, Bangkok, Thailand. Her research interests are applying the computational methods to the problems in the fields of mathematical physics including the topics in electromagnetic, acoustic, and potential scattering theory.

Michael A. Pohrivchak is working at Naval Research Laboratory (Washington, D.C., USA). His primary focus was on electromagnetic theory with an emphasis on nonhomogeneous media. Currently, he is working on the propagation of electromagnetic waves through the atmosphere. This requires obtaining an accurate solution to the parabolic wave equation which allows for the prediction of the path loss between two points.

Sergey N. Savenkov received his Ph.D. in Radiophysics 1996 and his Doctor of Science degree in Optics and Laser Physics in 2013 from Taras Shevchenko National University of Kyiv. His research interests are focused on the use of polarization of electromagnetic radiation in remote sensing, crystal optics, biomedical optics, and laser/radar technology. He is currently employed at Faculty of Radio Physics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv. Specific topics are the methods of structural and anisotropy property analysis of objects contained in their scattering matrices, development of the Mueller matrix measurement methods, optimization polarimetric sensors for remote sensing applications, and use of polarimetry to improve imaging in turbid media.

Knut Stamnes is a Professor in the Department of Physics and Engineering Physics, and Director of the Light and Life Laboratory at Stevens Institute of Technology, Hoboken New Jersey. His research interests include radiative transfer, remote sensing, and climate-related studies. He has published more than 200 research papers and two textbooks (Radiative Transfer in the Atmosphere and Ocean, Cambridge, 1999; Radiative Transfer in Coupled Environmental Systems, Wiley-VCH, 2015). He is a fellow of OSA, a member of SPIE, and was elected member of the Norwegian Academy of Technological Sciences in 2009. Stamnes earned his B.Sc. and M.Sc. in Physics from the University of Oslo, Norway, and his Ph.D. from the University of Colorado, USA.

Si-Chee Tsay is a Senior Physical Scientist in NASA Climate and Radiation Laboratory and serves as EOS/Terra deputy project scientist since 2000. Besides theoretical radiative transfer, his research experience includes science planning and operating remote sensing instruments and in situ probes from suborbital and ground-based platforms in field experiments to study aerosol and cloud properties, and to aid in the development of retrieval algorithms. He has published over a hundred of research papers and awarded *NASA Exceptional Scientific Achievement Medal* in 2002 and *NASA Outstanding Leadership Medal* in 2008, among numerous achievement awards. Tsay earned his B.S. in Atmospheric Sciences from the National Taiwan University, Taiwan, and M.S. and Ph.D. in Atmospheric Sciences from the University of Alaska.



Warren Wiscombe graduated from MIT with a B.S. in Physics, then from CalTech with a Ph.D. in Applied Mathematics. He joined the ARPA Climate Dynamics Program in 1971 and helped found the new field of climate science. He specialized in atmospheric radiation with particular application to clouds. He worked at NCAR in the 1970s, then at NYU as a Professor, and then at NASA Goddard for 30 years before retiring in 2013. His work until 1990 was largely theoretical, but increasingly afterward became measurement-oriented, leading ultimately to his capstone job as DOE ARM Chief Scientist.

Min Xu obtained his Ph.D. in Physics from the City University of New York in 2001 and is currently Associate Professor of Physics at Fairfield University, CT, USA. He has been actively involved in biophotonics since 2001 with over 50 peer-reviewed journal papers, books and book chapters, and five patents. His research focuses on random photonics, and spectroscopy and tomography in biomedical applications. In particular, he is interested in mathematical modeling and applications of multiply scattered light in complex systems. Dr. Xu is currently developing novel mesoscopic and microscopic quantitative imaging techniques for lighting up the static structure and dynamic processes in biological systems; and photonic cancer screening, diagnosis, and prognosis. He pioneered the unified Mie and fractal model for light scattering by complex systems such as cell and tissue, and the electric field Monte Carlo method to simulate coherence phenomenon of multiple scattered light. He is a Senior Member of OSA.

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Part I
Radiative Transfer

The Discrete Ordinate Algorithm, DISORT for Radiative Transfer

Istvan Laszlo, Knut Stamnes, Warren J. Wiscombe and Si-Chee Tsay

Abstract The discrete ordinate method for the transfer of monochromatic unpolarized radiation in non-isothermal, vertically inhomogeneous media, as implemented in the computer code Discrete-Ordinate-Method Radiative Transfer, DISORT, is reviewed. Both the theoretical background and its algorithmic implementation are covered. Among others, described are the reduction of the order of the standard algebraic eigenvalue problem to increase efficiency in both the homogenous and particular solutions of the system of coupled ordinary differential equations, application of the scaling transformation to make the solution unconditionally stable for arbitrary large values of optical depth, application of the δ-M method to handle highly anisotropic scattering, the correction of intensities by the Nakajima-Tanaka method, and the implementation of a realistic bidirectional bottom boundary. Numerical considerations that make the implementation robust and efficient are also discussed. Examples of setting up DISORT runs are shown by using test cases with increasing complexity. Brief summaries of the versions released to date are provided, as well.

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A. Kokhanovsky (ed.), *Light Scattering Reviews, Volume 11*,
Springer Praxis Books, DOI 10.1007/978-3-662-49538-4_1

1 Introduction

Studies of propagation of electromagnetic radiation in a medium (e.g., stellar and planetary atmospheres) require the solution of an equation, the radiative transfer equation, which mathematically describes the interaction between emission, absorption, and scattering by which the medium affects the transfer of radiation. One such solution is the discrete ordinate approximation; a systematic development of which is presented by Chandrasekhar (1960). The strength of the approximation is in the transformation of an integro-differential equation describing radiative transfer to a system of ordinary differential equations for which solutions in terms of eigenvectors and eigenvalues can be found. Computer implementation of the discrete ordinate solutions proposed by investigators (e.g., Chandrasekhar 1960; Liou 1973; Asano 1975), however, had numerical difficulties as discussed by Stamnes and Swanson (1981), who also showed a way to overcome these difficulties. The discrete ordinate method has gained considerable popularity after the publication of the paper by Stamnes et al. (1988a) that presented a detailed summary of treating numerical ill-conditioning, computation of the eigenvalues and eigenvectors, efficient inversion of the matrix needed for determining the constants of integration, and especially after its implementation in the computer code Discrete Ordinate Method Radiative Transfer, or DISORT, in 1988 was made readily available to the public.

DISORT is a discrete ordinate algorithm for monochromatic unpolarized radiative transfer in non-isothermal, vertically inhomogeneous, but horizontally homogeneous media. It can treat thermal emission, absorption, and scattering with an arbitrary phase function covering the electromagnetic spectrum from the ultraviolet to radio. The medium may be driven by parallel or isotropic diffuse radiation incident at the top boundary, by internal thermal sources and thermal emission from the boundaries, as well as by bidirectional reflection at the surface. It calculates intensities (radiances), fluxes (irradiances), and mean intensities at user-specified angles and levels.

Our goal is to review the discrete ordinate approximation as it is implemented in DISORT. The primary source used in this review is the DISORT Report v1.1 (Stamnes et al. 2000). Most of the material is taken from that report with little or no modification. However, some parts, e.g., the treatment of the bidirectionally reflecting lower boundary, are expanded on. We also include recent advances that appeared in Lin et al. (2015), and which were not present in the v1.1 Report. We first describe the theoretical basis for DISORT, and then discuss numerical considerations that must be dealt with in order to make the implementation robust and efficient. Next, taking from the many test cases provided with the code, we show examples of how to correctly set up a DISORT run, and finally, we provide brief summaries of the versions released to date.

2 Equation of Transfer in DISORT

We consider a plane-parallel horizontally homogeneous medium (a slab), the optical properties of which are characterized by its optical thickness (defined as the difference between the optical depth at the bottom and that at the top), the single-scattering albedo ω, and the scattering phase function P. As defined, ω gives the fraction of an incident beam which is scattered by an infinitesimal volume inside the medium, while P describes how much of the radiation incident from a given direction is scattered by that volume into another direction, that is, the angular scattering pattern.

Location in the medium is specified by one vertical coordinate, measured in optical depth units (τ) from the top down. Directions are described by two angular coordinates, zenith and azimuth angles (Fig. 1). Polar (zenith) angles (θ) are measured from the upward direction: straight up is 0° and straight down is 180°. In the rest of the discussion we use the cosine of the polar angle (μ) instead of θ to denote the polar direction. According to the above convention all upward directions have positive polar angle cosines ($+\mu$), while downward-directed intensities have negative polar angle cosines ($-\mu$). The exception is the cosine of the incident beam angle (μ_0) which, for historical reasons, is taken positive. Azimuth angles (ϕ) are measured in an absolute frame of reference between 0° and 360°. They can be measured either clockwise or counterclockwise from the zero azimuth when viewed downward from zenith. However, when a choice has been made it must be applied consistently for all directions (upward, downward, incident, reflection). We note that according to this definition the relative azimuth angle of sunglint is 0°.

The transfer of monochromatic radiation through the medium, subject to internal thermal emission in local thermodynamic equilibrium and illuminated at the top boundary by a parallel beam in the direction μ_0, ϕ_0, is described by the following pair of equations:

$$I_{\text{direct}}(\tau) = F_0 e^{-\tau/\mu_0} \delta(\mu - \mu_0) \delta(\phi - \phi_0), \tag{1}$$

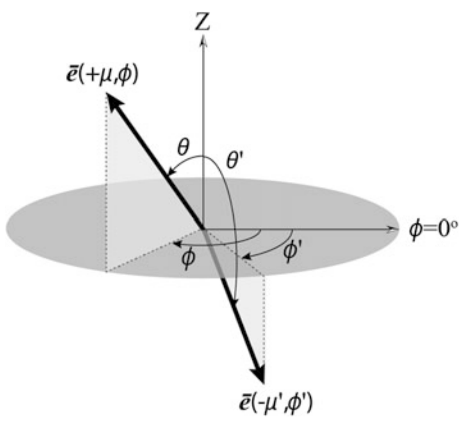

Fig. 1 Definition of upward, $\bar{e}(+\mu, \phi)$ and downward, $\bar{e}(-\mu, \phi)$ directions in DISORT. Polar (zenith) angles θ are measured from the upward normal pointing to Z. Azimuth angles ϕ are measured in a plane perpendicular to the upward normal, and in relative to the reference direction $\phi = 0°$

$$\mu \frac{dI(\tau, \mu, \phi)}{d\tau} = I(\tau, \mu, \phi) - S(\tau, \mu, \phi). \tag{2}$$

Here I_{direct} is the intensity of the direct beam at vertical optical depth τ, F_0 is the flux (irradiance) of the parallel beam normal to the direction of incidence at the top boundary, and δ is the delta function in units of per steradian. I is the diffuse specific intensity at τ in a cone of unit solid angle along direction μ, ϕ, and S is the "source function." S is the sum of the radiation scattered into the direction μ, ϕ from all other directions μ', ϕ', the "pseudobeam" source term $Q^{(\text{beam})}$, and the internal thermal source $Q^{(\text{thermal})}$ characterized by the Planck function $B(T)$ at temperature T at optical depth τ (cf. Stamnes et al. 2000):

$$\begin{aligned} S(\tau, \mu, \phi) = \frac{\omega(\tau)}{4\pi} \int_0^{2\pi} d\phi' \int_{-1}^{1} P(\tau, \mu, \phi; \mu', \phi') I(\tau, \mu', \phi') d\mu' \\ + Q^{(\text{beam})}(\tau, \mu, \phi) + Q^{(\text{thermal})}(\tau), \end{aligned} \tag{3}$$

where

$$\begin{aligned} Q^{(\text{beam})}(\tau, \mu, \phi) &= \frac{\omega(\tau)}{4\pi} P(\tau, \mu, \phi; -\mu_0, \phi_0) F_0 \, e^{-\tau/\mu_0}, \\ Q^{(\text{thermal})}(\tau) &= \{1 - \omega(\tau)\} B[T(\tau)]. \end{aligned} \tag{4}$$

Apart from the polar angles defining the direction all other quantities in (1)–(4) depend on the wavelength of radiation. The wavelength dependence is assumed to be understood and is omitted from the equations.

Equation (1) gives the solution for the transfer of the direct beam radiation. It says that I_{direct} decreases exponentially with the pathlength τ/μ_0, and it is nonzero only in the direction μ_0, ϕ_0. The solution of (2) provides the diffuse radiation propagating in the direction μ, ϕ at the optical depth τ. In the remainder of the document we describe the solution of (2) using the discrete ordinate method as implemented in DISORT. The solution, as we show below, is comprised of essentially three steps: (1) transforming (2) into a set of radiative transfer equations which are functions of the vertical coordinate τ and the angular coordinate μ only (separation of azimuth dependence); (2) transforming the integro-differential equations into a system of ordinary differential equations; and (3) solving the system of ordinary differential equations using robust linear algebra solvers.

2.1 Radiative Transfer Equation Uncoupled in Azimuth

The scatterers within the medium are assumed to have random orientations; thus, ω does not explicitly depend on the direction of the incident beam, and P depends only on the angle between the incident and scattered beam (the scattering angle, Θ), that is, $P(\tau, \mu, \phi; \mu', \phi') = P(\tau, \cos\Theta)$ where, from the cosine law of spherical trigonometry, $\cos\Theta = \mu\mu' + \sqrt{(1-\mu^2)(1-\mu'^2)}\cos(\phi - \phi')$. With this restriction on the form of P, we expand the phase function P into a series of Legendre polynomials P_ℓ with $2M$ terms ($\ell = 0, \ldots, 2M - 1$) (Chandrasekhar 1960, Chap. 1, Eq. 33; Thomas and Stamnes 1999, Eq. 6.28).

$$P(\tau, \cos\Theta) = \sum_{\ell=0}^{2M-1} (2\ell + 1)\, g_\ell(\tau) P_\ell(\cos\Theta), \tag{5}$$

where the expansion coefficients g_ℓ are given by

$$g_\ell(\tau) = \frac{1}{2}\int_{-1}^{+1} P_\ell(\cos\Theta) P(\tau, \cos\Theta) \mathrm{d}(\cos\Theta). \tag{6}$$

In DISORT we require the phase function to be normalized to unity, so $g_0 = 1$. The g's generally decrease monotonically, so we can expect that a finite number of terms $2M$ in the expansion is sufficient. However, for highly asymmetric phase functions (e.g., for clouds) the g's often decrease very slowly, and several hundred terms may be necessary in (5) to adequately represent the phase function (in Sect. 6.1 we show how DISORT mitigates this problem).

Applying the addition theorem for spherical harmonics (Chandrasekhar 1960, Chap. 6, Eq. 86; Thomas and Stamnes 1999, Eq. 6.30) to (5) we obtain

$$P(\tau, \mu, \phi; \mu', \phi') = \sum_{m=0}^{2M-1} (2 - \delta_{0m}) \left\{ \sum_{\ell=m}^{2M-1} (2\ell + 1) g_\ell(\tau) \Lambda_\ell^m(\mu) \Lambda_\ell^m(\mu') \right\} \cos m(\phi - \phi'). \tag{7}$$

Here Λ_ℓ^m are the normalized associated Legendre polynomials related to the associated Legendre polynomials P_ℓ^m by

$$\Lambda_\ell^m(\mu) = \sqrt{\frac{(\ell - m)!}{(\ell + m)!}} P_\ell^m(\mu).$$

Since (7) is essentially a Fourier expansion of P in azimuth, we may similarly expand the intensity in a Fourier cosine series (Chandrasekhar 1960, Chap. 6, Eq. 91; Thomas and Stamnes 1999, Eq. 6.34):

$$I(\tau, \mu, \phi) = \sum_{m=0}^{2M-1} I^m(\tau, \mu) \cos m(\phi_0 - \phi). \tag{8}$$

Substitution of this equation, as well as (3) and (7) into the radiative transfer equation (2) splits it into $2M$ independent integro-differential equations, one for each azimuthal intensity component I^m:

$$\mu \frac{dI^m(\tau, \mu)}{d\tau} = I^m(\tau, \mu) - S^m(\tau, \mu), \quad (m = 0, 1, \ldots, 2M - 1), \tag{9}$$

where the source function S is given by

$$S^m(\tau, \mu) = \int_{-1}^{1} D^m(\tau, \mu, \mu')I^m(\tau, \mu')d\mu' + Q^m(\tau, \mu). \tag{10}$$

The symbols D^m and Q^m are defined by

$$D^m(\tau, \mu, \mu') = \frac{\omega(\tau)}{2} \sum_{\ell=m}^{2M-1} (2\ell + 1)g_\ell(\tau)\Lambda_\ell^m(\mu)\Lambda_\ell^m(\mu'), \tag{11}$$

$$Q^m(\tau, \mu) = X_0^m(\tau, \mu)e^{-\tau/\mu_0} + \delta_{m0}\, Q^{(\text{thermal})}(\tau), \tag{12}$$

where

$$X_0^m(\tau, \mu) = \frac{\omega(\tau)\, F_0}{4\pi}(2 - \delta_{m0}) \sum_{\ell=m}^{2M-1} (-1)^{\ell+m}(2\ell + 1)g_\ell(\tau)\Lambda_\ell^m(\mu)\Lambda_\ell^m(\mu_0), \tag{13}$$

and δ_{m0} is the Kronecker delta

$$\delta_{m0} = \begin{cases} 1 & \text{if } m = 0, \\ 0 & \text{otherwise.} \end{cases}$$

The above procedure transforms (2) into a set of equations (9) which do not depend on the azimuth angle (ϕ). It also uncouples the various Fourier components I^m in (9); that is, I^m does not depend on any I^{m+k} for $k \neq 0$.

Using the same number of terms ($2M$) in the Fourier expansion of intensity (8) as in the Legendre polynomial expansion of the phase function (7) is not accidental. To explain why, let us consider the case when the number of terms is different: $2M$ in the expansion of P and $2K$ in the expansion of I, and assume that $K > M$. Substitution of the series expansions into (2) results in an equation containing terms that are proportional to integrals of the type

$$\int_0^{2\pi} \sum_{m=0}^{2M-1} \sum_{k=0}^{2M-1} \cos mx \cos kx\, dx + \int_0^{2\pi} \sum_{m=0}^{2M-1} \sum_{k=2M}^{2K-1} \cos mx \cos kx\, dx.$$

In this expression the second term is zero because m runs from 0 to $2M - 1$ and k runs from $2M$ to $2K - 1$; that is, for each term $k \neq m$, and in this case the integral is zero. The same argument holds for the case $M > K$, in which case the remaining (nonzero) integral has both k and m running from 0 to $2K - 1$. As a consequence the expansion of the phase function and that of the intensity will have the same number of terms; and that number is determined by the smaller of M and K. We note that the integrals with $k \neq m \neq 0$ in the first term are also zero, which leads to the uncoupling of the various Fourier components mentioned above.

We note that when the lower boundary of the medium is characterized by specular reflection, for example, at the bottom of atmosphere in the atmosphere–ocean system, specular reflection can be included by adding a reflected beam source term to (12)

$$X_0^m(\tau,\mu)\,\rho_s(-\mu_0,\phi_0)\,\mathrm{e}^{-(2\tau_L-\tau)/\mu_0},$$

where ρ_s is the specular reflection function. This term is, however, not included in the versions of DISORT reviewed here.

3 Discrete Ordinate Approximation—Matrix Formulation

The steps presented so far are common to many approaches used to solve (2). What sets the discrete ordinate method apart from these, and gives its name, is the next step. In this step, we approximate the integral in (10) by a quadrature sum. For later convenience, we choose even-order quadrature angles $2N$ in the sum so that we have the same number of polar angle cosines for $+\mu$ as for $-\mu$. Substitution of the integral with a quadrature sum transforms the integro-differential equation (9) into the following system of ordinary differential equations (cf. Stamnes and Dale 1981; Stamnes and Swanson 1981)

$$\mu_i \frac{\mathrm{d}I^m(\tau,\mu_i)}{\mathrm{d}\tau} = I^m(\tau,\mu_i) - S^m(\tau,\mu_i), \quad (i = \pm 1, \ldots, \pm N). \tag{14}$$

Each μ_i is called a "stream", and (14) represents a "$2N$—stream approximation".

Writing (10) in quadratured form, S^m becomes a linear combination of I^m values at all quadrature angles μ_j ($j = \pm 1, \ldots, \pm N$),

$$S^m(\tau,\mu_i) = \sum_{\substack{j=-N \\ j\neq 0}}^{N} w_j D^m\big(\tau,\mu_i,\mu_j\big) I^m\big(\tau,\mu_j\big) + Q^m(\tau,\mu_i). \tag{15}$$

This approach makes the system coupled in i, but not in m.

In DISORT we draw the μ_i from a Gaussian quadrature rule for [0, 1] and have them mirror symmetric ($\mu_{-i} = -\mu_i$, where $\mu_i > 0$) with weights $w_{-i} = w_i$. This scheme is the so-called "Double-Gauss" quadrature rule suggested by Sykes (1951) in which Gaussian quadrature is applied separately to the half-ranges $-1 < \mu < 0$ and $0 < \mu < 1$. The main advantage is that even-order quadrature points are distributed symmetrically around $|\mu| = 0.5$ and clustered both toward $|\mu| = 1$ and $\mu = 0$,