Algorithm of Numerical Calculation on Lorentz Mie Theory

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Abstract

In this work an improved algorithm is presented. The quantities related with the scattering coefficients are calculated by means of the downward or upward recurrences of Riccati-Bessel functions respectively, which are proved to be stable. Numerical calculation shows that the algorithm is efficient, reliable and robust in a wide range of particle size and refractive index.

Introduction

Techniques of particle size analysis based on light scattering have been developed for several decades and have been applied in a lot of fields. The measurements involve numerical analysis based on the scattering theory for spherical particles developed by Mie [1]. Its mathematical solution was obtained as an infinite series of terms. The development of computer technology has made it feasible to sum these terms numerically, and there have been many numerical computational studies of scattering functions, most of those were contributed by Infeld [2], Dave [3-5], Lentz [6], Wiscombe [7-8] and etc. However, the situation is still not so satisfying. The Mie scattering shows strong variations with scattering angle when the size of the particle is large compared to the wavelength. For some applications, it is desirable to evaluate the field of the scattered radiation at many scattering angles. Furthermore, when one is interested in scattering properties of a polydispersed particle system, it is necessary to compute the scattering light for several hundred values of particle size for good reliability. Such computational tasks can be very tedious and time consuming. Therefore, the computation speed should be efficient and the algorithm should be capable to give accurate and reliable solution for a wide range of particle size and refractive index.

In this work, we propose an efficient numerical procedure for computing the Mie scattering. Some exemplifying results will be presented.

Improved Algorithm

The Mie scattering coefficients are usually expressed as:

$$\begin{aligned} a_n &= \frac{\psi_n(\alpha)\psi_n'(m\alpha) - m\psi_n'(\alpha)\psi_n(m\alpha)}{\zeta_n(\alpha)\psi_n'(m\alpha) - m\zeta_n'(\alpha)\psi_n(m\alpha)} \\ b_n &= \frac{m\psi_n(\alpha)\psi_n'(m\alpha) - \psi_n'(\alpha)\psi_n(m\alpha)}{m\zeta_n(\alpha)\psi_n'(m\alpha) - \zeta_n'(\alpha)\psi_n(m\alpha)} \end{aligned} \tag{1}$$

which require the calculation of Riccati-Bessel functions $\psi_n(m\alpha)$ and $\zeta_n(\alpha)$. Here m is the ratio of the refractive index of the particle to the medium, α is the particle size parameter defined as $\pi x/\lambda$ where x is the particle diameter and λ is the wavelength. The calculation of $\psi_n(m\alpha)$ can be a problem because it may overflow if the particle is large and absorbent. So the logarithmic derivative of $\psi_n(m\alpha)$ was introduced, by Infeld [2] and Dave [3-5]. The Mie coefficients are then written as

$$\begin{aligned} a_n &= \frac{\psi_n(\alpha)L_n(m\alpha) - m\psi_n'(\alpha)}{\zeta_n(\alpha)L_n(m\alpha) - m\zeta_n'(\alpha)} \\ b_n &= \frac{m\psi_n(\alpha)L_n(m\alpha) - \psi_n'(\alpha)}{m\zeta_n(\alpha)L_n(m\alpha) - \zeta_n'(\alpha)} \end{aligned} \tag{2}$$

whereby $L_n(m\alpha)$ is the logarithmic derivative of $\psi_n(m\alpha)$ defined as

$$L_n(m\alpha) = \psi_n'(m\alpha)/\psi_n(m\alpha) \tag{3}$$

This might be the most important progress in Mie calculation, which solves the overflow problem. The calculation of $L_n(m\alpha)$ can be executed with a stable downward recurrence starting from an initial value of $L_{n^*}(m\alpha)$. The initial order n^* can refer to the criterion n_{stop} given by Wiscombe [7]. Usually, n^* is an integer larger than n_{stop}. The initial value of $L_{n^*}(m\alpha)$ can be expressed as a continued fractional function and be calculated with the method developed by Lentz [6]. The stopping order n_{stop} given by Wiscombe is

$$n_{wis} = \begin{cases} \alpha + 4\alpha^{1/3} + 1, & 0.02 \le \alpha \le 8 \\ \alpha + 4.05\alpha^{1/3} + 2, & 8 < \alpha < 4200 \\ \alpha + 4\alpha^{1/3} + 2, & 4200 \le \alpha \le 20000 \end{cases} \tag{4}$$

which is empirical and it lacks a clear explanation. So in this work we re-express the Mie coefficients with

$$\begin{aligned} a_n &= A_n(\alpha) \cdot T_{a_n}(m, \alpha) \\ b_n &= A_n(\alpha) \cdot T_{b_n}(m, \alpha) \end{aligned} \tag{5}$$

The parameters $A_n(\alpha)$, $T_{a_n}(m, \alpha)$ and $T_{b_n}(m, \alpha)$ are defined as

$$\begin{aligned} A_n(\alpha) &= \psi_n(\alpha)/\zeta_n(\alpha) \\ T_{a_n}(m, \alpha) &= \frac{L_n(m\alpha)/m - L_n(\alpha)}{L_n(m\alpha)/m - B_n(\alpha)} \\ T_{b_n}(m, \alpha) &= \frac{mL_n(m\alpha) - L_n(\alpha)}{mL_n(m\alpha) - B_n(\alpha)} \end{aligned} \tag{6}$$

where

$$B_n(\alpha) = \zeta_n'(\alpha)/\zeta_n(\alpha) \tag{7}$$

Therefore, the Mie calculation comes down to the calculation of $A_n(\alpha)$, $B_n(\alpha)$, $L_n(\alpha)$ and $L_n(m\alpha)$. $L_n(\alpha)$ and $L_n(m\alpha)$ can be calculated with the down ward recurrence starting from a pre-determined initial order n^*. Initial values of $L_{n^*}(\alpha)$ and $L_{n^*}(m\alpha)$ are calculated with the Lentz's method, which can be computed very fast when $n^* > \alpha$ or $n^* > |m\alpha|$. Values of $L_n(\alpha)$ are stored in an array for the further calculation of $A_n(\alpha)$ and $B_n(\alpha)$. The calculation of $A_n(\alpha)$ and $B_n(\alpha)$ can be executed with the upward recurrences given below

$$\begin{aligned} A_n(\alpha) &= A_{n-1}(\alpha) \cdot \frac{B_n(\alpha) + n/\alpha}{L_n(\alpha) + n/\alpha} \\ B_n(\alpha) &= -n/\alpha + [n/\alpha - B_{n-1}(\alpha)]^{-1} \end{aligned} \tag{8}$$

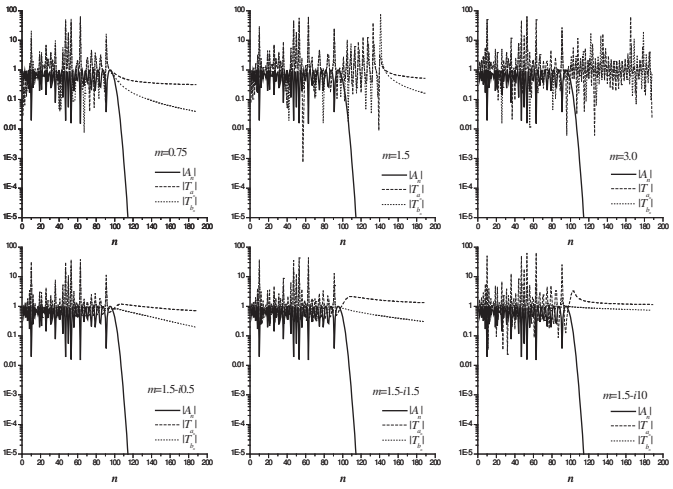

Figure 1: calculated results on $|A_n(\alpha)|$, $|T_{a_n}(m, \alpha)|$ and $|T_{b_n}(m, \alpha)|$ for $\alpha = 100$

The initial values are

$$\begin{aligned} A_1(\alpha) &= (1 + i\frac{\cos\alpha + \alpha\sin\alpha}{\sin\alpha - \alpha\cos\alpha})^{-1} \\ B_0(\alpha) &= -i \end{aligned} \tag{9}$$

$A_n(\alpha)$ should not start from $A_0(\alpha) = (1 + i\cot\alpha)^{-1}$ because it may leads to $A_n(\alpha) \equiv 0$ if α is times of π.

The numerical calculation shows that, for a certain particle size parameter α, the parameters $|A_n(\alpha)|$, $|T_{a_n}(m,\alpha)|$ and $|T_{b_n}(m,\alpha)|$, oscillate violently if the order n is less than α. As n is larger than α, $|T_{a_n}(m,\alpha)|$ and $|T_{b_n}(m,\alpha)|$ tend to decrease slowly and smoothly, while $|A_n(\alpha)|$ decreases very strongly (as shown in Fig.1). So the stopping order is mainly determined by the characteristic of $|A_n(\alpha)|$. Analyzing the numerical results in the range of $\alpha \in (0, 100000)$, we get the criterion of the stopping order for different precisions

$$n_{stop} = \begin{cases} \alpha + 7.5\alpha^{0.34} + 2 & |A_n(\alpha)| < 1e-18 \\ \alpha + 6\alpha^{1/3} + 2 & |A_n(\alpha)| < 1e-12 \\ \alpha + 4.88\alpha^{0.31} & |A_n(\alpha)| < 1e-5 \end{cases} \tag{10}$$

which offers a more detailed understanding of the stopping order and a possibility to control the precision of calculation.

Looking more into the detail, we find that the turning point of $|T_{a_n}(m,\alpha)|$ and $|T_{b_n}(m,\alpha)|$ from violent oscillation to smooth variation is slightly dependent on the refractive index m. However, this is not very important due to the fact that values of $|T_{a_n}(m,\alpha)|$ and $|T_{b_n}(m,\alpha)|$ are not larger than the particle size parameter α for $n > \alpha$.

The advantages of the improved algorithm presented here are that no restriction in the range of particle size and refractive index is found, the calculation is very stable and numerical results can be achieved accurately and very fast. Some exemplifying results are given in Table 1 comparing the accuracy of the calculation and in Table 2 for the comparison of the computation speed. The calculation is executed with a double-precision C++ code on a personal computer powered by a 2.66GHz P4 CPU. In Table 1, a complete match is found between the results calculated with different methods. From Table 2, we may find that the Lentz's method requires the most CPU time especially for calculating large particles and the method proposed in this work runs almost

Table 1: Comparison of k_{ext} and k_{sca} calculated with MIEV0, MIECPP [9] and in this work.

			k_{ext}		k_{sca}	
Case	m	α	MIEV0 MIECPP	This work	MIEV0 MIECPP	This work
(1)	0.75	0.099	7.41786e-5	7.41786e-5	7.41786e-5	7.41786e-5
(2)	0.75	0.101	8.03354e-6	8.03354e-6	8.03354e-6	8.03354e-6
(3)	0.75	10	2.23226	2.23226	2.23226	2.23226
(4)	0.75	1000	1.99791	1.99791	1.99791	1.99791
(5)	1.33-i 1e-5	100	2.10132	2.10132	2.09659	2.09659
(6)	1.33-i 1e-5	10000	2.00409	2.00409	1.72386	1.72386
(7)	1.5-i	0.055	0.101491	0.101491	1.13169e-5	1.13169e-5
(8)	1.5-i	0.056	0.1003347	0.1003347	1.21631e-5	1.21631e-5
(9)	1.5-i	100	2.09750	2.09750	1.28370	1.28370
(10)	1.5-i	1000	2.00437	2.00437	1.23657	1.23657
(11)	10-i10	1	2.53229	2.53229	2.04941	2.04941
(12)	10-i10	100	2.07112	2.07112	1.83679	1.83679
(13)	10-i10	10000	2.00591	2.00591	1.79539	1.79539

Table 2: Comparison of CPU time between different algorithms for computing k_{ext} and k_{sca}.

Case	Upward recursion Sec	Lentz's method Sec	This work Sec
(1)	9.28e-6	1.95e-5	1.55e-5
(2)	9.45e-6	1.91e-5	1.58e-5
(3)	3.70e-5	2.29e-4	5.73e-5
(4)	1.93e-3	2.51e-1	1.80e-3
(5)	2.40e-4	1.04e-2	2.60e-4
(6)	1.88e-2	6.51e+1	1.87e-2
(7)	1.32e-5	2.36e-5	1.39e-5
(8)	1.33e-5	2.28e-5	1.41e-5
(9)	2.47e-4	6.37e-3	2.55e-4
(10)	-	1.05e-1	1.80e-3
(11)	2.04e-5	1.78e-4	3.41e-5
(12)	-	2.14e-2	3.35e-4
(13)	-	6.80e+0	1.71e-2

as fast as the straight-forward method, except for the cases (4), (10), (12) and (13) where algorithm with the upward recursion fails due to the fact that the upward recursion breaks down before the summation of the terms is stopped by the criterion.

Conclusion

In this work, an improved algorithm of Mie calculation is proposed, whereby the Mie coefficients are reconstructed. In this way, the stopping order can be predetermined depending on the particle size parameter with controllable precision. Exemplifying results are given to check the accuracy, the stability and the robustness of the method. The CPU time is tabulated to compare the calculation speed between different methods. The algorithm is proved to be accurate, robust and efficient.

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