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Calculation of the T -matrix: general considerations and application of the point-matching method

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Abstract

The T -matrix method is widely used for the calculation of scattering by particles of sizes on the order of the illuminating wavelength. Although the extended boundary condition method (EBCM) is the most commonly used technique for calculating the T -matrix, a variety of methods can be used.

We consider some general principles of calculating T -matrices, and apply the point-matching method to calculate the T -matrix for particles devoid of symmetry. This method avoids the time-consuming surface integrals required by the EBCM.

Keywords: light scattering; electromagnetic scattering; nonspherical particles; T -matrix

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1 The T -matrix method

The T -matrix method in wave scattering involves writing the relationship between the wave incident upon a scatterer, expanded in terms of orthogonal eigenfunctions,

$$U_{\text{inc}} = \sum_n a_n \psi_n^{(\text{inc})}, \quad (1)$$

where a_n are the expansion coefficients for the incident wave, and the scattered wave, also expanded in terms of orthogonal eigenfunctions,

$$U_{\text{scat}} = \sum_k p_k \psi_k^{(\text{scat})}, \quad (2)$$

where p_k are the expansion coefficients for the scattered wave, is written as a simple matrix equation

$$p_k = \sum_n T_{kn} a_n \quad (3)$$

or, in more concise notation,

$$\mathbf{P} = \mathbf{T}\mathbf{A} \quad (4)$$

where T_{kn} are the elements of the T -matrix. The T -matrix method can be used for scalar waves or vector waves in a variety of geometries, with the only restrictions being that the geometry of the problem permits expansion of the waves as discrete series in terms of orthogonal eigenfunctions, that the response of the scatterer to the incident wave is linear, and that the expansion series for the

waves can be truncated at a finite number of terms. In general, one calculates the T -matrix, although it is conceivable that it might be measured experimentally.

The T -matrix depends only on the particle—its composition, size, shape, and orientation—and is independent of the incident field. This means that for any particular particle, the T -matrix only needs to be calculated once, and can then be used for repeated calculations. This is a significant advantage over many other methods of calculating scattering where the entire calculation needs to be repeated [1]. Some cases provide even more efficiency: if the waves are expanded in spherical functions, the averaging of scattering over various orientations of the particle compared to the direction of the incident wave can be performed analytically [2].

In the spherical geometry of elastic light scattering by a particle contained entirely within some radius r_0 , the eigenfunction expansions of the fields are made in terms of vector spherical wavefunctions (VSWFs) [1–7]:

$$\mathbf{M}_{nm}^{(1,2)}(kr) = N_n h_n^{(1,2)}(kr) \mathbf{C}_{nm}(\theta, \phi) \quad (5)$$

$$\begin{aligned} \mathbf{N}_{nm}^{(1,2)}(kr) &= \frac{h_n^{(1,2)}(kr)}{kr N_n} \mathbf{P}_{nm}(\theta, \phi) + \\ &N_n \left(h_{n-1}^{(1,2)}(kr) - \frac{nh_n^{(1,2)}(kr)}{kr} \right) \mathbf{B}_{nm}(\theta, \phi) \end{aligned} \quad (6)$$

where $h_n^{(1,2)}(kr)$ are spherical Hankel functions of the first and second kind, $N_n = 1/\sqrt{n(n+1)}$ are normalisation constants, and $\mathbf{B}_{nm}(\theta, \phi) = \mathbf{r} \nabla Y_n^m(\theta, \phi)$, $\mathbf{C}_{nm}(\theta, \phi) = \nabla \times (\mathbf{r} Y_n^m(\theta, \phi))$, and $\mathbf{P}_{nm}(\theta, \phi) = \hat{\mathbf{r}} Y_n^m(\theta, \phi)$ are the vector spherical harmonics [1–7], and $Y_n^m(\theta, \phi)$ are normalised scalar spherical harmonics. The usual polar spherical coordinates are used, where θ is the co-latitude measured from the $+z$ axis, and ϕ is the azimuth, measured from the $+x$ axis towards the $+y$ axis.

$\mathbf{M}_{nm}^{(1)}$ and $\mathbf{N}_{nm}^{(1)}$ are outward-propagating TE and TM multipole fields, while $\mathbf{M}_{nm}^{(2)}$ and $\mathbf{N}_{nm}^{(2)}$ are the corresponding inward-propagating multipole fields. Since these wavefunctions are purely incoming and purely outgoing, each has a singularity at the origin. Since fields that are free of singularities are of interest, it is useful to define the singularity-free regular vector spherical wavefunctions:

$$\mathbf{RgM}_{nm}(kr) = \frac{1}{2} [\mathbf{M}_{nm}^{(1)}(kr) + \mathbf{M}_{nm}^{(2)}(kr)], \quad (7)$$

$$\mathbf{RgN}_{nm}(kr) = \frac{1}{2} [\mathbf{N}_{nm}^{(1)}(kr) + \mathbf{N}_{nm}^{(2)}(kr)]. \quad (8)$$

Since the spherical Bessel functions $j_n(kr) = \frac{1}{2}(h_n^{(1)}(kr) + h_n^{(2)}(kr))$, the regular VSWFs are identical to the incoming and outgoing VSWFs except for the replacement of the spherical Hankel functions by spherical Bessel functions.

Since the incident field, in the absence of a scatterer, is singularity-free, the expansion

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n a_{nm}^{(3)} \mathbf{RgM}_{nm}(kr) + b_{nm}^{(3)} \mathbf{RgN}_{nm}(kr) \quad (9)$$

is generally used for the incident field. Alternatively, the purely incoming part of the incident field can be used:

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n a_{nm}^{(2)} \mathbf{M}_{nm}^{(2)}(kr) + b_{nm}^{(2)} \mathbf{N}_{nm}^{(2)}(kr). \quad (10)$$

In both cases, the scattered field is

$$\mathbf{E}_{\text{scat}}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n p_{nm}^{(1)} \mathbf{M}_{nm}^{(1)}(kr) + q_{nm}^{(1)} \mathbf{N}_{nm}^{(1)}(kr). \quad (11)$$

The two sets of expansion coefficients for the incident/incoming field are related, since $a_{nm}^{(3)} = 2a_{nm}^{(2)}$ and $b_{nm}^{(3)} = 2b_{nm}^{(2)}$. However, the scattered/outgoing field expansion coefficients will differ, as will the T -matrix. Using the regular expansion, the T -matrix in the absence of a scatterer is a zero matrix, while using the incoming field expansion, the no-scatterer T -matrix is the identity matrix. The

two expansions are essentially the same—the only difference is that the incident wave in the incident/scattered wave expansion includes part of the outgoing wave. T -matrices for the two expansions only differ by the identity matrix, so $\mathbf{T}^{(\text{in/out})} = 2\mathbf{T}^{(\text{inc/scat})} + \mathbf{I}$. The incident/scattered formulation is much more commonly used; the incoming/outgoing formulation gives simpler results for the transport of momentum and angular momentum (that is, optical force and torque) by the field. It should be noted that for plane wave illumination, for which the VSWF expansion is non-terminating, the incident/scattered formulation gives a scattered wave expansion that converges over all space, while the incoming/outgoing expansion, strictly used, would give a non-terminating, non-convergent outgoing field expansion. For focussed beam illumination with a finite VSWF expansion, the incoming/outgoing expansion directly gives the total outgoing field that would be experimentally measured. Since conversion from one formulation to the other is simple, either can be readily used for calculation of fields, forces, scattering matrices, or for orientation averaging.

In practice, the field expansions and the T -matrix are terminated at some $n = N_{\text{max}}$. For the case of a scatterer that is contained within a radius r_0 , $N_{\text{max}} \approx kr_0$ is usually adequate, but $N_{\text{max}} = kr_0 + 3\sqrt[3]{kr_0}$ is advisable if higher accuracy is needed [7]. Although we assume in this paper (as is usually the case) that the incident and scattered wave expansions are terminated at the same N_{max} (giving a square T -matrix), this is not necessary. It should be noted that convergence of the expansion of the incident field is not a necessary condition for the T -matrix method to be useful—indeed, for the most common application, scattering of an incident plane wave, the incident field expansion does not converge over all space. However, it does converge within the radius r_0 —which is the part of the field that can affect the scattering particle—and therefore, the field expansions and the T -matrix can be truncated at a finite N_{max} .

For the case of plane wave scattering, the plane wave expansion formula is useful:

$$a_{nm} = 4\pi i^n N_n \mathbf{C}_{nm}^* \cdot \mathbf{E}_0, \quad b_{nm} = 4\pi i^{n-1} N_n \mathbf{B}_{nm}^* \cdot \mathbf{E}_0. \quad (12)$$

The main case of interest for non-plane wave incident illumination is that of focussed beams. A variety of methods can be used, such as plane wave expansion [8], the localised approximation [9–12], or the point-matching method [13].

The only remaining requirement is that the T -matrix be calculated. This requires essentially a complete calculation of the scattering properties of the scatterer. This is almost universally done using the extended boundary condition method (EBCM), originally developed by Waterman [3], which is so strongly linked with the T -matrix method that the terms “EBCM” and “ T -matrix method” are often used interchangeably. In the next section, we consider some general principles involved in the calculation of the T -matrix, and show that an alternative method—column-by-column calculation using the point-matching method (PMM)—is computationally feasible and simply implemented for homogeneous isotropic particles devoid of symmetry.

Lastly, before we continue to consider calculation of T -matrices in more detail, we can note that while the incident and scattered fields are usually expanded in terms of VSWFs, other sets of eigenfunctions, such as cylindrical wavefunctions (for scatterers of infinite length in one dimension), or a Floquet expansion (planar periodic scatterers), are more appropriate for other geometries. There is no requirement that the modes into which the incident and scattered fields are expanded be the same, or even similar. In all of these cases, the T -matrix method remains applicable.

2 Calculating the T -matrix

If the field expansions and T -matrix are truncated at some N_{max} , there are $N_T = 2N_{\text{max}}(N_{\text{max}} + 2)$ expansion coefficients for each of the incident and scattered fields, and the T -matrix is $N_T \times N_T$. Since N_{max} is proportional to the radius enclosing the particle, r_0 , the number of expansion coefficients is proportional to r_0^2 , and the number of elements in the T -matrix is proportional to r_0^4 . This can be used to obtain an estimate of the scaling of computational time for different methods of calculation.

2.1 The extended boundary condition method

In principle, any method of calculating scattering by the particle can be used to calculate the T -matrix. However, the method of choice is almost universally the EBCM [1–4]. In the EBCM, the internal field within the particle is expanded in terms of regular VSWFs. Therefore, the method is restricted to homogeneous and isotropic particles. Rather than considering the coupling of the incident and scattered fields directly, the coupling between the incident and internal (the \mathbf{RgQ} matrix), and scattered and internal fields (the \mathbf{Q} matrix) is calculated, and the T -matrix found from these ($\mathbf{T} = -\mathbf{RgQQ}^{-1}$). The \mathbf{RgQ} and \mathbf{Q} matrices are the same size as the T -matrix, with $O(N_{\max}^4)$ elements. The elements of these matrices are found by integrating over the surface of the scatterer, an operation requiring $O(N_{\max}^2)$ time per element, so the calculation of the \mathbf{RgQ} and \mathbf{Q} matrices is expected to require $O(N_{\max}^6)$ computational time. The actual calculation of the T -matrix, if direct inversion is naively used, takes $O(N_{\max}^6)$ time. In practice, the calculation of the \mathbf{RgQ} and \mathbf{Q} matrices dominates the computational time [14].

From this, it can be seen that the EBCM can be expected to be very slow for large particles. However, most applications of the EBCM have been for the special case of scattering particles rotationally symmetric about the z axis. In this case, scattered modes $\mathbf{M}_{n'm'}^{(1)}$ and $\mathbf{N}_{n'm'}^{(1)}$ only couple to incident modes \mathbf{RgM}_{nm} and \mathbf{RgN}_{nm} if $m' = m$, greatly reducing the number of matrix elements that need to be calculated, and the surface integral over the particle surface reduces to a one-dimensional integral over θ , since the azimuthal integration over ϕ can be simply done analytically [4]. This results in a great improvement in performance, and, in terms of computational time, EBCM is clearly the method of choice for axisymmetric particles. Numerical problems do occur when the scatterer is highly non-spherical. The discrete sources method is designed to overcome these problems [15]. For the even more symmetric case of a spherical scatterer, the scattered and incident modes only couple if $n' = n$ and $m' = m$, the T -matrix becomes diagonal, and all of the integrals can be performed analytically, and Mie's solution to scattering by a sphere [16] is simply obtained.

In a similar manner, scatterers with point-group rotational symmetry allow significant improvement of the computational time required through exploitation of the symmetry [14, 17, 18].

Methods have also been developed to calculate T -matrices for clusters of particles and for layered particles [1].

The efficiency of the EBCM for the calculation of the T -matrix is such that alternative methods need only be considered if the EBCM is inapplicable (such as when the particle is inhomogeneous or anisotropic), numerical difficulties are encountered using the EBCM (such as for extremely non-spherical particles), or if the scattering particle has no symmetries that can be used to optimise the computation of the T -matrix.

2.2 Methods other than the EBCM

Methods other than the EBCM can be used to calculate the T -matrix. In general, one would calculate the scattered field, given a particular incident field. The most direct way in which to use this to produce a T -matrix is to solve the scattering problem when the incident field is equal to a single spherical mode—that is, a single VSWF such as $\mathbf{E}_{\text{inc}}(\mathbf{r}) = \mathbf{RgM}_{11}(kr)$, $\mathbf{E}_{\text{inc}}(\mathbf{r}) = \mathbf{RgN}_{11}(kr)$, $\mathbf{E}_{\text{inc}}(\mathbf{r}) = \mathbf{RgM}_{21}(kr)$, etc, and repeat this for all VSWFs that need to be considered (up to $n = N_{\max}$). The expansion coefficients for the scattered field can be found in each case, if necessary, by using the orthogonal eigenfunction transform (the generalised Fourier transform), and each scattering calculation gives a single column of the T -matrix.

Therefore, the calculation of a T -matrix requires that $2N_{\max}(N_{\max} + 2)$ separate scattering problems are solved. This provides a criterion for deciding whether it is desirable to calculate a T -matrix: if more than $2N_{\max}(N_{\max} + 2)$ scattering calculations will be performed, then it is more efficient to calculate the T -matrix and use this for the repeated calculations than it is to use the original scattering method repeatedly. Repeated calculations are expected if orientation averaging is to be carried out, or if inhomogeneous illumination is to be considered, such as, for example, scattering by focussed beams, where there are generally 6 degrees of freedom, namely the three-dimensional position of the scatterer within the beam, and the three-dimensional orientation of the scatterer. Even if only a

modest number of points are considered along each degree of freedom, the total number of scattering calculations required rapidly becomes very large, and even if the T -matrix takes many hours to calculate, the total time saved by doing so can make an otherwise computationally infeasible problem tractable.

Volume methods are of interest, since they can readily be used for inhomogeneous or anisotropic particles. The two most likely candidates are the finite-difference time-domain method (FDTD) [1, 19] and the discrete dipole approximation (DDA). In FDTD, the Maxwell equations are discretised in space and time, and, beginning from a known initial state, the electric and magnetic fields at each spatial grid point are calculated for successive steps in time. The number of grid points required is $O(N_{\max}^3)$ for three-dimensional scattering, and $O(N_{\max})$ time steps required, so FDTD solutions scale as $O(N_{\max}^4)$. Therefore, calculation of the T -matrix using FDTD should scale as $O(N_{\max}^6)$, which is the same scaling as the EBCM. However, the grid required must be closely spaced compared to the wavelength, and the space outside the scatterer must also be discretised, making FDTD substantially slower than EBCM, especially for smaller particles. However, FDTD is an extremely general technique, and has potential as a method for the calculation of T -matrices.

We should add that there is an additional consideration that makes FDTD potentially attractive as a method for calculating the T -matrix: FDTD does not assume that the incident wave is monochromatic. Consider the case when the illumination is a brief pulse with a Gaussian envelope. The frequency spectrum of the incident wave is Gaussian, and the scattering of a range of frequencies can be found by taking the Fourier transform of the scattered field [20]. Even if we are not interested in other than monochromatic illumination, we will frequently be interested in scattering by size distributions of particles. Since varying the frequency for a particular particle is equivalent to varying the size of the particle for a fixed incident frequency, the T -matrices for a range of particle sizes can be calculated simultaneously.

The other major volume method for computational scattering, the discrete dipole approximation (DDA), also known as the coupled-dipole method, has been recently applied to the calculation of the T -matrix by Mackowski [21], who obtained good results, with reasonable computational efficiency using a moment method to solve the DDA system of equations. DDA lacks the main disadvantages of FDTD, namely the need to discretise space outside the particle, and the need to implement suitable boundary conditions to prevent non-physical reflections from the boundary of the computational domain. Mackowski's method scales as $O(N_{\max}^7)$ for large N_{\max} . There is no need to discuss his method in detail here, and the interested reader is referred to his recent description of the method [21].

Finally, we consider the point-matching method. Like the T -matrix method and the EBCM, the point-matching method involves expansion of fields in terms of VSWFs. In the point-matching method, the internal field within the scatterer and the scattered field are expanded as series of VSWFs, and the incident, internal, and scattered fields are matched at points on the particle surface, using the usual boundary condition of continuity of tangential components of the electric and magnetic fields. This gives a system of equations from which the unknown expansion coefficients of the internal and scattered fields can be found. Typically, enough points are used for matching the fields so as to give an overdetermined system of equations, which is then solved in a least-squares sense. Solving the system of $O(N_{\max}^2)$ unknowns using direct matrix inversion can be expected to be an $O(N_{\max}^6)$ problem, with the result that the total computational time is $O(N_{\max}^8)$. In practice, faster methods can be used, and our results indicate a performance of about $O(N_{\max}^7)$ for our implementation.

The point-matching method is an attractive candidate since a T -matrix implementation will generally include routines to calculate VSWFs, making the implementation of a point-matching T -matrix calculator simple. The only further requirement is a routine for solving overdetermined linear systems. Since the scattered field is calculated in terms of VSWFs, the conversion of the results of a single PMM calculation to a T -matrix column is trivial.

Naturally, multiple expansion methods (the generalised multipole technique, or the multiple multipole method) can be used. Since multipole methods exist for anisotropic media [22], the method can be used for anisotropic scatterers.

Our implementation of the point-matching method, and its performance, is discussed in the next section.

3 Point-matching method

Our implementation of the PMM T -matrix calculation uses an incoming/outgoing field expansion (equations (10) and (11)), rather than the usual incident/scattered wave expansion (equations (9) and (11)), and the internal field is expanded in terms of regular VSWFs:

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n a_{nm} \mathbf{M}_{nm}^{(2)}(kr) + b_{nm} \mathbf{N}_{nm}^{(2)}(kr), \quad (13)$$

$$\mathbf{E}_{\text{scat}}(\mathbf{r}) = \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n p_{nm} \mathbf{M}_{nm}^{(1)}(kr) + q_{nm} \mathbf{N}_{nm}^{(1)}(kr), \quad (14)$$

$$\mathbf{E}_{\text{int}}(\mathbf{r}) = \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n c_{nm} \mathbf{RgM}_{nm}(kr) + d_{nm} \mathbf{RgN}_{nm}(kr). \quad (15)$$

We use this particular expansion since we are interested in calculating optical forces and torques within optical traps [23,24] and this results in simpler expressions for these quantities.

We considered a single scatterer, centred on the origin, contained entirely within a radius r_0 , and with a surface specified by a function of angle:

$$r = r(\theta, \phi) \quad (16)$$

The boundary conditions—matching the tangential fields on the surface of the scatterer—are

$$\hat{\mathbf{n}} \times (\mathbf{E}_{\text{inc}}(\mathbf{r}) + \mathbf{E}_{\text{scat}}(\mathbf{r})) = \hat{\mathbf{n}} \times \mathbf{E}_{\text{int}}(\mathbf{r}), \quad (17)$$

$$\hat{\mathbf{n}} \times (\mathbf{H}_{\text{inc}}(\mathbf{r}) + \mathbf{H}_{\text{scat}}(\mathbf{r})) = \hat{\mathbf{n}} \times \mathbf{H}_{\text{int}}(\mathbf{r}), \quad (18)$$

where $\hat{\mathbf{n}}$ is a unit vector normal to the surface of the particle.

The magnetic fields are given by expansions similar to those for the electric fields:

$$\mathbf{H}_{\text{inc}}(\mathbf{r}) = \frac{1}{k_{\text{medium}}} \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n a_{nm} \mathbf{N}_{nm}^{(2)}(kr) + b_{nm} \mathbf{M}_{nm}^{(2)}(kr), \quad (19)$$

$$\mathbf{H}_{\text{scat}}(\mathbf{r}) = \frac{1}{k_{\text{medium}}} \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n p_{nm} \mathbf{N}_{nm}^{(1)}(kr) + q_{nm} \mathbf{M}_{nm}^{(1)}(kr), \quad (20)$$

$$\mathbf{H}_{\text{int}}(\mathbf{r}) = \frac{1}{k_{\text{particle}}} \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n c_{nm} \mathbf{RgN}_{nm}(kr) + d_{nm} \mathbf{RgM}_{nm}(kr). \quad (21)$$

where k_{medium} and k_{particle} are the wavenumbers of the field in the surrounding medium and inside the particle, respectively.

There are $4N_{\text{max}}(N_{\text{max}} + 2)$ unknown variables—the expansion coefficients c_{nm} , d_{nm} , p_{nm} , and q_{nm} . Since the fields are vector fields, each point gives multiple equations—four independent equations per point. We generate a grid of $2N_{\text{max}}(N_{\text{max}} + 2)$ points with equal angular spacings in each of the θ and ϕ directions, giving $8N_{\text{max}}(N_{\text{max}} + 2)$ independent equations. Equal angle spaced points are used for simplicity, although points uniformly distributed about a sphere would be better [25].

The values of the VSWFs at these points on the particle surface are calculated, and used in the column-by-column calculation of the T -matrix.

The computation time (which is independent of the particle shape, depending only on the containing radius r_0) is shown in table 1. The calculations were carried out in MATLAB [26] on a 1.5 GHz PC. The times taken are reasonable in comparison to computation times for EBCM for particles with no symmetry [14].

Results of a sample calculation are shown in figure 2, where the diagonal scattering matrix elements are shown, calculated using the PMM T -matrix. The scattering matrix elements S_{11} and S_{22} are shown for scattering in two different planes; the effect of non-axisymmetry is evident.

The accuracy and validity of the PMM-calculated T -matrix will be essentially the same as the accuracy and validity of the point-matching algorithm used in the calculation. Thus, a detailed analysis of our simple proof-of-principle implementation serves little purpose. It is obviously useful to

N_{\max}	$kr_{0\max}$	Time
1	0.033	0.041 s
2	0.21	0.16 s
3	0.55	0.85 s
4	1.00	7.00 s
5	1.54	30.3 s
6	2.14	1.86 min
7	2.78	4.95 min
8	3.46	12.2 min
9	4.17	26.8 min
10	4.90	56.3 min
11	5.66	1.91 h
12	6.42	3.53 h
13	7.21	6.35 h

Table 1: Computation times for calculating T -matrices. The calculations were carried out in MATLAB on a 1.5 GHz PC. The maximum size parameter kr_0 for which the truncation is expected to always be well-convergent is shown. Reasonable convergence can also be expected for size parameters $kr_0 \approx N_{\max}$

use the best, sufficiently fast, point-matching code available. In view of the mathematical similarity between the T -matrix method and the point-matching method, it should be a simple task to adapt any PMM code to the task of generating T -matrix columns.

4 Conclusions

The point-matching method is suitable for the calculation of the T -matrix for particles with no symmetry, provided that the particles are not too large. The method has the advantage of being extremely simple to implement within a general T -matrix package, since most of the required routines will be shared with the existing T -matrix code. This results from the mathematical formalisms of the T -matrix method and the point-matching method being essentially the same. Any point-matching algorithm can be used, with multiple expansion origins, automatic convergence checks, and so on. Since the PMM uses the same field expansions as the EBCM, the same numerical difficulties are to be expected for scatterers with large aspect ratios; in such cases, multiple expansion origin algorithms will be necessary. The accuracy of the PMM T -matrix will be the same as the PMM which is used to calculate it. Naturally, the usual conditions of applicability of the PMM, such as the validity of the Rayleigh hypothesis, need to be considered.

The PMM explicitly depends on the Rayleigh hypothesis—the assumption that the fields can be represented by the expansions (13)—(15) over all space rather than just outside and inside spherical surfaces circumscribing and inscribing the surface of the scatterer. The validity of this assumption for arbitrary scatterers is unknown. However, the use of an overdetermined system of equation may well extend the method somewhat beyond the strict range of applicability of the Rayleigh hypothesis by providing a least squares approximation of the fields between the circumscribing and inscribing surfaces where the VSWF expansions might be non-convergent. One advantage of relying on the Rayleigh hypothesis is that the fields are given everywhere, including the fields internal to the scatterer (a $T^{(\text{int})}$ -matrix can be used to relate the internal and incident fields). This applies generally to methods that make use of the Rayleigh hypothesis, such as the generalised separation of variables method [27]. In contrast to this, the EBCM, which avoids the Rayleigh hypothesis, gives the tangential surface fields on the surface of the scatterer, rather than the internal fields.

The point-matching method lacks the generality of DDA and FDTD. In this respect, the recent discrete dipole moment method T -matrix calculations by Mackowski [21] are particularly promising.

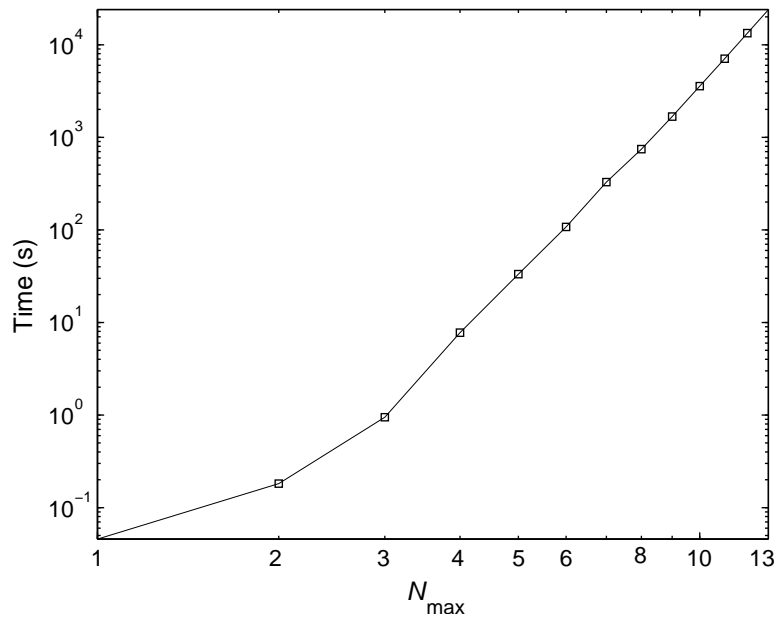


Figure 1: Computation times for calculating T -matrices. The calculations were carried out in MATLAB on a 1.5 GHz PC. The time taken scales as $O(N_{\max}^{6.8})$ for $N_{\max} > 2$.

Lastly, we note again that FDTD may prove to be a useful method for T -matrix calculation since it can be used to calculate T -matrices simultaneously for a range of particle sizes.

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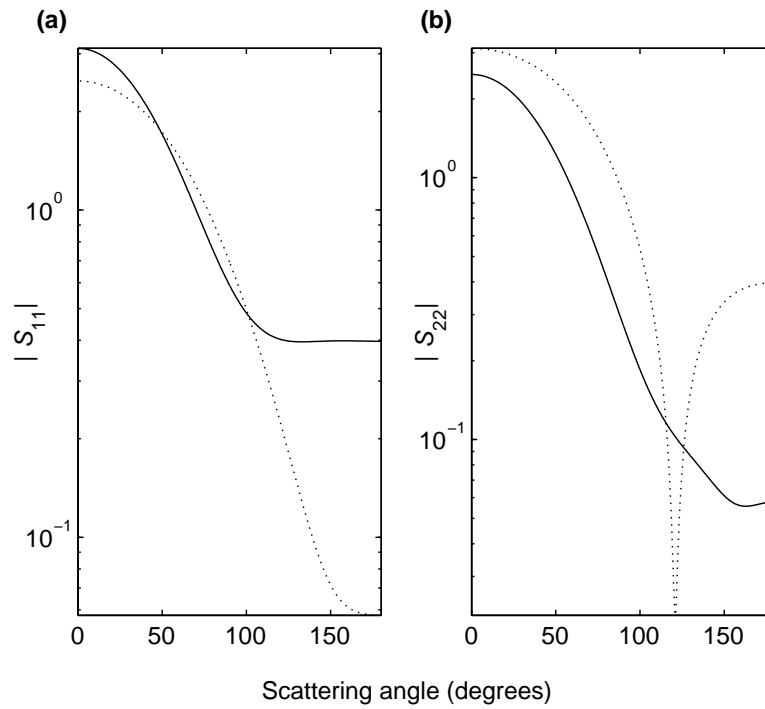


Figure 2: (a) S_{11} and (b) S_{22} scattering matrix elements for an ellipsoidal particle with axes of length $a = 1\lambda$, $b = 0.2\lambda$, and $c = 0.5\lambda$, and relative refractive index $m = 1.5$. The incident illumination is directed along the c axis of the ellipsoid. The solid line shows scattering in the ac plane (containing the largest area cross-section of the ellipsoid), and the dotted line shows scattering in the bc plane (the smallest cross-sectional area).

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