Journal of Computational and Applied Mathematics 228 (2009) 104–114

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Numerical performance of stability enhancing and speed increasing steps in radiative transfer solution methods☆

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ARTICLE INFO

Article history:
Received 13 June 2006
Received in revised form 25 June 2008

MSC:
45J05
65R20
65Y20
85A25

Keywords:
Radiative transfer
Solution method
Numerical performance
Stability
Speed
Accuracy

ABSTRACT

Methods for solving the radiative transfer problem, which is crucial for a number of sectors of industry, involve several numerical challenges. This paper gives a systematic presentation of *the effect* of the steps that are needed or possible to make *any* discrete ordinate radiative transfer solution method numerically efficient. This is done through studies of the numerical performance of the stability enhancing and speed increasing steps used in modern tools like DISORT or DORT2002.

Performance tests illustrate the effect of steps that are taken to improve the stability and speed. It is shown how the steps together give a stable solution procedure to a problem previously considered numerically intractable, and how they together decrease the computation time compared to a naive implementation with a factor 1000 in typical cases and far beyond in extreme cases. It is also shown that the speed increasing steps are not introduced at the cost of reduced accuracy. Further studies and developments, which can have a positive impact on computation time, are suggested.

1. Introduction

Radiative transfer solution methods are important tools for modelling the interaction of radiation with turbid (scattering and absorbing) media. Applications range from stellar atmospheres and infrared and visible light in space and in the atmosphere, to optical tomography and diffusion of neutrons. An industrially important application is light scattering in textile, paint, pigment films, paper and print, and accurate calculation methods are crucial for these sectors of industry.

Discrete ordinate solution methods for radiative transfer problems have been studied throughout the last century. In the beginning most radiative transfer problems were considered intractable because of numerical difficulties. Therefore coarse approximations were used, and methods developed slowly due to the lack of mathematical tools. The first approximate solution to the radiative transfer problem was presented by Schuster [11], and Wick [20] gave the first general treatment of discrete ordinate methods. Chandrasekhar described a method using spherical harmonics [1], but having read Wick's article, he adopted the discrete ordinate method, and further refined it [2]. Later, he wrote a classic exposition on radiative transfer theory in book form [3], and since then the area has expanded tremendously. Mudgett and Richards [8,9] described a discrete ordinate method for use in technology, and reported on numerical difficulties, as have many before and after them.

Through a great effort, ranging over several years, Stamnes and coworkers [17,15] presented in a series of papers the successive development of a stable discrete ordinate algorithm, and provided a software package, DISORT. Thomas and

☆ This work was financially supported by the Swedish printing research program T2F, 'TryckTeknisk Forskning'.
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doi:10.1016/j.cam.2008.08.045

Stamnes [19] also wrote a textbook on radiative transfer in the atmosphere. In a recent paper, Edström [4] presented a systematic review of the stability enhancing and speed increasing steps used in modern discrete ordinate radiative transfer algorithms. Edström also presented the solution method Dort2002, which is adapted to light scattering simulations in paper and print, but which is also designed for methodical numerical experiments through its modularized design and ability to give any kind of intermediate results and performance data.

The point of this paper is to give a systematic presentation of *the effect* of the steps that are needed or possible to make *any* discrete ordinate radiative transfer solution method numerically efficient, and in particular the effect of the most important steps used in modern tools like Disort or Dort2002. To the author's knowledge, this has not been summarized in one single publication before, in particular not with the focus on quantifying the effect of the steps.

First, a short overview of a generic solution method is given. Then the resulting improvements, quantified in terms of reduced condition number and increased speed compared to a naive implementation, are illustrated. The speed increasing steps are also analyzed to verify that speed is not introduced at the cost of reduced accuracy. Finally, some studies and developments that can have a positive impact on computation time are suggested.

2. Solution method overview

This section gives a short introduction to the radiative transfer problem, and the structure of a modern generic discrete ordinate solution method.

Edström [4] states the equation of radiative transfer as

$$u\frac{\mathrm{d}I(\tau,u,\varphi)}{\mathrm{d}\tau}=I(\tau,u,\varphi)-\frac{a}{4\pi}\int_0^{2\pi}\int_{-1}^{1}p(u',\varphi';u,\varphi)I(\tau,u',\varphi')\mathrm{d}u'\mathrm{d}\varphi'. \tag{1}$$

The unknown intensity, I, at optical depth τ is considered as non-interacting beams of radiation in all directions. The phase function, p, specifies the probability distribution of scattering from incident direction (u',φ') to direction (u,φ), where u is cosine of polar angle, and φ is azimuthal angle. The shape of the phase function may be controlled by a parameter called the asymmetry factor, g, ranging from complete forward scattering ($g=1$) over isotropic scattering ($g=0$) to complete backward scattering ($g=-1$), or it may be defined by any number of discrete phase space moments. The single scattering albedo, a, is the probability for scattering given an extinction event, and is defined as $a=\sigma_s/(\sigma_a+\sigma_s)$, where σ_s and σ_a are the scattering and absorption coefficients of the medium. The first term on the right-hand side in the radiative transfer equation (1) thus gives intensity absorbed when traversing a thickness $\mathrm{d}\tau$, while the integral term gives the intensity scattered from all incoming directions at a point to a specified direction.

The common procedure in discrete ordinate methods is to use Fourier analysis on the azimuthal angle to turn the integro-differential equation (1) into a number of uncoupled equations, one for each Fourier component of the unknown intensity, which are then discretized using numerical quadrature. By introducing the function

$$p^m(u',u)=\sum_{l=m}^{2N-1}(2l+1)\chi_l\Lambda_l^m(u')\Lambda_l^m(u),$$

where the χ_l are Legendre expansion coefficients and the $\Lambda_l^m(u)$ are normalized associated Legendre functions, the phase function can be expressed in a Fourier cosine series as

$$p(u',\varphi';u,\varphi)=\sum_{m=0}^{2N-1}(2-\delta_{0m})p^m(u',u)\cos(m(\varphi'-\varphi)),$$

and the intensity can be expanded in a similar way as

$$I(\tau,u,\varphi)=\sum_{m=0}^{2N-1}I^m(\tau,u)\cos(m(\varphi_0-\varphi)),$$

where $2N$ is the number of quadrature points. The Double-Gauss quadrature formula, proposed by Sykes [18], approximates an integral over the two hemispheres separately,

$$\int_{-1}^{1}f(u)\mathrm{d}u=\int_0^1 f^+(\mu)\mathrm{d}\mu+\int_0^1 f^-(\mu)\mathrm{d}\mu\approx\sum_{j=1}^{N}\omega_j f^+(\mu_j)+\sum_{j=1}^{N}\omega_j f^-(\mu_j),$$

where the quadrature points μ_j and weights ω_j are chosen for the "half interval" [0, 1] according to ordinary Gaussian quadrature on the interval $0\le\mu\le 1$ (the plus and minus signs designate quantities in the upper and lower hemispheres). Application of the Double-Gauss quadrature rule is what is called the discrete ordinate approximation, and this gives for each Fourier component (where the superscript m has been dropped)