



Program description

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TMATRIX is a Fortran 90 program to compute the scattering and absorption of electromagnetic waves by particles with arbitrary geometries using the \mathbf{T} -matrix method. The program is intended for science professionals, engineers and graduate students working in optics, electromagnetics, biomedical optics, atmospheric radiation and remote sensing. We assume that the reader is familiar with the fundamentals of classical electromagnetics and optics.

1 Theoretical background

In the \mathbf{T} -matrix method, the scattered and internal fields are approximated by the complete set of localized vector spherical wave functions $\mathbf{M}_{mn}(k\mathbf{r})$ and $\mathbf{N}_{mn}(k\mathbf{r})$, where n is the expansion order index, $n = \max(1, |m|), \dots, N_{\text{rank}}$, m is the azimuthal index, $m = 0, \pm 1, \dots, \pm M_{\text{rank}}$, \mathbf{r} is the position vector and k is the wave number. The truncation indices N_{rank} and M_{rank} are the maximum expansion and azimuthal orders, respectively, and an important part of the code is the convergence procedure which finds reliable estimates of N_{rank} and M_{rank} . For particles with extremely aspherical surfaces, the use of distributed vector spherical wave functions (lowest-order multipoles)

$$\mathcal{M}_{mn}(k\mathbf{r}) = \mathbf{M}_{m,|m|+l}[k(\mathbf{r} - z_n\mathbf{e}_z)], \quad \mathcal{N}_{mn}(k\mathbf{r}) = \mathbf{N}_{m,|m|+l}[k(\mathbf{r} - z_n\mathbf{e}_z)],$$

improves the numerical stability of the \mathbf{T} -matrix calculations. Here, $\{z_n\}$ is a dense set of points on the z -axis, \mathbf{e}_z is the unit vector in the direction of the z -axis, $n = 1, 2, \dots, N_{\text{rank}}$, $m = 0, \pm 1, \dots, \pm M_{\text{rank}}$, and $l = 1$ if $m = 0$ and $l = 0$ if $m \neq 0$. For distributed vector spherical wave functions, N_{rank} is the number of discrete sources, and by convention, N_{rank} will be also referred to as the maximum expansion order. The vector spherical wave functions are expressed in terms of spherical and normalized associated Legendre functions, and we recall that the radiating localized vector spherical wave functions are singular at the origin ($\mathbf{r} = 0$), while the radiating distributed vector spherical wave functions are singular at $\mathbf{r} = z_n\mathbf{e}_z$.

Everywhere outside the (smallest) sphere circumscribing the particle it is appropriate to expand the scattered field in terms of radiating vector spherical

wave functions

$$\mathbf{E}_s(\mathbf{r}) = \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} \sum_{n=\max(1,|m|)}^{N_{\text{rank}}} f_{mn} \mathbf{M}_{mn}^3(k_s \mathbf{r}) + g_{mn} \mathbf{N}_{mn}^3(k_s \mathbf{r}). \quad (1)$$

and the incident field in terms of regular vector spherical wave functions

$$\mathbf{E}_e(\mathbf{r}) = \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} \sum_{n=\max(1,|m|)}^{N_{\text{rank}}} a_{mn} \mathbf{M}_{mn}^1(k_s \mathbf{r}) + b_{mn} \mathbf{N}_{mn}^1(k_s \mathbf{r}). \quad (2)$$

Due to the linearity relations of the Maxwell equations and the constitutive relations, the relation between the scattered and incident field coefficients must be linear. This relation is given by the so-called transition matrix \mathbf{T} as follows:

$$\begin{bmatrix} f_{mn} \\ g_{mn} \end{bmatrix} = \mathbf{T} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} = \begin{bmatrix} \mathbf{T}^{11} & \mathbf{T}^{12} \\ \mathbf{T}^{21} & \mathbf{T}^{22} \end{bmatrix} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix}. \quad (3)$$

Essentially, the transition matrix depends on the physical and geometrical characteristics of the particle and is independent on the propagation direction and polarization states of the incident and scattered field. The standard scheme for computing the \mathbf{T} matrix relies on the null-field method. For a homogeneous particle, the transition matrix relating the expansion coefficients of the scattered and incident fields is given by

$$\mathbf{T} = -\mathbf{Q}^{11}(k_s, k_i) [\mathbf{Q}^{31}(k_s, k_i)]^{-1}. \quad (4)$$

where the expressions of the matrices \mathbf{Q}^{31} and \mathbf{Q}^{11} follow from the extinction theorem and Huygens principle, respectively. The elements of the matrices \mathbf{Q}^{31} and \mathbf{Q}^{11} are expressed as integrals over the particle surface and the number of integration points N_{int} is an additional parameter of the convergence analysis. In fact, the \mathbf{T} -matrix calculation is directly influenced by the three parameters N_{int} , N_{rank} and M_{rank} .

If the \mathbf{T} matrix is known, the scattering characteristics, describing the scattered field in the far-field region, can be readily computed. These include the far-field pattern, the differential scattering cross sections, the amplitude matrix, the optical cross sections and the phase and extinction matrices. We consider a global coordinate system $OXYZ$ with the origin inside the particle and denote by α_p , β_p and γ_p the particle orientation angles. For an incident wave traveling in the direction (β, α) we denote by

$$\mathbf{E}_s(\mathbf{r}) = \frac{e^{jk_s r}}{r} \left\{ \mathbf{E}_{s\infty}(\mathbf{e}_r) + O\left(\frac{1}{r}\right) \right\}, \quad r \rightarrow \infty,$$

the scattered field in the direction (θ, φ) , where $\mathbf{E}_{s\infty}(\mathbf{e}_r)$ is the far-field pattern, and $\mathbf{e}_r = \mathbf{r}/r$ is the radial unit vector. Using the decomposition

$$\mathbf{E}_{s\infty} = E_{s\infty, \theta} \mathbf{e}_\theta + E_{s\infty, \varphi} \mathbf{e}_\varphi$$

where $(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi)$ are the spherical unit vectors of the scattering direction (θ, φ) , we define the differential scattering cross sections for parallel and perpendicular polarizations as $\sigma_{\text{dp}} = |E_{s\infty, \theta}|^2$ and $\sigma_{\text{ds}} = |E_{s\infty, \varphi}|^2$. The differential scattering cross sections have the dimension of area, and a dimensionless quantity are the normalized differential scattering cross sections $\sigma_{\text{dppn}} = |E_{s\infty, \theta}|^2 / \pi a_c^2$ and $\sigma_{\text{dspn}} = |E_{s\infty, \varphi}|^2 / \pi a_c^2$, where a_c is a characteristic dimension of the particle. The incident vector plane wave can be expressed as

$$\mathbf{E}_e(\mathbf{r}) = \mathbf{E}_{e0} e^{i\mathbf{k}_e \cdot \mathbf{r}}, \quad \mathbf{E}_{e0} \cdot \mathbf{e}_k = 0, \quad (5)$$

where \mathbf{k}_e is the wave vector, $\mathbf{k}_e = k_s \mathbf{e}_k$, \mathbf{E}_{e0} is the complex amplitude vector,

$$\mathbf{E}_{e0} = E_{e0, \beta} \mathbf{e}_\beta + E_{e0, \alpha} \mathbf{e}_\alpha,$$

and $E_{e0, \beta}$ and $E_{e0, \alpha}$ are the complex amplitudes in the β - and α -direction, respectively. An equivalent representation for \mathbf{E}_{e0} is

$$\mathbf{E}_{e0} = |\mathbf{E}_{e0}| \mathbf{e}_{\text{pol}}, \quad (6)$$

where \mathbf{e}_{pol} is the complex polarization unit vector, $|\mathbf{e}_{\text{pol}}| = 1$, and

$$\mathbf{e}_{\text{pol}} = \frac{1}{|\mathbf{E}_{e0}|} (E_{e0, \beta} \mathbf{e}_\beta + E_{e0, \alpha} \mathbf{e}_\alpha).$$

Inserting (6) into (5), gives the representation

$$\mathbf{E}_e(\mathbf{r}) = |\mathbf{E}_{e0}| \mathbf{e}_{\text{pol}} e^{i\mathbf{k}_e \cdot \mathbf{r}}, \quad \mathbf{e}_{\text{pol}} \cdot \mathbf{e}_k = 0,$$

and obviously, $|\mathbf{E}_e(\mathbf{r})| = |\mathbf{E}_{e0}|$. For a linearly polarized wave, the polarization unit vector is real and is given by

$$\mathbf{e}_{\text{pol}} = \cos \alpha_{\text{pol}} \mathbf{e}_\beta + \sin \alpha_{\text{pol}} \mathbf{e}_\alpha, \quad (7)$$

where α_{pol} is the polarization angle.

In Figs. 1, 2 and 3 we illustrate the particle orientation angles α_p , β_p and γ_p , the transformation from the global coordinate system $OXYZ$ to the particle coordinate system $Oxyz$, and the incident and scattering direction (β, α) and (θ, φ) , respectively.

The amplitude matrix is given by

$$\begin{bmatrix} E_{s\infty, \theta}(\mathbf{e}_r) \\ E_{s\infty, \varphi}(\mathbf{e}_r) \end{bmatrix} = \mathbf{S}(\mathbf{e}_r, \mathbf{e}_k) \begin{bmatrix} E_{e0, \beta} \\ E_{e0, \alpha} \end{bmatrix}, \quad (8)$$

where $E_{e0, \beta}$ and $E_{e0, \alpha}$ do not depend on the incident direction. Essentially, the amplitude matrix is a generalization of the scattering amplitudes including polarization effects. The amplitude matrix provides a complete description of the far-field patterns and depends on the incident and scattering directions as

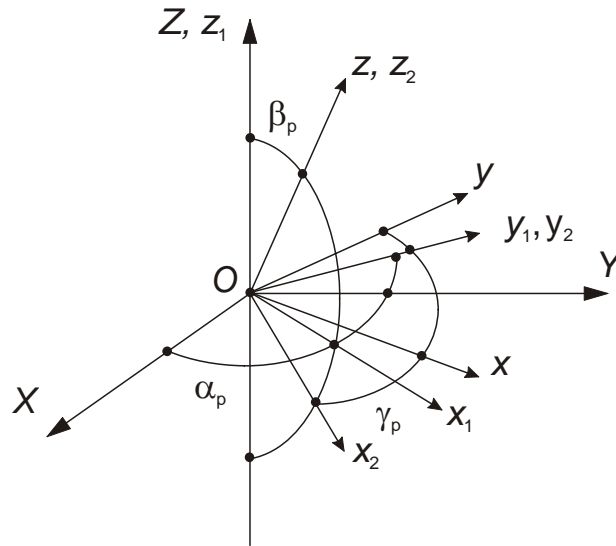


Figure 1: Particle orientation angles and the transformation from the global coordinate system $OXYZ$ to the particle coordinate system $Oxyz$ through three rotations.

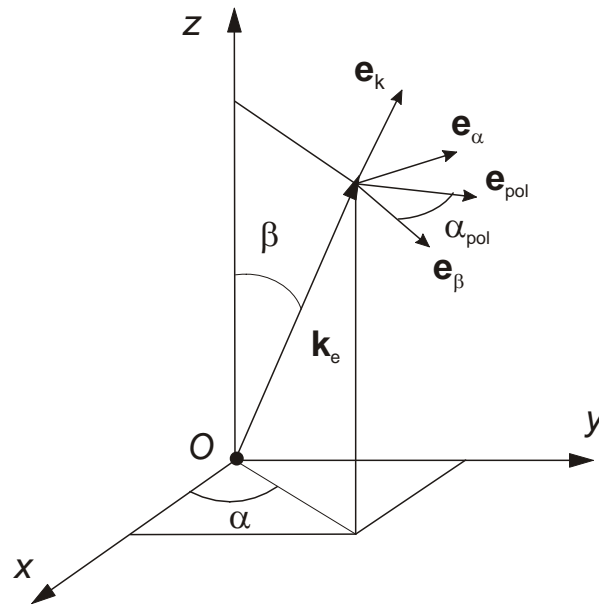


Figure 2: Incident direction (β, α) .

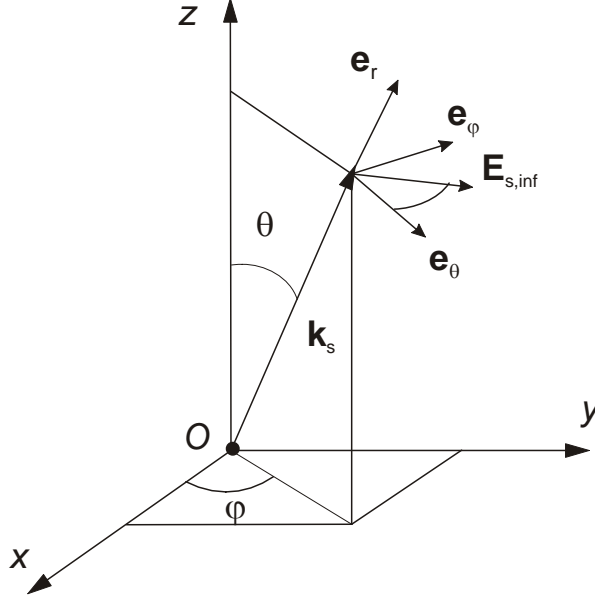


Figure 3: Scattering direction (θ, φ) .

well on the size, optical properties and orientation of the particle. Assuming that the incident vector plane wave is of unit amplitude and setting

$$\mathbf{S} = \begin{bmatrix} S_{\theta\beta} & S_{\theta\alpha} \\ S_{\varphi\beta} & S_{\varphi\alpha} \end{bmatrix},$$

we see that for a vector plane wave linearly polarized in the β -direction, $S_{\theta\beta} = E_{s\infty,\theta}$ and $S_{\varphi\beta} = E_{s\infty,\varphi}$, while for a vector plane wave linearly polarized in the α -direction, $S_{\theta\alpha} = E_{s\infty,\theta}$ and $S_{\varphi\alpha} = E_{s\infty,\varphi}$. In general for a linearly polarized wave of unit amplitude, we have

$$E_{s\infty,\theta} = S_{\theta\beta} \cos \alpha_{\text{pol}} + S_{\theta\alpha} \sin \alpha_{\text{pol}}$$

and

$$E_{s\infty,\varphi} = S_{\varphi\beta} \cos \alpha_{\text{pol}} + S_{\varphi\alpha} \sin \alpha_{\text{pol}}.$$

The Stokes vectors \mathbf{I}_e and \mathbf{I}_s describe the polarization characteristics of the incident and scattered fields, respectively. They are given by

$$\mathbf{I}_e = \begin{bmatrix} I_e \\ Q_e \\ U_e \\ V_e \end{bmatrix} \quad \text{and} \quad \mathbf{I}_s(r\mathbf{e}_r) = \frac{1}{r^2} \begin{bmatrix} I_s(\mathbf{e}_r) \\ Q_s(\mathbf{e}_r) \\ U_s(\mathbf{e}_r) \\ V_s(\mathbf{e}_r) \end{bmatrix},$$

where the first Stokes parameter I , is the intensity of the wave, while the Stokes parameters Q , U and V describe the polarization state of the wave. The Stokes parameters are defined with respect to a reference plane containing the direction of wave propagation, and Q and U depend on the choice of the reference frame. The phase matrix \mathbf{Z} relates the Stokes vectors of the incident and scattered fields, i.e.,

$$\mathbf{I}_s(r\mathbf{e}_r) = \frac{1}{r^2} \mathbf{Z}(\mathbf{e}_r, \mathbf{e}_k) \mathbf{I}_e$$

and note that the elements of the phase matrix can be expressed in terms of the elements of the amplitude matrix.

A scattering particle can change the state of polarization of the incident beam after it passes the particle. This phenomenon is called dichroism and a complete description of the extinction process requires the introduction of the extinction matrix \mathbf{K} . The extinction matrix \mathbf{K} is defined as

$$\mathbf{I}(r\mathbf{e}_k) \Delta S \approx \mathbf{I}_e \Delta S - \mathbf{K}(\mathbf{e}_k) \mathbf{I}_e,$$

where \mathbf{I} is the Stokes vector of the total field in the forward-scattering direction ($\mathbf{e}_r = \mathbf{e}_k$) and ΔS is an elementary surface situated in the far-field region. Note that according to the optical theorem, the elements of the extinction matrix can be expressed in terms of the forward-scattering amplitude matrix.

The scattering and absorption cross sections C_{scat} and C_{abs} represents the electromagnetic powers removed from the incident wave as a result of scattering and absorption of the incident radiation, while the extinction cross section C_{ext} gives the total electromagnetic power removed from the incident wave by the combined effect of scattering and absorption. The optical cross sections have the dimension of area and depend on the direction and polarization state of the incident wave as well on the size, optical properties and particle orientation. For an incident wave of unit amplitude, the scattering cross section is given by

$$C_{\text{scat}} = \int_{\Omega} |\mathbf{E}_{s\infty}|^2 d\Omega,$$

where the integral is taken over the unit sphere Ω . In practice, the scattering cross section can be computed as

$$C_{\text{scat}} = \frac{\pi}{k_s^2} \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} \sum_{n=\max(1,|m|)}^{N_{\text{rank}}} |f_{mn}|^2 + |g_{mn}|^2 \quad (9)$$

where f_{mn} and g_{mn} are the expansion coefficients of the scattered field. The scattering efficiency is a dimensionless quantity and is given by

$$Q_{\text{scat}} = \frac{C_{\text{scat}}}{G},$$

where G is the particle cross-sectional area projected onto a plane perpendicular to the incident beam. Taking into account the definition of the normalized

differential scattering cross section, we set $G = \pi a_c^2$, where a_c is the area-equivalent-circle radius. In view of the optical theorem and for an incident wave of unit amplitude, the extinction cross section can be computed as

$$C_{\text{ext}} = \frac{4\pi}{k_s^2} \text{Im} \{ \mathbf{E}_{e_0}^* \cdot \mathbf{E}_{s\infty}(\mathbf{e}_k) \}.$$

In terms of the expansion coefficients of the incident and scattered field, we have

$$C_{\text{ext}} = -\frac{\pi}{k_s^2} \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} \sum_{n=\max(1,|m|)}^{N_{\text{rank}}} \text{Re} \{ f_{mn} a_{mn}^* + g_{mn} b_{mn}^* \} \quad (10)$$

where a_{mn} and b_{mn} are the expansion coefficients of the incident wave. As before, the extinction efficiency or the extinction efficiency factor is given by

$$Q_{\text{ext}} = \frac{C_{\text{ext}}}{G}.$$

The phase function is related to the differential scattering cross section by the relation

$$p(\mathbf{e}_r, \mathbf{e}_k) = \frac{4\pi}{C_{\text{scat}}} |\mathbf{E}_{s\infty}(\mathbf{e}_r)|^2,$$

whence, taking into account the definition of the scattering cross section, we see that p is dimensionless and normalized, i.e.,

$$\frac{1}{4\pi} \int_{\Omega} p \, d\Omega = 1.$$

The mean direction of propagation of the scattered radiation is defined as

$$\mathbf{g} = \frac{1}{C_{\text{scat}}} \int_{\Omega} |\mathbf{E}_{s\infty}(\mathbf{e}_r)|^2 \mathbf{e}_r \, d\Omega(\mathbf{e}_r) \quad (11)$$

and we note the decomposition

$$\mathbf{g} = g_{\beta} \mathbf{e}_{\beta} + g_{\alpha} \mathbf{e}_{\alpha} + g_k \mathbf{e}_k,$$

where $g_k = \langle \cos \Theta \rangle = \mathbf{g} \cdot \mathbf{e}_k$ is the asymmetry parameter (the dot product between the vector \mathbf{g} and the incident direction \mathbf{e}_k). The asymmetry parameter can be expressed as

$$\langle \cos \Theta \rangle = \mathbf{g} \cdot \mathbf{e}_k = \frac{1}{4\pi} \int_{\Omega} p(\mathbf{e}_r, \mathbf{e}_k) \cos \Theta \, d\Omega(\mathbf{e}_r),$$

where $\cos \Theta = \mathbf{e}_r \cdot \mathbf{e}_k$, and it is apparent that the asymmetry parameter is the average cosine of the scattering angle Θ . If the particle scatters more light toward the forward direction ($\Theta = 0$), $\langle \cos \Theta \rangle$ is positive and $\langle \cos \Theta \rangle$ is negative

if the scattering is directed more toward the backscattering direction ($\Theta = 180^\circ$). If the scattering is symmetric about a scattering angle of 90° , $\langle \cos \Theta \rangle$ vanishes.

The scattering medium consisting of an ensemble of randomly oriented, identical particles is macroscopically isotropic, i.e., the scattering characteristics are independent of the incident and scattering directions \mathbf{e}_k and \mathbf{e}_r . For this type of scattering problem, it is convenient to direct the Z -axis of the global coordinate system along the incident direction and to choose the XZ -plane as the scattering plane. The phase matrix of a volume element containing randomly oriented particles can be written as

$$\mathbf{Z}(\mathbf{e}_r, \mathbf{e}_k) = \mathbf{Z}(\theta, \varphi = 0, \beta = 0, \alpha = 0),$$

where, in general, θ and φ are the polar angles of the scattering direction \mathbf{e}_r , and β and α are the polar angles of the incident direction \mathbf{e}_k . The phase matrix $\mathbf{Z}(\theta, 0, 0, 0)$ is known as the scattering matrix \mathbf{F} and relates the Stokes parameters of the incident and scattered fields defined with respect to the scattering plane. The phase matrix $\mathbf{Z}(\theta, \varphi, \beta, \alpha)$ can then be expressed in terms of the scattering matrix $\mathbf{F}(\theta)$ by using the rotation transformation rule for the incident and scattered fields

$$\mathbf{Z}(\theta, \varphi, \beta, \alpha) = \mathbf{L}(-\sigma_2) \mathbf{F}(\Theta) \mathbf{L}(\sigma_1),$$

where

$$\begin{aligned} \cos \Theta &= \mathbf{e}_k \cdot \mathbf{e}_r = \cos \beta \cos \theta + \sin \beta \sin \theta \cos(\varphi - \alpha), \\ \cos \sigma_1 &= \mathbf{e}'_\alpha \cdot \mathbf{e}_\alpha = -\frac{\sin \beta \cos \theta - \cos \beta \sin \theta \cos(\varphi - \alpha)}{\sin \Theta}, \\ \cos \sigma_2 &= \mathbf{e}'_\varphi \cdot \mathbf{e}_\varphi = \frac{\cos \beta \sin \theta - \sin \beta \cos \theta \cos(\varphi - \alpha)}{\sin \Theta}. \end{aligned}$$

The scattering matrix of a volume element containing randomly oriented particles has only ten independent elements,

$$\mathbf{F}(\theta) = \begin{bmatrix} F_{11}(\theta) & F_{12}(\theta) & F_{13}(\theta) & F_{14}(\theta) \\ F_{12}(\theta) & F_{22}(\theta) & F_{23}(\theta) & F_{24}(\theta) \\ -F_{13}(\theta) & -F_{23}(\theta) & F_{33}(\theta) & F_{34}(\theta) \\ F_{14}(\theta) & F_{24}(\theta) & -F_{34}(\theta) & F_{44}(\theta) \end{bmatrix}. \quad (12)$$

If each particle has a plane of symmetry, or equivalently, the particles and their mirror-symmetric particles are present in equal number, the scattering mediums called macroscopically and mirror-symmetric. The scattering matrix for macroscopically isotropic and mirror-symmetric media has a block-diagonal structure, so that only eight elements of the scattering matrix are nonzero and only six of them are independent,

$$\mathbf{F}(\theta) = \begin{bmatrix} F_{11}(\theta) & F_{12}(\theta) & 0 & 0 \\ F_{12}(\theta) & F_{22}(\theta) & 0 & 0 \\ 0 & 0 & F_{33}(\theta) & F_{34}(\theta) \\ 0 & 0 & -F_{34}(\theta) & F_{44}(\theta) \end{bmatrix}. \quad (13)$$

For an ensemble of randomly oriented particles, the waves scattered by different particles are random in phase, and the Stokes parameters of these incoherent waves add up. Therefore, the scattering matrix for the ensemble is the sum of the scattering matrices of the individual particles,

$$\mathbf{F} = N \langle \mathbf{F} \rangle,$$

where N is number of particles and $\langle \mathbf{F} \rangle$ denotes the ensemble-average scattering matrix per particle. Similar relations hold for the extinction matrix and optical cross sections. Because the particles are identical, the ensemble-average of a scattering quantity X is the orientation-averaged quantity

$$\langle X \rangle = \int_0^{2\pi} \int_0^{2\pi} \int_0^\pi X(\alpha_p, \beta_p, \gamma_p) p(\alpha_p, \beta_p, \gamma_p) \sin\beta_p \, d\beta_p d\alpha_p d\gamma_p,$$

where α_p , β_p and γ_p are the particle orientation angles and p is the probability density function satisfying the normalization condition,

$$\int_0^{2\pi} \int_0^{2\pi} \int_0^\pi p(\alpha_p, \beta_p, \gamma_p) \sin\beta_p \, d\beta_p d\alpha_p d\gamma_p = 1.$$

Random particle orientation means that the orientation distribution of the particle is uniform. For a complete uniform orientation distribution function, the Euler angles α_p , β_p and γ_p are uniformly distributed in the intervals $(0, 360^\circ)$, $(0, 180^\circ)$ and $(0, 360^\circ)$, respectively and

$$p(\alpha_p, \beta_p, \gamma_p) = \frac{1}{8\pi^2}.$$

For an ensemble of randomly oriented particles illuminated by a vector plane wave of unit amplitude and polarization vector $\mathbf{e}_{\text{pol}} = e_{\text{pol},\beta} \mathbf{e}_\beta + e_{\text{pol},\alpha} \mathbf{e}_\alpha$, the average differential scattering cross sections in the scattering plane φ are given by

$$\begin{aligned} \langle \sigma_{\text{dp}}(\theta) \rangle &= \langle |E_{s\infty,\theta}(\theta)|^2 \rangle = \langle |S_{\theta\beta}(\theta)|^2 \rangle |E'_{e0,\beta}|^2 \\ &+ \langle |S_{\theta\alpha}(\theta)|^2 \rangle |E'_{e0,\alpha}|^2 \\ &+ 2 \operatorname{Re} \{ \langle S_{\theta\beta}(\theta) S_{\theta\alpha}^*(\theta) \rangle E'_{e0,\beta} E_{e0,\alpha}'^* \}, \end{aligned} \quad (14)$$

and

$$\begin{aligned} \langle \sigma_{\text{ds}}(\theta) \rangle &= \langle |E_{s\infty,\varphi}(\theta)|^2 \rangle = \langle |S_{\varphi\beta}(\theta)|^2 \rangle |E'_{e0,\beta}|^2 \\ &+ \langle |S_{\varphi\alpha}(\theta)|^2 \rangle |E'_{e0,\alpha}|^2 \\ &+ 2 \operatorname{Re} \{ \langle S_{\varphi\beta}(\theta) S_{\varphi\alpha}^*(\theta) \rangle E'_{e0,\beta} E_{e0,\alpha}'^* \}, \end{aligned} \quad (15)$$

where

$$\begin{aligned} E'_{e0,\beta} &= e_{\text{pol},\beta} \cos \varphi + e_{\text{pol},\alpha} \sin \varphi, \\ E'_{e0,\alpha} &= -e_{\text{pol},\beta} \sin \varphi + e_{\text{pol},\alpha} \cos \varphi. \end{aligned}$$

It should be noted that for macroscopically isotropic and mirror-symmetric media,

$$\begin{aligned} \langle S_{\theta\beta}(\theta) S_{\theta\alpha}^*(\theta) \rangle &= 0, \\ \langle S_{\varphi\beta}(\theta) S_{\varphi\alpha}^*(\theta) \rangle &= 0, \end{aligned}$$

and the expressions of $\langle \sigma_{\text{dp}}(\theta) \rangle$ and $\langle \sigma_{\text{ds}}(\theta) \rangle$ simplify considerably. The non-zero elements of the average extinction matrix are given by

$$\langle K_{ii} \rangle = -\frac{2\pi}{k_s^2} \text{Re} \left\{ \sum_n (2n+1) (t_n^{11} + t_n^{22}) \right\}, \quad i = 1, 2, 3, 4, \quad (16)$$

and

$$\begin{aligned} \langle K_{14} \rangle = \langle K_{41} \rangle &= \frac{2\pi}{k_s^2} \text{Re} \left\{ \sum_n (2n+1) (t_n^{12} + t_n^{21}) \right\}, \\ \langle K_{23} \rangle = -\langle K_{32} \rangle &= \frac{2\pi}{k_s^2} \text{Im} \left\{ \sum_n (2n+1) (t_n^{12} + t_n^{21}) \right\}. \end{aligned} \quad (17)$$

where the coefficients t_n^{ij} are expressed in terms of the \mathbf{T} -matrix elements

$$t_n^{ij} = \frac{1}{2n+1} \sum_{m'} T_{m'n, m'n}^{ij}.$$

For macroscopically isotropic and mirror-symmetric media, the identities $t_n^{12} = t_n^{21} = 0$, imply

$$\langle K_{14} \rangle = \langle K_{41} \rangle = \langle K_{23} \rangle = \langle K_{32} \rangle = 0.$$

In this specific case, the orientation-averaged extinction matrix becomes diagonal with diagonal elements being equal to the orientation-averaged extinction cross section per particle, $\langle \mathbf{K} \rangle = \langle C_{\text{ext}} \rangle \mathbf{I}$.

The average optical cross sections are given by

$$\langle C_{\text{scat}} \rangle = \frac{1}{I_e} (\langle C_{\text{scat}} \rangle_I I_e + \langle C_{\text{scat}} \rangle_V V_e),$$

and

$$\langle C_{\text{ext}} \rangle = \frac{1}{I_e} (\langle C_{\text{ext}} \rangle_I I_e + \langle C_{\text{ext}} \rangle_V V_e),$$

where as before, (I_e, Q_e, U_e, V_e) are the Stokes parameters of the incident wave,

$$\langle C_{\text{scat}} \rangle_{\text{I}} = \frac{2\pi}{k_s^2} \sum_n (2n+1) (\hat{t}_n^{11} + \hat{t}_n^{22}), \quad (18)$$

$$\langle C_{\text{ext}} \rangle_{\text{I}} = \langle K_{11} \rangle, \quad (19)$$

$$\langle C_{\text{scat}} \rangle_{\text{V}} = 2\pi \int_0^\pi \langle F_{14}(\theta) \rangle \sin \theta \, d\theta, \quad (20)$$

$$\langle C_{\text{ext}} \rangle_{\text{V}} = \langle K_{14} \rangle, \quad (21)$$

and

$$\hat{t}_n^{11} = \frac{1}{2n+1} \sum_{m', n_1, m_1} |T_{m_1 n_1, m' n}^{11}|^2 + |T_{m_1 n_1, m' n}^{21}|^2,$$

$$\hat{t}_n^{22} = \frac{1}{2n+1} \sum_{m', n_1, m_1} |T_{m_1 n_1, m' n}^{12}|^2 + |T_{m_1 n_1, m' n}^{22}|^2.$$

For macroscopically isotropic and mirror-symmetric media, $\langle C_{\text{scat}} \rangle_{\text{V}} = 0$ and $\langle C_{\text{ext}} \rangle_{\text{V}} = 0$, and the optical cross sections are independent of the direction and polarization of the incident wave.

For the asymmetry parameter, we have similar relations, i.e.,

$$\langle \cos \Theta \rangle = \frac{\langle C_{\text{scat}} \rangle_{\text{I}}}{\langle C_{\text{scat}} \rangle} \frac{1}{I_e} (\langle \cos \Theta \rangle_{\text{I}} I_e + \langle \cos \Theta \rangle_{\text{V}} V_e),$$

where

$$\langle \cos \Theta \rangle_{\text{I}} = \frac{2\pi}{\langle C_{\text{scat}} \rangle_{\text{I}}} \int_0^\pi \langle F_{11}(\theta) \rangle \sin \theta \cos \theta \, d\theta, \quad (22)$$

and

$$\langle \cos \Theta \rangle_{\text{V}} = \frac{2\pi}{\langle C_{\text{scat}} \rangle_{\text{I}}} \int_0^\pi \langle F_{14}(\theta) \rangle \sin \theta \cos \theta \, d\theta. \quad (23)$$

Note that for macroscopically isotropic and mirror-symmetric media, $\langle \cos \Theta \rangle_{\text{V}} = 0$.

It should be mentioned that for an ensemble of randomly oriented particles (not necessarily a macroscopically isotropic and mirror-symmetric medium), illuminated by linearly polarized vector plane wave, we also have $\langle C_{\text{scat}} \rangle = \langle C_{\text{scat}} \rangle_{\text{I}}$, $\langle C_{\text{ext}} \rangle = \langle C_{\text{ext}} \rangle_{\text{I}}$ and $\langle \cos \Theta \rangle = \langle \cos \Theta \rangle_{\text{I}}$.

2 Program structure

The package contains the following directories:

- TMATSOURCEs,

- INPUTFILES,
- GEOMFILES,
- OUTPUTFILES, and
- TMAFILES.

The executable program must be created in the directory TMAFILES and must include the main program “TMATRIX.f90” and all F90 routines contained in this directory. To compile the code on a Unix system use the Makefile supplied in the directory TMAFILES, but edit the Makefile to provide the desired compiler option. To compile the code on a PC (using for instance, Compaq Visual Fortran or Microsoft Developer Studio) create a project in the directory TMAFILES and add all F90 files to the project.

2.1 Directory TMA_SOURCES

The main program “TMATRIX.f90” calls a T-matrix routine for solving a specific scattering problem. These routines compute the \mathbf{T} matrix of

- homogeneous, dielectric (isotropic, chiral) and perfectly conducting, axisymmetric particles (“TAXSYM.f90”),
- homogeneous, dielectric (isotropic, uniaxial anisotropic, chiral) and perfectly conducting, nonaxisymmetric particles (“TNONAXSYM.f90”),
- axisymmetric, composite particles (“TCOMP.f90”),
- axisymmetric, layered particles (“TLAY.f90”),
- an inhomogeneous, dielectric, axisymmetric particle with an arbitrarily shaped inclusion (“TINHOM.f90”),
- an inhomogeneous, dielectric sphere with a spherical inclusion (“TINHOM2SPH.f90”),
- an inhomogeneous, dielectric sphere with an arbitrarily shaped inclusion (“TINHOMSPH.f90”),
- an inhomogeneous, dielectric sphere with multiple spherical inclusions (“TINHOMSPHREC.f90”),
- clusters of arbitrarily shaped particles (“TMULT.f90”),
- two homogeneous, dielectric spheres (“TMULT2SPH.f90”),
- clusters of homogeneous, dielectric spheres (“TMULTSPH.f90” and “TMULTSPHREC.f90”),
- concentrically layered spheres (“TSPHERE.f90”) and

- a homogeneous, dielectric or perfectly conducting, axisymmetric particle on or near a plane surface (“TPARTSUB.f90”).

The code

- performs convergence tests and write the results to the output file “/OUTPUTFILES/Output.dat”,
- computes and stores the \mathbf{T} matrix in the file “/TMATFILES/FileTmat”, and
- compute the scattering characteristics and write the results to the files “/OUTPUTFILES/FileDSCS” and “/OUTPUTFILES/FileScat”.

Three other routines are called by the main program:

- “SCT.f90” computes the scattering characteristics of a particle using the previously calculated \mathbf{T} matrix,
- “SCTAVRGSPH.f90” computes the scattering characteristics of an ensemble of polydisperse, homogeneous spherical particles, and
- “EFMED.f90” computes the effective wave number of a medium with randomly distributed spheroidal particles.

Detailed descriptions of the routines invoked by the main program are given in the comment lines included at the top of each routine.

Specific \mathbf{T} -matrix calculations are performed by several routines which are included in the following files:

- “AdditionTh.f90” provides routines for computing the translation addition coefficients, the rotation functions and the coupling coefficients,
- “BesLeg.f90” contains routines for computing the spherical Bessel and Hankel functions, the cylindrical Bessel functions and the associated Legendre functions,
- “Check.f90” provides routines for checking the input data,
- “GeomLib.f90” is a library of particle geometries,
- “GeomTrans.f90” provides routines for geometric transformations,
- “IncCoeff.f90” contains routines for computing the incident field coefficients for a vector plane wave and a Gaussian beam,
- “InputOutput.f90” supplies routines for reading and writing the data,
- “Integr.f90” provides numerical integration routines,
- “Interp.f90” supplies interpolation routines,

- “MachParam.f90” contains routines for computing the machine constants,
- “MatrixOp.f90” provides routines for performing elementary matrix operations,
- “MatrixQ.f90” contains routines for computing the (partial) \mathbf{Q} matrices and the incident matrices at a specific integration point,
- “MatrixSolv.f90” supplies routines for solving linear algebraic equations,
- “MatrixTrans.f90” provides matrix transformation routines,
- “Parameter.f90” defines the constant parameters of the codes,
- “PostProces1.f90” and “PostProces2.f90” provide routines for computing the scattering characteristics for a particle in a fixed or a random orientation,
- “PostProces3.f90” provides analytical size averaging routines for spherical particles,
- “Proces1.f90” supplies routines for computing the complete \mathbf{Q} matrices and the incident matrices for axisymmetric and nonaxisymmetric particles,
- “Proces2.f90” supplies routines for computing the complete \mathbf{Q} matrices and the incident matrices for composite and layered particles,
- “Proces3.f90” supplies routines for computing the scattered field coefficients for spheres and the complete \mathbf{Q} matrices for uniaxial anisotropic particles and particles on or near a plane surface, and
- “SVWF.f90” provides routines for computing the localized and distributed vector spherical wave functions.

The programs are written in a modular form, so that modifications, if required, should be fairly straightforward. In this context, the routines contained in the files:

- “BesLeg.f90”,
- “GeomLib.f90”,
- “Integr.f90”,
- “Interp.f90”,
- “MachParam.f90”,
- “MatrixOp.f90”,
- “MatrixSolv.f90”, and

- “SVWF.f90”

can be replaced by more efficient routines.

The code performs calculations with double- or extended-precision floating point variables. The precision control parameter `O` is defined in the file “Parameters.f90”. For double-precision calculation, set `O = kind(1.d0)`, while for extended-precision calculation, use the statement `O = kind(1.q0)`. The extended-precision codes are slower than the double-precision codes by a factor of 5-6, but allow computations for larger particles. It should also be mentioned that the CPU time consumption rapidly increases with increasing the particle size and asphericity.

T-matrix calculations involve matrix inversions which can be performed with the LU-factorization. For large matrices, the stabilized version of Bi-Conjugate-Gradients with preconditioning can be used. In general, matrix inversion is an ill-conditioned process and the round-off errors become significant with increasing the particle size and/or aspect ratio. As a result, **T**-matrix computations can become divergent. Efficient ways of dealing with this numerical instability is to use extended precision or distributed vector spherical wave functions. Distributed sources can be used for axisymmetric particles and are preferable for highly aspherical particles. For highly elongated particles, the sources are distributed along the axis of symmetry of the particle, while for highly flattened particles, the sources are distributed in the complex plane. Error messages are printed to the screen and messages appear explaining the cause of termination. **However, we are convinced that we were not able to imagine all conflicting situations. Therefore, we recommend to analyze carefully the significance of the input parameters.**

2.2 Directory INPUTFILES

Input to the program is by means of user supplied input files. In fact, the input parameters are divided between several groups each specified by a keyword that is recognized by the program. Once a keyword has been read, the program expects certain parameters to follow. The following points should be noted:

- Each parameter is specified on a single line and free format input is used throughout.
- Comments are included at the end of each group.
- Character input must be enclosed by quotes.
- When file names are supplied, they should not be greater than 80 characters long.

The general structure of a group of variables is:

< keyword of the group of variables >

< value of variable 1 >

...

```

< value of variable n >
Variables:
< name and short description of variable 1 >
...
< name and short description of variable n >

```

Note that the lines after the line `< value of variable n >` are comments. For example, the group of variables `MatProp`, contained in the input file `"InputAXSYM.dat"`, read as

```

MatProp
.false.
.false.
0.1
Variables:
- perfectcond - if perfectcond = t, the particle is perfectly conducting.
- chiral - if chiral = t, the particle is optical active (chiral).
- kb - parameter of chirality.

```

In general, the required input parameters are specified in three input files:

- the file `"/INPUTFILES/InputXXX.dat"` provides the variables specifying the optical properties, geometry, type of discrete sources and error tolerances,
- the file `"/INPUTFILES/InputSCT.dat"` provides the variables specifying the scattering characteristics calculation, and
- the file `"/INPUTFILES/Input.dat"` specifies the model control parameters.

Here `XXX` stands for `AXSYM`, `NONAXSYM`, `COMP`, `LAY`, `INHOM`, `INHOM2SPH`, `INHOMSPH`, `INHOMSPHREC`, `MULT`, `MULT2SPH`, `MULTSPH`, `MULTSPHREC`, `SPHERE`, `PARTSUB`, `EFMED` and `SCTAVRGSPH`.

2.2.1 "InputXXX.dat"

Exhaustive descriptions of the parameters required by the input files `"InputXXX.dat"` are given in the comment lines of each **T**-matrix routine.

2.2.2 "InputSCT.dat"

The scattering characteristics depend on the type of the orientation distribution function. By convention, the uniform distribution function is called complete if the Euler angles α_p , β_p and γ_p are uniformly distributed in the intervals $(0, 360^\circ)$, $(0, 180^\circ)$ and $(0, 360^\circ)$, respectively. The normalization constant is 4π for axisymmetric particles and $8\pi^2$ for nonaxisymmetric particles. The uniform distribution function is called incomplete if the Euler angles α_p , β_p and γ_p are uniformly distributed in the intervals $(\alpha_{p \min}, \alpha_{p \max})$, $(\beta_{p \min}, \beta_{p \max})$,

and $(\gamma_{\text{p min}}, \gamma_{\text{p max}})$, respectively. For axisymmetric particles, the orientational average is performed over α_{p} and β_{p} , and the normalization constant is

$$(\alpha_{\text{p max}} - \alpha_{\text{p min}}) (\cos \beta_{\text{p min}} - \cos \beta_{\text{p max}}),$$

while for nonaxisymmetric particles, the orientational average is performed over α_{p} , β_{p} and γ_{p} , and the normalization constant is

$$(\alpha_{\text{p max}} - \alpha_{\text{p min}}) (\cos \beta_{\text{p min}} - \cos \beta_{\text{p max}}) (\gamma_{\text{p max}} - \gamma_{\text{p min}}).$$

The scattering characteristics computed by the code are summarized below.

Complete uniform distribution function

For the complete uniform distribution function, the external excitation is a vector plane wave propagating along the Z -axis of the global coordinate system and the scattering plane is the XZ -plane. The code computes the following orientation-averaged quantities:

- the scattering matrix $\langle \mathbf{F} \rangle$ at a set of $N_{\theta, \text{RND}}$ scattering angles,
- the extinction matrix $\langle \mathbf{K} \rangle$,
- the scattering and extinction cross sections $\langle C_{\text{scat}} \rangle$ and $\langle C_{\text{ext}} \rangle$, and
- the asymmetry parameter $\langle \cos \Theta \rangle$.

The scattering angles, at which the scattering matrix is evaluated, are uniformly spaced in the interval $(\theta_{\text{min, RND}}, \theta_{\text{max, RND}})$. The elements of the scattering matrix are expressed in terms of the ten average quantities

$$\begin{aligned} &\langle |S_{\theta\beta}|^2 \rangle, \langle |S_{\theta\alpha}|^2 \rangle, \langle |S_{\varphi\beta}|^2 \rangle, \langle |S_{\varphi\alpha}|^2 \rangle, \langle S_{\theta\beta} S_{\varphi\alpha}^* \rangle, \\ &\langle S_{\theta\alpha} S_{\varphi\beta}^* \rangle, \langle S_{\theta\beta} S_{\theta\alpha}^* \rangle, \langle S_{\theta\beta} S_{\varphi\beta}^* \rangle, \langle S_{\theta\alpha} S_{\varphi\alpha}^* \rangle, \langle S_{\varphi\beta} S_{\varphi\alpha}^* \rangle, \end{aligned}$$

for macroscopically isotropic media, and the six average quantities

$$\langle |S_{\theta\beta}|^2 \rangle, \langle |S_{\theta\alpha}|^2 \rangle, \langle |S_{\varphi\beta}|^2 \rangle, \langle |S_{\varphi\alpha}|^2 \rangle, \langle S_{\theta\beta} S_{\varphi\alpha}^* \rangle, \langle S_{\theta\alpha} S_{\varphi\beta}^* \rangle,$$

for macroscopically isotropic and mirror-symmetric media. $\langle S_{pq} S_{p_1 q_1}^* \rangle$ are computed at $N_{\theta, \text{GS}}$ scattering angles, which are uniformly spaced in the interval $(0, 180^\circ)$. The scattering matrix is calculated at the same sample angles and polynomial interpolation is used to evaluate the scattering matrix at any polar angle θ in the range $(\theta_{\text{min, RND}}, \theta_{\text{max, RND}})$. The average quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ can be computed by using a numerical procedure or the analytical orientation-averaging approach. The numerical orientation-averaging procedure chooses the angles α_{p} , β_{p} and γ_{p} to sample the intervals $(0, 360^\circ)$, $(0, 180^\circ)$ and $(0, 360^\circ)$, respectively. The prescription for choosing the angles is to

- uniformly sample in α_{p} ,

- uniformly sample in $\cos \beta_p$ or nonuniformly sample in β_p , and
- uniformly sample in γ_p .

The integration over α_p and γ_p are performed with Simpson's rule, and the number of integration points N_α and N_γ must be odd numbers. The integration over β_p can also be performed with Simpson's rule, and in this specific case, the algorithm samples uniformly in $\cos \beta_p$, and the number of integration points N_β is an odd number. Alternatively, Gauss-Legendre quadrature method can be used for averaging over β_p , and N_β can be any integer number. For the analytical orientation-averaging approach, the maximum expansion and azimuthal orders N_{rank} and M_{rank} (specifying the dimensions of the \mathbf{T} matrix) can be reduced. In this case, a convergence test over the extinction and scattering cross sections gives the effective values $N_{\text{rank}}^{\text{eff}}$ and $M_{\text{rank}}^{\text{eff}}$.

The orientation-averaged extinction matrix $\langle \mathbf{K} \rangle$ is computed by using (16) and (17), and note that for macroscopically isotropic and mirror-symmetric media the off-diagonal elements are zero and the diagonal elements are equal to the orientation-averaged extinction cross section per particle.

For macroscopically isotropic and mirror-symmetric media, the orientation-averaged scattering and extinction cross sections $\langle C_{\text{scat}} \rangle = \langle C_{\text{scat}} \rangle_{\text{I}}$ and $\langle C_{\text{ext}} \rangle = \langle C_{\text{ext}} \rangle_{\text{I}}$ are calculated by using (18) and (19), respectively, while for macroscopically isotropic media, the code additionally computes $\langle C_{\text{scat}} \rangle_{\text{V}}$ accordingly to (20), and $\langle C_{\text{ext}} \rangle_{\text{V}}$ as $\langle C_{\text{ext}} \rangle_{\text{V}} = \langle K_{14} \rangle$.

The asymmetry parameter $\langle \cos \Theta \rangle$ is determined by angular integration over the scattering angle θ . The number of integration points is $N_{\theta, \text{GS}}$ and Simpson's rule is used for calculation. For macroscopically isotropic and mirror-symmetric media, the asymmetry parameter $\langle \cos \Theta \rangle = \langle \cos \Theta \rangle_{\text{I}}$ is calculated by using (22), while for macroscopically isotropic media, the code supplementarily computes $\langle \cos \Theta \rangle_{\text{V}}$ accordingly to (23).

The physical correctness of the computed results is tested by using the inequalities

$$\begin{aligned}
\langle F_{11} \rangle &\geq |\langle F_{ij} \rangle|, \quad i, j = 1, 2, 3, 4, \\
(\langle F_{11} \rangle + \langle F_{22} \rangle)^2 - 4 \langle F_{12} \rangle^2 &\geq (\langle F_{33} \rangle + \langle F_{44} \rangle)^2 + 4 \langle F_{34} \rangle^2, \\
\langle F_{11} \rangle - \langle F_{22} \rangle &\geq |\langle F_{33} \rangle - \langle F_{44} \rangle|, \\
\langle F_{11} \rangle - \langle F_{12} \rangle &\geq |\langle F_{22} \rangle - \langle F_{12} \rangle|, \\
\langle F_{11} \rangle + \langle F_{12} \rangle &\geq |\langle F_{22} \rangle + \langle F_{12} \rangle|,
\end{aligned} \tag{24}$$

given by Hovenier and van der Mee. The message that the test is not satisfied means that the computed results may be wrong.

The code also computes the average differential scattering cross sections $\langle \sigma_{\text{dp}} \rangle$ and $\langle \sigma_{\text{ds}} \rangle$ for a specific incident polarization state and at a set of $N_{\theta, \text{GS}}$ scattering angles (cf. (14) and (15)). These scattering angles are uniformly spaced in the interval $(0, 180^\circ)$ and coincide with the sample angles at which the average quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ are computed. The polarization state of the incident vector plane wave is specified by the complex amplitudes $E_{e0, \beta}$ and $E_{e0, \alpha}$, and the

differential scattering cross sections are calculated for the complex polarization unit vector

$$\mathbf{e}_{\text{pol}} = \frac{1}{\sqrt{|E_{e0,\beta}|^2 + |E_{e0,\alpha}|^2}} (E_{e0,\beta} \mathbf{e}_\beta + E_{e0,\alpha} \mathbf{e}_\alpha). \quad (25)$$

Note that $N_{\theta,\text{GS}}$ is the number of scattering angles at which $\langle S_{pq} S_{p_1 q_1}^* \rangle$, $\langle \sigma_{\text{dp}} \rangle$ and $\langle \sigma_{\text{ds}} \rangle$ are computed, and also gives the number of integration points for calculating $\langle C_{\text{scat}} \rangle_V$, $\langle \cos \Theta \rangle_I$ and $\langle \cos \Theta \rangle_V$. Because the integrals are computed with Simpson's rule, $N_{\theta,\text{GS}}$ must be an odd number.

Incomplete uniform distribution function

For the incomplete uniform distribution function, we use a global coordinate system to specify both the direction of propagation and the states of polarization of the incident and scattered waves, and the particle orientation. A special orientation with a constant orientation angle can be specified by setting $N_\delta = 1$ and $\delta_{\text{min}} = \delta_{\text{max}}$, where δ stands for α_p , β_p and γ_p . For example, uniform particle orientation distributions around the Z -axis can be specified by setting $N_\beta = 1$ and $\beta_{p\text{min}} = \beta_{p\text{max}}$.

The scattering characteristics are averaged over the particle orientation by using a numerical procedure. The prescriptions for choosing the sample angles and the significance of the parameters are as above. For each particle orientation we compute the following quantities:

- the phase matrix \mathbf{Z} at N_φ scattering planes,
- the extinction matrix \mathbf{K} for a plane wave incidence,
- the scattering and extinction cross sections C_{scat} and C_{ext} for incident parallel and perpendicular linear polarizations, and
- the mean direction of propagation of the scattered field \mathbf{g} for incident parallel and perpendicular linear polarizations.

The azimuthal angles describing the positions of the scattering planes at which the phase matrix is computed are $\varphi(1), \varphi(2), \dots, \varphi(N_\varphi)$. In each scattering plane i , $i = 1, 2, \dots, N_\varphi$, the number of zenith angles is $N_\theta(i)$, while the zenith angle varies between $\theta_{\text{min}}(i)$ and $\theta_{\text{max}}(i)$. For each particle orientation, the phase and extinction matrices \mathbf{Z} and \mathbf{K} are computed, while the scattering and extinction cross sections C_{scat} and C_{ext} are calculated accordingly to (9) and (10), respectively.

The mean direction of propagation of the scattered field \mathbf{g} is evaluated by angular integration over the scattering angles θ and φ (cf. (11)), and the numbers of integration points are $N_{\theta,\text{asym}}$ and $N_{\varphi,\text{asym}}$. The integration over φ is performed with Simpson's rule, while the integration over θ can be performed with Simpson's rule or Gauss-Legendre quadrature method. We note that the optical cross sections and the mean direction of propagation of the scattered field are computed for linearly polarized incident waves (vector plane waves and Gaussian beams) by choosing $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$ (cf. (7)).

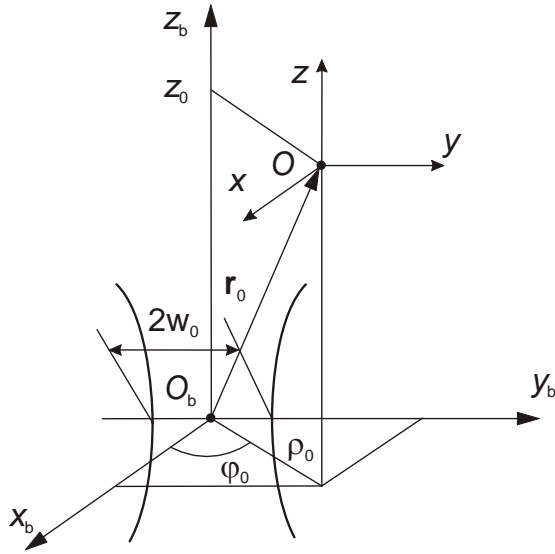


Figure 4: Geometry of a Gaussian beam.

The code also calculates the average differential scattering cross sections σ_{dp} and σ_{ds} in the azimuthal plane φ_{GS} and at a set of $N_{\theta,GS}$ scattering angles. The average differential scattering cross sections can be computed for scattering angles ranging from 0° to 180° in the azimuthal plane φ_{GS} and from 180° to 0° in the azimuthal plane $\varphi_{GS} + 180^\circ$, or for scattering angles ranging from 0° to 180° in the azimuthal plane φ_{GS} . The calculations are performed for elliptically polarized vector plane waves (characterized by the complex polarization unit vector \mathbf{e}_{pol} as in (25)) and linearly polarized Gaussian beams (characterized by the polarization angle α_{pol}). The geometry for a Gaussian beam excitation is shown Fig. 4.

For spherical particles, the code chooses a single orientation $\alpha_{p\ min} = \alpha_{p\ max} = 0^\circ$, $\beta_{p\ min} = \beta_{p\ max} = 0^\circ$ and $\gamma_{p\ min} = \gamma_{p\ max} = 0^\circ$, and sets $M_{rank} = N_{rank}$. The input parameters specified in the file "InputSCT.dat" are listed below.

- wavelength (real) - wavelength in the surrounding medium.
- FileTmat (character(80)) - name of the file containing the \mathbf{T} matrix.
- Mrank, Nrank (integers) - are the variables M_{rank} and N_{rank} and represent the number of azimuthal modes and the maximum expansion order, respectively. These parameters give the dimensions of the \mathbf{T} matrix.
- axsym (logical) - if axsym = t, the scatterer is a rotationally symmetric particle (axisymmetric particle).

| particle | axsym | sphere | chiral |
|-------------------------------|-------|--------|--------|
| axisymmetric and chiral | t | f | t |
| axisymmetric and nonchiral | t | f | f |
| sphere (always nonchiral) | t | t | f |
| nonaxisymmetric and chiral | f | f | t |
| nonaxisymmetric and nonchiral | f | f | f |

Table 1: Values of the logical variables axsym, sphere and chiral.

- sphere (logical) - if sphere = t, the scatterer is a spherical particle. Note that for a spherical particle we must set: sphere = .true. **and** axsym = .true.
- chiral (logical) - if chiral = t, the scatterer is an optical active particle (chiral particle). The possible values of the logical variables axsym, sphere and chiral are as in Table 1.

The above parameters must be specified if the main program calls the routine "SCT.f90", i.e., if we compute the scattering characteristics of a particle using the previously calculated T matrix. Otherwise these parameters are ignored.

- RandomOrientation (logical) - if RandomOrientation = t, the uniform distribution function is complete and the particle is randomly oriented with respect to the global coordinate system. The Euler orientation angles α_p , β_p and γ_p are uniformly distributed in the intervals $(0^\circ, 360^\circ)$, $(0^\circ, 180^\circ)$ and $(0^\circ, 360^\circ)$, respectively. If RandomOrientation = f, the uniform distribution function is incomplete and the Euler orientation angles are uniformly distributed in the intervals $(\alpha_{p \min}, \alpha_{p \max})$, $(\beta_{p \min}, \beta_{p \max})$, and $(\gamma_{p \min}, \gamma_{p \max})$, respectively.

The following input parameters must be specified for a complete uniform distribution function, i.e., for RandomOrientation = .true.

- MirrorSym (logical) - if MirrorSym = t, the scattering medium is isotropic and mirror-symmetric.
- DoNumAvrg (logical) - if DoNumAvrg = t, the average quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ are computed by using a numerical orientation-averaging procedure. Otherwise, an analytical orientation-averaging procedure is employed.
- NthetaGS (integer) - is the variable $N_{\theta,GS}$ and gives the number of scattering angle at which the average quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ are computed. The scattering angles are uniformly spaced and $N_{\theta,GS}$ must be an **odd number**. The scattering matrix and the differential scattering cross section are also computed at $N_{\theta,GS}$ scattering angles, while the asymmetry parameter is calculated with Simpson's rule by integrating $\langle F_{11}(\theta) \rangle$ over the $N_{\theta,GS}$ scattering angles.

- ReducedOrder (logical) - if ReducedOrder = t, the analytical orientation-averaging procedure (DoNumAvrg = f) computes the average quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ for reduced values of N_{rank} and M_{rank} . The effective values $N_{\text{rank}}^{\text{eff}}$ and $M_{\text{rank}}^{\text{eff}}$ are computed by analyzing the convergence of the extinction and scattering cross sections.
- deltaOrder (real) - error tolerance for the convergence test over the extinction and scattering cross sections. This parameter is used for computing $N_{\text{rank}}^{\text{eff}}$ and $M_{\text{rank}}^{\text{eff}}$.
- UseSimpson (logical) - if UseSimpson = t, the integration over the orientation angle β_p is transformed into an integration over $\cos \beta_p$ and the Simpson rule is used for numerical integration (uniformly sample in $\cos \beta_p$). If UseSimpson = f, the integration is performed with the Gauss-Legendre quadrature method.
- Nalpha, Nbeta, Ngamma (integers) - are the variables N_α , N_β and N_γ , and give the numbers of division points for averaging the quantities $\langle S_{pq} S_{p_1 q_1}^* \rangle$ over the Euler orientation angles α_p , β_p and γ_p (when DoNumAvrg = t). The integration over α_p and γ_p are performed with Simpson's rule and N_α and N_γ must be **odd numbers**. If the numerical integration over β_p is performed with Simpson's rule (UseSimpson = t), N_β must be also an **odd number**.
- anorm (real) - is the variable a_c and specifies the characteristic length of the particle which is used to normalize the average differential scattering cross sections and the optical cross sections.
- ComputeDSCS (logical) - if ComputeDSCS = t, the average differential scattering cross sections are computed in the azimuthal plane φ_{GS} and for the complex polarization unit vector \mathbf{e}_{pol} . The complex polarization unit vector \mathbf{e}_{pol} is computed from the complex amplitudes $E_{e0,\beta}$ and $E_{e0,\alpha}$. If ComputeDSCS = f, this calculation is not performed.
- EI_betaGI (complex) - is the variable $E_{e0,\beta}$ and represents the parallel component of the complex amplitude vector (in the β -direction) for a plane wave incidence.
- EI_alphaGI (complex) - is the variable $E_{e0,\alpha}$ and represents the perpendicular component of the complex amplitude vector (in the α -direction) for a plane wave incidence.
- phiGS (real) - is the variable φ_{GS} and specifies the scattering plane in which the average differential scattering cross sections are computed.
- normalized (logical) - if normalized = t, the average differential scattering cross sections are normalized by πa_c^2 , where a_c is the characteristic length of the particle.

- FileDSCS (character(80)) - name of the file to which the average differential scattering cross sections are written.
- ComputeScatPar (logical) - if ComputeScatPar = t, the extinction and scattering cross sections, the asymmetry parameter, and the extinction and scattering matrix are computed.
- NthetaRND (integer) - is the variable $N_{\theta,RND}$ and gives the number of zenith angle values in the interval $(\theta_{min,RND}, \theta_{max,RND})$ at which the scattering matrix is computed. The zenith angles are uniformly spaced.
- thetaminRND, thetamaxRND (reals) - are the variables $\theta_{min,RND}$ and $\theta_{max,RND}$, and specify the minimal and maximal values of the zenith angle θ at which the scattering matrix is computed.
- FileSCAT (character(80)) - name of the file to which the scattering characteristics are written.
- Nelem (integer) - number of scattering matrix elements to be printed out in the output file FileSCAT.
- MatrixElem (integer array) - set of matrix elements to be printed. The permissive values are: 11, 12, 13, 14, 15, 21, 22, 23, 24, 31, 32, 33, 34, 41, 42, 43, 44. The default set of elements is: 11, 21, 31, 41, 12, 13 and Nelem = 6.

The following input parameters must be specified for an incomplete uniform distribution function, i.e., for RandomOrientation = .false.

- UseSimpson (logical) - if UseSimpson = t, the integration over the orientation angle β_p is transformed into an integration over β_p and the Simpson rule is used for numerical integration (uniformly sample in $\cos \beta_p$). Furthermore, if UseSimpson = t, the integration over the scattering angle θ for computing the asymmetry parameter and the mean direction of propagation of the scattered radiation is also performed with Simpson's rule. If UseSimpson = f, the integrations are performed with the Gauss-Legendre quadrature method.
- alphamin, alphamax, betamin, betamax, gammamin, gammamax (reals) - are the variables $\alpha_{p\ min}$, $\alpha_{p\ max}$, $\beta_{p\ min}$, $\beta_{p\ max}$, $\gamma_{p\ min}$ and $\gamma_{p\ max}$, and specify the minimal and maximal values of the Euler orientation angles α_p , β_p and γ_p .
- Nalpha, Nbeta, Ngamma (integers) - are the variables N_α , N_β and N_γ , and give the numbers of division points for averaging the scattering characteristics over the Euler orientation angles α_p , β_p and γ_p . The integration over α_p and γ_p are performed with Simpson's rule and N_α and N_γ must be **odd numbers**. If the numerical integration over β_p is performed with Simpson's rule (UseSimpson = t), N_β must be also an **odd number**.

- `anorm` (real) - is the variable a_c and represents the characteristic length of the particle which is used to normalize the average differential scattering cross sections and the optical cross sections.
- `TypeExcit` (character(5)) - specifies the type of the external excitation. `TypeExcit = 'PLANE'`, for a plane wave excitation, and `TypeExcit = 'GAUSS'` for a Gaussian beam excitation.
- `betaGI`, `alphaGI` (reals) - are the variables β and α , and specify the angular coordinates of the incident direction in the global coordinate system.
- `x0`, `y0`, `z0` (reals) - are the variables x_0 , y_0 and z_0 , and represent the Cartesian coordinates of the middle of the Gaussian beam waist.
- `w0` (real) - is the variable w_0 and represents the waist radius of the Gaussian beam.
- `ComputeDSCS` (logical) - if `ComputeDSCS = t`, the average differential scattering cross sections are computed in the azimuthal plane φ_{GS} . For a plane wave incidence, the calculation is performed for the complex polarization unit vector \mathbf{e}_{pol} . The complex polarization unit vector \mathbf{e}_{pol} is computed from the complex amplitudes $E_{e0,\beta}$ and $E_{e0,\alpha}$. In the case of a Gaussian beam illumination, the calculation is performed for a linearly polarized wave. The state of polarization of the Gaussian beam is described by the polarization angle $\alpha_{pol,gauss}$. If `ComputeDSCS = f`, this calculation is not performed.
- `EI_betaGI` (complex) - is the variable $E_{e0,\beta}$ and specify the parallel component of the complex amplitude vector (in the β -direction) for a plane wave incidence.
- `EI_alphaGI` (complex) - is the variable $E_{e0,\alpha}$ and specify the perpendicular component of the complex amplitude vector (in the α -direction) for a plane wave incidence.
- `alphapGauss` (real) - is the variable $\alpha_{pol,gauss}$ and represents the polarization angle of the Gaussian beam. If $(\mathbf{e}_k, \mathbf{e}_\beta, \mathbf{e}_\alpha)$ are the spherical unit vectors of the incident direction (β, α) , then $\alpha_{pol,gauss}$ is the angle between the electric field vector and the unit vector \mathbf{e}_β .
- `phiGS` (real) - is the variable φ_{GS} and specifies the scattering plane in which the average differential scattering cross sections are computed.
- `NthetaGS` (integer) - is the variable $N_{\theta,GS}$ and gives the number of scattering angle at which the average differential scattering cross sections are computed. The scattering angles are uniformly spaced.
- `ExtThetaDom` (logical) - if `ExtThetaDom = t` the DSCS are computed for scattering angles ranging from 0° to 180° in the azimuthal plane φ_{GS} , and from 180° to 0° in the azimuthal plane $\varphi_{GS} + 180^\circ$. The total number of

scattering angles is $N_{\theta,GS}$. If `ExtThetaDom = f` the DSCS are computed for scattering angles ranging from 0° to 180° in the azimuthal plane φ_{GS} .

- `normalized (logical)` - if `normalized = t`, the average differential scattering cross sections are normalized by πa_c^2 , where a_c is the characteristic length of the particle.
- `FileDSCS (character(80))` - name of the file to which the average differential scattering cross sections are written.
- `ComputeScatPar (logical)` - if `ComputeScatPar = t`, the scattering characteristics are computed at specified scattering directions. The following average quantities are computed: the extinction and scattering cross sections for incident parallel and perpendicular linear polarizations, the mean direction of propagation of the scattered radiation for incident parallel and perpendicular linear polarizations, and the phase and extinction matrices. Note that the extinction matrix is computed only for a plane wave excitation. The azimuthal angles describing the positions of the scattering planes at which the phase matrix is computed are $\varphi(1), \dots, \varphi(N_\varphi)$. In each scattering plane i , $i = 1, \dots, N_\varphi$, the number of zenith angles is $N_\theta(i)$, while the zenith angle varies between $\theta_{\min}(i)$ and $\theta_{\max}(i)$.
- `Nphi (integer)` - is the variable N_φ and gives the number of scattering planes at which the phase matrix is computed.
- `phi (real array)` - is the array $\varphi(1), \dots, \varphi(N_\varphi)$ of all azimuthal angles specifying the scattering planes at which the phase matrix is computed.
- `Ntheta (integer array)` - is the array $N_\theta(1), \dots, N_\theta(N_\varphi)$, and gives the number of zenith angle values in each scattering plane at which the phase matrix is computed.
- `thetamin, thetamax (real arrays)` - are the arrays $\theta_{\min}(1), \dots, \theta_{\min}(N_\varphi)$ and $\theta_{\max}(1), \dots, \theta_{\max}(N_\varphi)$, and specify the minimal and maximal values of the zenith angle in each scattering plane at which the phase matrix is computed.
- `FileSCAT (character(80))` - name of the file to which the scattering characteristics are written.
- `Nelem (integer)` - number of phase matrix elements to be printed out in the output file `FileSCAT`.
- `MatrixElem (integer array)` - set of matrix elements to be printed. The permissible values are: 11, 12, 13, 14, 15, 21, 22, 23, 24, 31, 32, 33, 34, 41, 42, 43, 44. The default set of elements is: 11, 21, 31, 41, 12, 13 and `Nelem = 6`.
- `ComputeAsymPar (logical)` - if `ComputeAsymPar = t`, the mean direction of propagation of the scattered wave is computed.

- $N_{\theta, \text{asym}}$, $N_{\phi, \text{asym}}$ (integers) - are the variables $N_{\theta, \text{asym}}$ and $N_{\phi, \text{asym}}$, and give the numbers of integration points for computing the the mean direction of propagation of the scattered radiation. If the integration over θ is performed with Simpson's rule ($\text{UseSimpson} = \text{t}$), $N_{\theta, \text{asym}}$ must be an **odd number**.
- PrnProgress (logical) - if $\text{PrnProgress} = \text{t}$, the progress of calculation is printed.
- WriteInputInfo (logical) - if $\text{WriteInputInfo} = \text{t}$, the input parameters of the scattering problem are written to the output files FileDSCS and FileSCAT .

Note that all input parameters specifying lengths must be provided in the same units of lengths.

The process of computing the scattering characteristics is shown by the following logical scheme.

```

if (  $\text{RandomOrientation}$  ) then
   $\text{TypeExcit} = \text{'PLANE'}$ ,  $\beta = \alpha = 0$  (the incident wave is an arbitrarily
  polarized vector plane wave propagating along the  $Z$ -axis of the
  global coordinate system)
  < read the integer variable  $N_{\theta, \text{GS}}$  from the input file "Input.SCT.dat" >
  if (  $\text{.not. DoNumAvrg}$  ) then
    < read the logical variable  $\text{ReducedOrder}$  from the file
    "InputSCT.dat" >
    < compute  $\langle S_{pq} S_{p_1 q_1}^* \rangle$  at  $N_{\theta, \text{GS}}$  discrete angles,
    and  $\langle C_{\text{ext}} \rangle_{\text{I}}$  and  $\langle C_{\text{scat}} \rangle_{\text{I}}$  by using the analytical
    integration procedure; if  $\text{ReducedOrder} = \text{t}$ , the effective
    values  $N_{\text{rank}}^{\text{eff}}$  and  $M_{\text{rank}}^{\text{eff}}$  are computed by using a
    convergence test over the extinction and scattering cross
    sections >
  else
     $\text{ReducedOrder} = \text{.false.}$ 
    < read the variables  $\text{UseSimpson}$ ,  $N_{\alpha}$ ,  $N_{\beta}$  and  $N_{\gamma}$ 
    from the file "InputSCT.dat" >
    < compute  $\langle S_{pq} S_{p_1 q_1}^* \rangle$  at  $N_{\theta, \text{GS}}$  discrete angles,
    and  $\langle C_{\text{ext}} \rangle_{\text{I}}$  and  $\langle C_{\text{scat}} \rangle_{\text{I}}$  by using the numerical
    integration procedure; if  $\text{UseSimpson} = \text{t}$ , the integration over
     $\beta$  is performed with Simpson's rule >
  end if
  if (  $\text{ComputedDSCS}$  ) then
    < read the variables  $\varphi_{\text{GS}}$ ,  $E_{e0, \beta}$  and  $E_{e0, \alpha}$  from
    the file "InputSCT.dat" >
    < compute the complex polarization unit vector  $\mathbf{e}_{\text{pol}}$  >
    if (  $\text{.not. MirrorSym}$  ) < compute  $\langle C_{\text{ext}} \rangle_{\text{V}}$  and  $\langle C_{\text{scat}} \rangle_{\text{V}}$ ;
    the number of integration points for computing  $\langle C_{\text{scat}} \rangle_{\text{V}}$  is
  
```

$N_{\theta,GS}$ and the Simpson rule is used for calculation >
 < for an elliptically polarized vector plane wave, characterized
 by the complex polarization unit vector \mathbf{e}_{pol} , compute
 $\langle \sigma_{dp} \rangle$ and $\langle \sigma_{ds} \rangle$ at $N_{\theta,GS}$ scattering angles in the azimuthal
 plane φ_{GS} >
 < write $\langle \sigma_{dp} \rangle$ and $\langle \sigma_{ds} \rangle$ together with $\langle C_{ext} \rangle_I$, $\langle C_{scat} \rangle_I$,
 $\langle C_{ext} \rangle_V$ and $\langle C_{scat} \rangle_V$ to the file FileDSCS; note that
 $\langle C_{ext} \rangle_I$, $\langle C_{scat} \rangle_I$, $\langle C_{ext} \rangle_V$ and $\langle C_{scat} \rangle_V$ do not depend on
 the polarization state of the incident vector plane wave >
end if
if (ComputeScatPar) then
 < read the variables $N_{\theta,RND}$, $\theta_{min,RND}$ and $\theta_{max,RND}$
 from the file "InputSCT.dat" >
 < compute the average extinction matrix for macroscopically
 isotropic media; if the scattering medium is mirror symmetric,
 the extinction matrix is a diagonal matrix >
 < compute the average asymmetry parameter $\langle \cos \Theta \rangle_I$,
 and for macroscopically isotropic media, additionally compute
 $\langle \cos \Theta \rangle_V$; the number of integration points for computing
 the asymmetry parameters is $N_{\theta,GS}$ and the Simpson rule is
 used for calculation >
if (.not. MirorSym) < compute $\langle C_{ext} \rangle_V$ and $\langle C_{scat} \rangle_V$;
 the number of integration points for computing $\langle C_{scat} \rangle_V$ is
 $N_{\theta,GS}$ and the Simpson rule is used for calculation >
 < compute the scattering matrix at $N_{\theta,RND}$ scattering angles
 (uniformly spaced in the interval $(\theta_{min,RND}, \theta_{max,RND})$),
 and write the results together with the average extinction matrix,
 asymmetry parameter and optical cross sections to the file
 FileSCAT; note that these quantities are independent on the
 polarization state of the incident vector plane wave >
end if
else
 < read the logical variable UseSimpson (specifying the type of
 integration method for the orientational average procedure) from
 the file "InputSCT.dat" >
 < read the minimal and the maximal values of the Euler orientation
 angles: $\alpha_{p min}$, $\alpha_{p max}$, $\beta_{p min}$, $\beta_{p max}$, $\gamma_{p min}$ and $\gamma_{p max}$,
 and the number of integration points N_α , N_β and N_γ >
 < read the variables TypeExcit ('PLANE' or 'GAUSS'), β
 and α from the file "InputSCT.dat"; note that the incident field
 is a linearly polarized Gaussian beam or a vector plane wave
 propagating in the direction (β, α) >
if (ComputeDSCS) then
 < read the variables φ_{GS} , $N_{\theta,GS}$, $E_{e0,\beta}$, $E_{e0,\alpha}$
 and $\alpha_{pol,gauss}$ from the file "InputSCT.dat" >

```

< for a plane wave incidence, compute the complex polarization
unit vector  $\mathbf{e}_{\text{pol}}$  >
 $\langle C_{\text{ext}} \rangle = 0$ ,  $\langle C_{\text{scat}} \rangle = 0$ ,  $\langle \sigma_{\text{dp}} \rangle = 0$ ,  $\langle \sigma_{\text{ds}} \rangle = 0$ 
for < each particle orientation  $(\alpha_p, \beta_p, \gamma_p)$  > do
  < for an elliptically polarized vector plane wave, characterized
  by the complex polarization unit vector  $\mathbf{e}_{\text{pol}}$ , or for a linearly
  polarized Gaussian beam, characterized by the polarization
  angle  $\alpha_{\text{pol,gauss}}$ , compute the cross sections  $C_{\text{ext}}$  and
   $C_{\text{scat}}$ , and  $\sigma_{\text{dp}}$  and  $\sigma_{\text{ds}}$  at  $N_{\theta,\text{GS}}$  scattering angles
  in the azimuthal plane  $\varphi_{\text{GS}}$  >
   $\langle C_{\text{ext}} \rangle = \langle C_{\text{ext}} \rangle + C_{\text{ext}}/N_{\text{config}}$ 
   $\langle C_{\text{scat}} \rangle = \langle C_{\text{scat}} \rangle + C_{\text{scat}}/N_{\text{config}}$ 
   $\langle \sigma_{\text{dp}} \rangle = \langle \sigma_{\text{dp}} \rangle + \sigma_{\text{dp}}/N_{\text{config}}$ ,  $\langle \sigma_{\text{ds}} \rangle = \langle \sigma_{\text{ds}} \rangle + \sigma_{\text{ds}}/N_{\text{config}}$ 
end for
  < write the average quantities to the file FileDSCS >
end if
if ( ComputeScatPar ) then
  < read the variables ComputeAsymPar,  $N_{\theta,\text{asym}}$  and  $N_{\varphi,\text{asym}}$ 
  from the file "InputSCT.dat" >
  < read the variables  $N_{\varphi}$  and  $\varphi(i)$ ,  $N_{\theta}(i)$ ,  $\theta_{\text{min}}(i)$ 
  and  $\theta_{\text{max}}(i)$  for  $i = 1, \dots, N_{\varphi}$ , from the file "InputSCT.dat" >
   $\langle C_{\text{ext,p}} \rangle = 0$ ,  $\langle C_{\text{ext,s}} \rangle = 0$ ,  $\langle C_{\text{scat,p}} \rangle = 0$ ,  $\langle C_{\text{scat,s}} \rangle = 0$ 
   $\langle \mathbf{g}_p \rangle = 0$ ,  $\langle \mathbf{g}_s \rangle = 0$ ,  $\langle \mathbf{Z} \rangle = 0$ ,  $\langle \mathbf{K} \rangle = 0$ 
  for < each particle orientation  $(\alpha_p, \beta_p, \gamma_p)$  > do
    < assume linearly polarized incident waves (vector plane waves
    or Gaussian beams) and compute the cross sections  $C_{\text{ext,p}}$ ,
     $C_{\text{ext,s}}$ ,  $C_{\text{scat,p}}$  and  $C_{\text{scat,s}}$  for incident parallel and
    perpendicular linear polarizations, that is for  $\alpha_{\text{pol}} = 0^\circ$  and
     $\alpha_{\text{pol}} = 90^\circ$  >
    if ( ComputeAsymPar ) then
      < assume linearly polarized incident waves (vector plane
      waves or Gaussian beams) and compute the mean
      direction of propagation of the scattered radiation  $\mathbf{g}_p$  and
       $\mathbf{g}_s$  for incident parallel and perpendicular linear
      polarizations, that is for  $\alpha_{\text{pol}} = 0^\circ$  and  $\alpha_{\text{pol}} = 90^\circ$ ;
      the number of integration points for computing  $\mathbf{g}_p$  and
       $\mathbf{g}_s$  are  $N_{\theta,\text{asym}}$  and  $N_{\varphi,\text{asym}}$ , and Simpson's rule
      is used for the integration over  $\varphi$ , while, according to
      the value of the logical variable UseSimpon, the Simpson
      rule or the Gauss-Legendrequadrature method is used
      for the integration over  $\theta$  >
    end if
    < for a plane wave incidence, compute the extinction matrix  $\mathbf{K}$  >
    < compute the phase matrix  $\mathbf{Z}$  at  $N_{\varphi}$  scattering planes >
     $\langle C_{\text{ext,p}} \rangle = \langle C_{\text{ext,p}} \rangle + C_{\text{ext,p}}/N_{\text{config}}$ 
     $\langle C_{\text{ext,s}} \rangle = \langle C_{\text{ext,s}} \rangle + C_{\text{ext,s}}/N_{\text{config}}$ 
  end for

```

```

    <Cscat,p> = <Cscat,p> + Cscat,p/Nconfig
    <Cscat,s> = <Cscat,s> + Cscat,s/Nconfig
    if ( ComputeAsymPar ) then
        <gp> = <gp> + gp/Nconfig
        <gs> = <gs> + gs/Nconfig
    end if
    <Z> = <Z> + Z/Nconfig, <K> = <K> + K/Nconfig
end for
    < write the average quantities to the file FileSCAT >
end if
end if

```

2.2.3 “Input.dat”

The model control parameters specified in the input file “Input.dat” are listed below.

- TypeMatrSolv (character array) - specifies the method for solving linear algebraic equations. The permissive values are: ‘LU1’ - LU decomposition method from Numerical Recipes, ‘LU2’ - LU decomposition method from Lapack library, ‘LU3’ - LU decomposition method from Lapack library with solution improvement, and ‘BICG’ - Bi-Conjugate-Gradients method. The recommended value is ‘LU2’.
- itmax (integer) - maximum number of iteration for the ‘LU3’ method or ‘BICG’ method. The recommended value of this parameter is 100.
- TypePrecond (character array) - specifies the type of preconditioning for the ‘BICG’ method. The permissive values are: ‘NEUMANN’ - incomplete Neumann series, ‘SILU’ - incomplete LU factorization, ‘ ’ - diagonal elements of the matrix. The recommended value is ‘ ’.
- NPrecOrder (integer) - truncation order of the Neumann series. This parameter is used if TypePrecond = ‘NEUMANN’. The recommended value is 6.
- epsilon (real) - solution tolerance for the ‘BICG’ method. The recommended value is 1.e-6.
- TypeInterp (character array) - specifies the type of interpolation method for scattering matrix calculation. The scattering matrix is computed at a set of sample angles and polynomial interpolation is used to evaluate the scattering matrix at any zenith angle. The permissive values are: ‘LINEAR’, ‘SPLINE’ and ‘HERMITE’. The recommended value of this parameter is ‘LINEAR’.
- TypeIntegr (character array) - specifies the source of the numerical integration routines Gauss-Legendre, Laguerre, Simpson and trapez method.

The permissive values are: ‘MET1’ - routines from Numerical Recipes, ‘MET2’ - modified routines from Slatec library. The recommended value is ‘MET1’.

- epsGauss (real) - tolerance for computing the roots of the Legendre polynoms. The accuracy of the **T**-matrix calculation strongly depends on epsGauss. The value of this parameter should be set **as small as possible**. For double precision arithmetic, epsGauss = 1.e-15,...,1.e-12.
- epsLaguerre (real) - tolerance for computing the roots of the Laguerre polynomials. The routine “TPARTSUB.f90” computes the scattering characteristics of a particle on or near a plane surface. In this case, the integrals appearing in the expression of the reflection matrix are calculated by using the Laguerre quadrature method. The recommended value for double precision arithmetic is 1.e-10.
- TypeRND (character array) - specifies the type of the random number generator. The routines “TMULTSPHREC.f90” and “TINHOMSPHREC.f90” compute the scattering characteristics of a cluster of spherical particles and of an inhomogeneous sphere with multiple spherical inclusions. In both cases, the spherical particles are randomly distributed and random distributions of particles are simulated by using random number generators. The permissive values are: ‘SLAT’ - modified routine from SLATEC library, ‘LPCK’ - modified routine from LAPACK library and ‘ZIGG’ - Ziggurat method of Marsaglia and Tsang. The recommended value is ‘SLAT’.

2.3 Directory GEOMFILES

The routines “TAXSYM.f90” and “TNONAXSYM.f90” can read the particle geometry information from the file FileFEM. The name of the file FileFEM is specified in the input files “InputAXSYM.dat” and “InputNONAXSYM.dat”, while the file FileFEM is contained in the directory GEOMFILES (as provided). More informations concerning the structure of file FileFEM are given in the comment lines of the routines “TAXSYM.f90” and “TNONAXSYM.f90”.

2.4 Directories OUTPUTFILES and TMAFILES

As mentioned before, the code produces several ASCII files:

- the file “/OUTPUTFILES/Output.dat” contains the results of the convergence analysis,
- the file FileTmat in the directory TMAFILE contains the transition matrix,
- the file InfoFileTmat in the directory TMAFILE contains the values of the maximum expansion and azimuthal orders (which serve as INPUT PARAMETERS for other programs),

- the files FileDSCS and FileScat in the directory OUTPUTFILES contain the differential scattering cross section and the scattering characteristics.

The name of the file FileTmat is supplied by the input file “InputXXX.dat”, while the name of the files FileDSCS and FileScat are specified in the input file “InputSCT.dat”. The values provided by the information file InfoFileTmat must be specified in the input files of all programs which read the **T** matrix from file (“TINHOM.f90”, “TINHOMSPH.f90”, “TMULT.f90” and “SCT.f90”). The name of the information file InfoFileTmat **is not** explicitly provided. The codes produce an information file with the name

name of InfoFileTmat = “Info”//name of FileTmat,

i.e., for FileTmat = “TmatSph.dat”, the information file is InfoFileTmat = “InfoTmatSph.dat”.

3 Flow Diagrams

In Fig. 5 we show the flow diagram of the routines “TAXSYM.f90” and “TNON-AXSYM.f90”. The flow diagram of the routines “TCOMP.f90”, “TLAY.f90”, “TINHOM2SPH.f90”, “TINHOMSPHREC.f90”, “TMULT2SPH.f90”, “TMULT-SPH.f90” and “TMULTSPHREC.f90” are as in Fig. 5 without the block C, which provide a discretization of the particle geometry. In Table 2 we indicate the changes with respect to Fig. 5 for the routines “TXXX.f90”, “TPART-SUB.f90” and “TSPHERE.f90”, where “TXXX.f90” stands for “TINHOM.f90”, “TINHOMSPH.f90” and “TMULT.f90”. Finally, the changes with respect to Fig. 5 for the routines “SCT.f90”, “SCTAVRGSPH.f90” and “EFMED.f90” are given in Table 3.

Let us summarize the steps for computing the electromagnetic scattering with the TMATRIX program. For this purpose we consider an axisymmetric particle. The user must

- specify the optical properties, geometry, type of discrete sources and error tolerances in the input file “/INPUTFILES/InputAXSYM.dat”,
- provide the variables specifying the scattering characteristics calculation in the input file “/INPUTFILES/InputSCT.dat”;
- set the model control parameters in the input file “/INPUTFILES/Input.dat”;
- run the main program “TMATRIX.f90” by calling the routine “TAXSYM.f90”;
- perform convergence test and analyse the results written to the file “/OUTPUTFILES/Output.dat”; if convergence is achieved the program will write the **T** matrix to the file FileTmat in the directory TMATFILES, and the differential scattering cross sections and the scattering characteristics to the files FileDSCS and FileScat in the directory OUTPUTFILES;

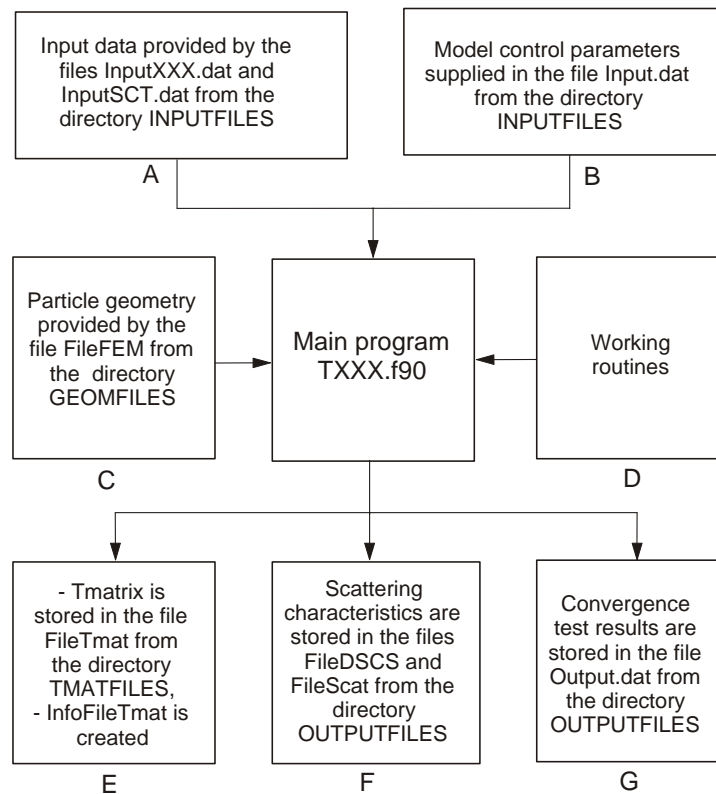


Figure 5: Flow diagrams of the routines "TAXSYM.f90" and "TNON-AXSYM.f90".

| Block | TXXX.f90 | TPARTSUB.f90 | TSPHERE.f90 |
|-------|--|--|--|
| A | as in Figure 5 | Input data provided by the file InputPARTSUB.dat from the directory INPUTFILES | as in Figure 5 |
| C | T matrix of the inclusion/particle provided by the file FileTmat from the directory TMAFILES | not used | not used |
| E | as in Figure 5 | not used | T vector is stored in the file FileTmat from the directory TMAFILES |
| F | as in Figure 5 | Scattering characteristics are stored in the files FileDSCS and FileEFM from the directory OUTPUTFILES | as in Figure 5 |

Table 2: Peculiarities of the flow diagrams of the routines "TXXX.f90", "TPARTSUB.f90" and "TSPHERE.f90".

| Block | SCT.f90 | SCTAVRGSPH.f90 | EFMED.f90 |
|-------|--|--|--|
| A | Input data provided by the file InputSCT.dat from the directory INPUTFILES | Input data provided by the file InputSCATAVRGSPH.dat from the directory INPUTFILES | Input data provided by the file InputEFMED.dat from the directory INPUTFILES |
| C | T matrix of the particle provided by the file FileTmat from the directory TMAFILES | not used | not used |
| E | not used | not used | not used |
| F | as in Figure 5 | as in Figure 5 | Results are stored in the file Output.dat from the directory OUTPUTFILES |
| G | not used | not used | not used |

Table 3: Peculiarities of the flow diagrams of the routines "SCT.f90", "SCATAVRGSPH.f90" and "EFMED.f90".

- for new scattering characteristics calculation, modify the input file “/INPUTFILES/InputSCT.dat” and run the main program “TMATRIX.f90” by calling the routine “SCT.f90”.

For computing the scattering characteristics of inhomogeneous particles with nonspherical inclusions (routines “TINHOM.f90” and “TINHOMSPH.f90”) and of clusters of particles (routine “TMULT.f90”), the user must first compute the individual (free-field) \mathbf{T} matrix of the inclusion (embedded in a medium with the same refractive index as the host particle) and of each particle in the cluster.

4 Note

We would like to point out that there are two main drawbacks of the present software package:

- The code is time consuming as compared to other \mathbf{T} -matrix programs. Our intention was to cover a large class of electromagnetic problems and therefore we sacrifice the speed in favour of the flexibility and code modularization. The code shares several modules which are of general use and are not devoted to a specific application.
- The code is not user-friendly because no automatic built-in convergence criteria are used. In fact we believe that the user can understand the capabilities and limitations of the method by performing his own convergence tests.