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T-matrix computations of light scattering by large spheroidal particles

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Abstract

It is well known that T-matrix computations of light scattering by nonspherical particles may suffer from the ill-conditionality of the process of matrix inversion, which has precluded calculations for particle size parameters larger than about 25. It is demonstrated that calculating the T-matrix using extended-precision instead of double-precision floating-point variables is an effective approach for suppressing the numerical instability in computations for spheroids and allows one to increase the maximum particle size parameter for which T-matrix computations converge by as significant a factor as 2–2.7. Yet this approach requires only a negligibly small extra memory, an affordable increase in CPU time consumption, and practically no additional programming effort. As a result, the range of particle size parameters, for which rigorous T-matrix computations of spheroidal scattering can be performed, now covers a substantial fraction of the gap between the domains of applicability of the Rayleigh and geometrical optics approximations.

It is well known that light scattering by nonspherical particles much smaller and much larger than a wavelength of light is well described by the Rayleigh and geometrical optics approximations, respectively [1–3]. On the other hand, scattering properties of particles with sizes comparable to the wavelength (so-called resonance particles) are complicated functions of the particle size parameter, shape, and refractive index and should be computed by directly solving Maxwell's equations. Apparently, the fastest and most powerful numerical tool for rigorously computing nonspherical light scattering in the resonance region of size parameters is the T-matrix method [4]. However, even with this method, computations were rarely reported for size parameters exceeding 25, which is explained by the numerical instability of the method at higher frequencies. The origin of this numerical instability is discussed in Ref. [5]. In brief, in the T-matrix method the electric fields incident on (superscript i) and scattered by (superscript s) a particle are expanded in series of vector spherical functions as follows:

$$\boldsymbol{E}^{\mathrm{i}}(\boldsymbol{r}) = \sum_{nm} [a_{mn}\,\mathrm{Rg}\boldsymbol{M}_{mn}(k\boldsymbol{r}) + b_{mn}\,\mathrm{Rg}\boldsymbol{N}_{mn}(k\boldsymbol{r})]\,, \tag{1}$$

$$\boldsymbol{E}^{\mathrm{s}}(\boldsymbol{r}) = \sum_{nm} [p_{mn}\boldsymbol{M}_{mn}(k\boldsymbol{r}) + q_{mn}\boldsymbol{N}_{mn}(k\boldsymbol{r})]\,, \tag{2}$$

where $k = 2\pi/\lambda$ is a free-space wavenumber and λ is a free-space wavelength. The vector spherical functions $\mathrm{Rg}\boldsymbol{M}_{mn}$ and $\mathrm{Rg}\boldsymbol{N}_{mn}$ in Eq. (1) have a Bessel function radial dependence, while the functions $\boldsymbol{M}_{mn}$

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and N_{mn} in Eq. (2) have a Hankel function radial dependence. The expansion coefficients of the incident plane wave a_{mn} and b_{mn} are given by simple analytical expressions (see, e.g., Ref. [6]), whereas the expansion coefficients of the scattered field p_{mn} and q_{mn} are initially unknown. Because of the linearity of Maxwell's equations, the relation between the expansion coefficients of the incident and scattered fields is linear and is given by a transition matrix (or T matrix) **T** as follows:

$$\begin{bmatrix} \boldsymbol{p} \\ \boldsymbol{q} \end{bmatrix} = \mathbf{T} \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{bmatrix}, \tag{3}$$

where compact matrix notations are used. The elements of the T matrix are independent of the incident and scattered fields and depend only on the shape, size parameter, and refractive index of the scattering particle as well as on its orientation with respect to the reference frame. Thus, to calculate the scattered field, the T matrix should be computed beforehand for a given scattering particle. The T matrix can be represented in the form $\mathbf{T} = -\mathbf{Q}^{-1}\,\mathrm{Rg}\mathbf{Q}$, where the elements of the matrices **Q** and Rg**Q** can be computed for given particle shape, refractive index, and size parameter by using formulas derived by Waterman [4]. Although theoretically the expansions (1) and (2) and, therefore, the matrices **T**, **Q** and Rg**Q** are of infinite size, in practical computer calculations they must be truncated to a finite maximum size. This maximum size depends on the required accuracy of computations and is determined by increasing the size of the matrices **Q** and Rg**Q** in unit steps until some convergence criteria (like those described in Refs. [7] and [8]) are satisfied. Unfortunately, calculation of the inverse matrix $\mathbf{Q}^{-1}$ is an ill-conditioned process strongly influenced by round-off errors. The ill-conditioning means that even small numerical errors in the computed elements of the matrix **Q** may result in (very) big errors in the elements of the inverse matrix $\mathbf{Q}^{-1}$. The round-off errors become increasingly significant with increasing particle size and/or aspect ratio and rapidly accumulate with increasing size of the matrix **Q**. As a result, for large and/or highly aspherical particles, for which the convergent size of the T matrix should be large, T-matrix computations may become very slowly convergent or even divergent.

To ameliorate the problem of numerical instability of the T-matrix method, the so-called iterative extended boundary condition method (IEBCM) [9] has recently been developed. However, the numerical stability of IEBCM is achieved at the expense of a considerable increase in computer code complexity and CPU time consumption. As a result, this method has not been used, to our knowledge, in computations of nonspherical scattering for large size parameters.

An alternative method for dealing with the ill-conditioning of the numerical inversion of the matrix **Q** is to improve the accuracy with which this matrix is calculated and inverted. To do that, we calculated the elements of this matrix and performed the matrix inversion using extended-precision (REAL*16 and COMPLEX*32) instead of double-precision (REAL*8 and COMPLEX*16) floating-point variables. We performed our calculations on IBM RISC workstations for which the accuracy of double-precision and extended-precision variables is approximately 15 and 31 decimal digits, respectively. Table 1 compares the results obtained using both types of variables and shows the maximum size parameter for which convergence within a given accuracy can be achieved depending on the asphericity of the scattering particle. The calculations have been carried out for randomly oriented spheroids using the analytical orientational averaging method developed in Ref. [10]. The refractive indices are 1.5+0.02i and 1.0925+0.248i. The first of these indices is typical of mineral tropospheric aerosols [11], while the second one corresponds to water ice at $\lambda = 11$ μm [12]. The aspect ratio of a spheroid is defined as the ratio of the major to minor spheroidal semi-axes. The spheroidal size parameter x_s is defined as the wavenumber times the major semi-axis, while the equal-surface-area-sphere size parameter x is defined as the wavenumber times the radius of the sphere having the surface area equal to that of the spheroid. The convergence criterion is described in detail in Ref. [8]. The T-matrix computations were considered convergent if the relative accuracy of computing the extinction and scattering cross sections was better than 10^{-4}. The effect of using extended accuracy variables is also demonstrated in Fig. 1 which shows the relative accuracy of computing the extinction and scattering cross sections for randomly oriented prolate spheroids as a function of the parameter $n_{\max}$

Table 1
Maximum convergent equal-surface-area-sphere size parameter x^{max} and spheroidal size parameter x_s^{max} for randomly oriented spheroids with refractive indices 1.5+0.02i and 1.0925+0.248i and aspect ratios 2, 3, and 4 depending on the type of computer variables.

Aspect ratio	Double precision		Extended precision	
	x^{max}	x_s^{max}	x^{max}	x_s^{max}
	1.5+0.02i Prolate spheroids			
2	29	44	61	93
3	10	19	26	49
4	6	13	16	35
	Oblate spheroids			
2	34	40	76	91
3	15	19	39	50
4	11	14	29	34
	1.0925+0.248i Prolate spheroids			
2	34	52	69	105
3	13	24	28	53
4	7	15	17	37
	Oblate spheroids			
2	41	49	87	104
3	19	24	42	54
4	13	17	29	38

specifying the maximum value of the index n in expansions (1) and (2). The refractive index of the spheroids is 1.5+0.02i and their equal-surface-area-sphere size parameter is $x=16$.

It is readily seen from Table 1 that using extended-precision variables is indeed a powerful tool enabling one to increase the maximum convergent size parameter by as significant a factor as 2–2.7. Timing tests performed on an IBM RISC Model 37T workstation show that the use of extended-precision instead of double-precision variables slows computations down by a factor of only 5–6. Taking into account that the T-matrix method, especially in application to randomly oriented scatterers [8,10], is orders of magnitude faster than any alternative method for rigorously calculating nonspherical scattering, this factor of 5–6 seems to be a reasonable cost of being able to compute much bigger nonspherical particles than ever

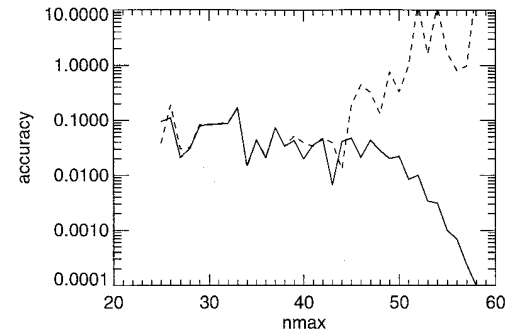

Fig. 1. Relative accuracy of computing the extinction and scattering cross sections for randomly oriented prolate spheroids versus parameter n_{max}, specifying the largest value of the index n in expansions (1) and (2). The spheroidal aspect ratio is 4, the equal-surface-area-sphere size parameter is $x=16$, and the index of refraction is 1.5+0.02i. The solid and dashed lines show results obtained using extended-precision and double-precision variables, respectively.

before (cf. Refs. [13–22]). An additional advantage of this approach is that it does not require any additional programming effort. Also, the use of extended-precision instead of double-precision variables requires only a negligibly small extra memory. Indeed, for rotationally symmetric particles the T matrix in the natural reference frame with the z-axis along the axis of rotation is composed of $n_{max}+1$ independent square $[2n_{max}\times 2n_{max}]$ submatrices corresponding to different values of the azimuthal mode m [6,7]. Since these m-submatrices are independent of one another, they can be successively computed using the same auxiliary two-dimensional $[2n_{max}\times 2n_{max}]$ array and then stored in a three-dimensional $[(n_{max}+1)\times 2n_{max}\times 2n_{max}]$ array. If extended-precision instead of double-precision variables are used to compute bigger and/or more aspherical particles, only the small auxiliary array doubles its size, while the big three-dimensional array containing already computed T matrix elements may preserve its type (COMPLEX*16 or COMPLEX*8) and, thus, its size.

We have extensively tested the accuracy of our T-matrix code versus previously published computations for spheroids [13,16,17,20] and so-called Chebyshev particles [7]. Since no nonspherical data have been published for the largest size parameters that our code can handle, we tested our computations in that size parameter range versus Mie calculations for spheres and rigorous inequalities that must be satis-

fied by any physically correct scattering matrices [23–25].

To demonstrate the capabilities of the new approach, Fig. 2 shows the degree of linear polarization (i.e., the ratio $-F_{12}/F_{11}$ of the elements of the scattering matrix [2]) for monodisperse spheres and surface-area-equivalent randomly oriented oblate spheroids with the aspect ratio 3. The index of refraction is 1.5+0.022i. We have chosen linear polarization for this example because spherical/nonspherical differences are much more pronounced in polarization than in intensity. In particular, even the sign of polarization may be different for spheres and surface-equivalent nonspherical particles of the same refractive index. For spheres, the polarization is shown as a function of the size parameter kr, where r is the sphere radius. For the spheroids, the polarization is displayed as a function of the equal-surface-area-sphere size parameter x. It is seen that for spheres, the diagram is essentially a field of sharp local maxima and minima resulting from the optical interference phenomena for monodisperse particles (cf. Fig. 19 in Ref. [2]). For the highly aspherical randomly oriented spheroids, the interference structure is much less pronounced, thus demonstrating the smoothing effect of averaging over orientations of a nonspherical particle [13]. It is also seen that for nonspherical particles, the geometrical optics regime (polarization is independent of x) may be reached at smaller size parameters than for surface-equivalent spheres. Apparently, this can be explained by the smoothing effect of the orientational averaging. The spheroidal polarization is positive at most scattering angles, especially for larger size parameters. An interesting feature of the spheroidal pattern is the bridge of positive polarization at side-scattering angles, which extends upwards from the region of Rayleigh scattering (size parameters less than about 1) and separates two regions of negative polarization at small and large scattering angles. This bridge of positive polarization at side-scattering angles may be a common property of nonspherical scattering and was first found by Perry et al. [26] in their laboratory measurements for wavelength-sized nearly cubically shaped NaCl particles and then by Asano and Sato [13] in their theoretical computations for spheroids. Note that the lower panel in Fig. 2 involves calculations for 400 spheroids in random orientation and was computed in 50 hours on the IBM RISC Model 37T workstation.

In conclusion, it follows from our calculations and discussion that the T-matrix method has no fundamental limitations on the upper size parameter and aspect ratio of spheroids. To calculate light scattering by bigger and/or more aspherical particles, one must just increase the number of decimal digits with which the matrix **Q** is computed and inverted. In particular, we have demonstrated that, for a given aspect ratio, the use of extended-precision instead of double-precision variables in computing the T matrix results in an increase of the maximum convergent size parameter by a factor of 2–2.7. Yet this approach requires only a negligibly small extra memory, an affordable increase in CPU time consumption, and practically no additional programming effort. Using extended-precision variables, T-matrix calculations of spheroidal scattering can be performed in a substantial fraction of the resonance region of particle size parameters (ranging from about 0.1 to about 100) where the Rayleigh approximation cannot be used because particles are too large, while the geometrical optics approximation is not applicable because particles are too small. Moreover, our illustrative computations show that nonspherical particles can reach the geometrical optics regime at smaller size parameters than surface-equivalent spheres. The results of this Communication may have important practical implications. In particular, they make the T-matrix method applicable in studies of nonspherical tropospheric aerosols in the visible and cirrus cloud particles in the infrared spectral regions [27–30]. Finally, we note that numerical instability similar to that for the T-matrix method was reported by Asano [31] for his method of separation of variables in the spheroidal coordinate system. Since Asano carried out his calculations with double-precision arithmetic, it would be interesting to see whether the use of extended-precision variables can improve the performance of the Asano method as well. Apparently, this problem would also affect Farafonov's [32,22] version of the separation of variables method.

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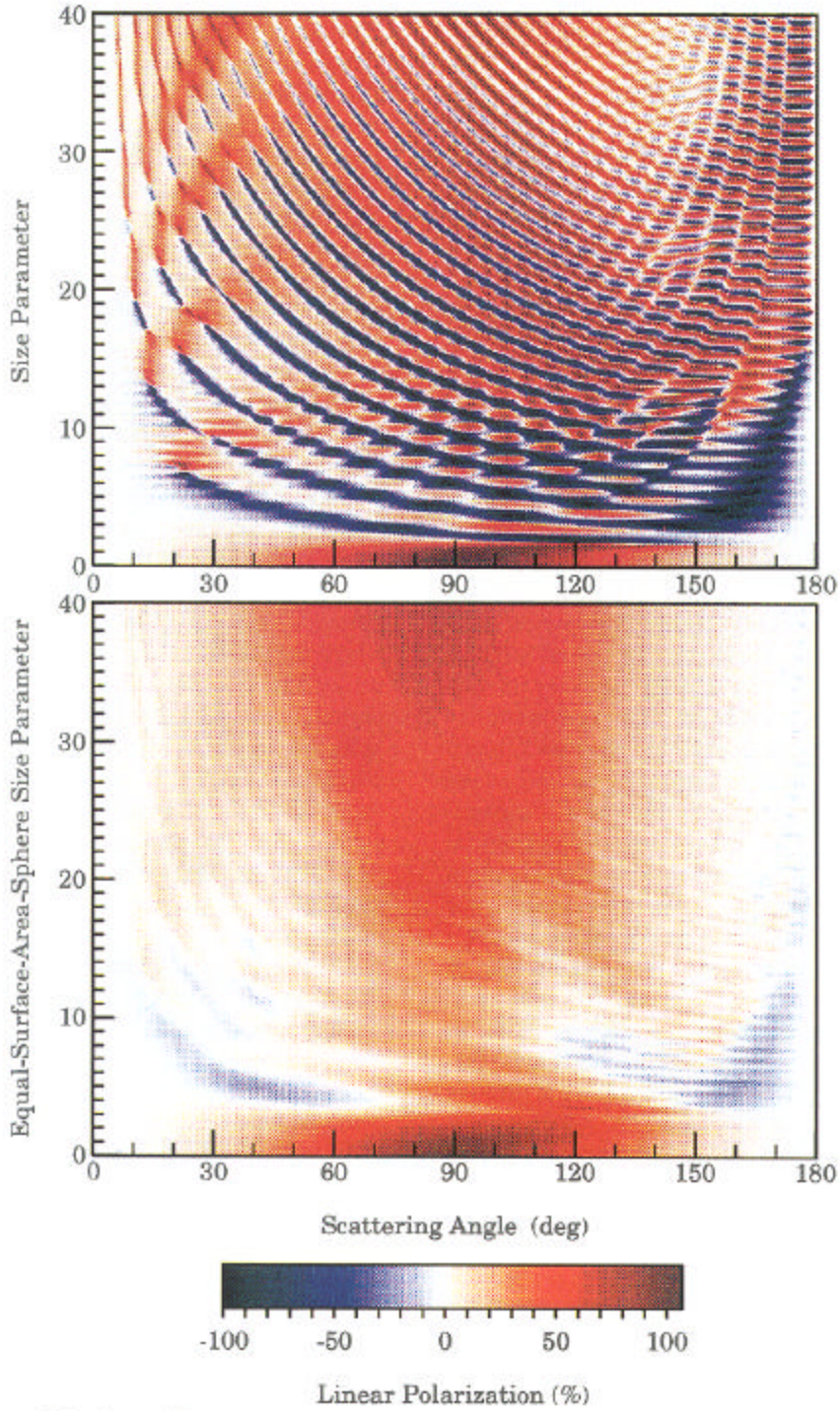

Fig. 2. Color diagram of the degree of linear polarization as a function of the scattering angle and size parameter. Calculations for monodisperse spheres (upper panel) are compared with computations for randomly oriented surface-equivalent oblate spheroids with the aspect ratio 4 (lower panel). The refractive index is 1.5+0.022i.

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