

UTILIZATION OF THE RCTMA TO CALCULATE THE OPTICAL PROPERTIES OF AN ENSEMBLE OF N DIELECTRIC SPHERES

The numerical simulation involves the following steps

- 1) Parametrization of the calculation
- 2) Calculation of the One particle T-Matrix
- 3) Calculation of the H matrices.
- 4) Calculation of the N-Particles Centered T-Matrices (RCTMA).
- 5) Calculation of the J Matrices.
- 6) Calculation of the orientation average extinction cross-sections

1 Parametrization of the input parameters.

The input parameters can be either read from an output text file, or directly initialized within the source code.

Description	Symbol
Wavelength of the incident radiation	λ
Index of refraction (real part only) of the surrounding medium	n_0
The number of particles in the system	N
For each particle:	
The radius	R^i
The index of refraction (real and imaginary parts)	Ren^i, Imn^i
The cartesian coordinates in the main reference frame	(X^i, Y^i, Z^i)
The truncation index	n_{max}^i

2 Calculation of the One particle T-Matrix

For each particle, calculate the One-Particle T Matrix

Type	Description	Symbol
INPUT	Wavelength of the incident radiation	λ
	Index of refraction (real part only) of the surrounding medium	n_0
	The radius	R^i
	The index of refraction (real and imaginary parts)	Ren^i, Imn^i
	The truncation index	n_{max}^i
OUTPUT	One Particle T-Matrix	$\tilde{\mathbf{T}}^i$

3 Calculation of the $H(i,j)$ matrices

The calculation of the translational matrix $\bar{H}^{(i,j)}$ is realized in three steps:

1. Calculation the position of particle j in the reference frame of particles I in spherical coordinates
2. Calculation of all distance size $kd_{ij} = 2\pi n_0 d_{ij}/\lambda$
3. Calculation of the $\bar{H}^{(i,j)}$

Type	Description	Symbol
INPUT	Position of particles i	(X^i, Y^i, Z^i)
	Position of particle j	(X^j, Y^j, Z^j)
OUPUT	Distance between particles i and j	d_{ij}
	Polar angle	θ_{ij}
	Azimuthal angle	ϕ_{ij}

Type	Description	Symbol
INPUT	Distance between particles i and j	d_{ij}
	Wavelength of the incident radiation	λ
	Index of refraction (real part only) of the surrounding medium	n_0
OUPUT	The distance size parameters between particles i and j	kd_{ij}

Type	Description	Symbol
INPUT	Wave vector Distance between particles	kd_{ij}
	Polar angle	θ_{ij}
	Azimuthal angle	ϕ_{ij}
	Truncation index of particle i	n_{max}^i
	Truncation index of particle j	n_{max}^j
OUPUT	Translational matrix	$\bar{H}^{(i,j)}$

4 Calculation of the N-Particles Centered T-Matrix (RCTMA)

The N-Centered T-Matrices $\bar{T}^{(i,j)}$ are calculated via the use of the RCTMA.

Type	Description	Symbol
INPUT	All the one particle T-Matrices	\bar{T}^i
	All the $H(i,j)$ Matrices	$\bar{H}^{(i,j)}$
OUPUT	All the N-Particles Centered T-Matrices	$\bar{T}^{(i,j)}$

5 Calculation of the $\bar{J}(i,j)$ matrices

The calculation of the translational matrix $\bar{J}^{(i,j)}$ are easily realized as all the input parameters have already been calculated.

Type	Description	Symbol
INPUT	Wave vector Distance between particles	kd_{ij}
	Polar angle	θ_{ij}
	Azimuthal angle	ϕ_{ij}
	Truncation index of particle i	n_{max}^i
	Truncation index of particle j	n_{max}^j
OUTPUT	Translational matrix	$\bar{J}^{(i,j)}$

6 Orientation average extinction cross-sections

The orientation average extinction cross-section $\langle C_{ext}^T \rangle$ of the N-Particles system is calculated from all the N-Particles Centered T-Matrices $\bar{T}^{(i,j)}$.

$$\langle C_{ext}^T \rangle = \frac{2\pi}{k_0^2} \sum_{i=1}^{i=N} \sum_{j=1}^{n=N} Tr[\bar{T}^{(i,j)} \cdot \bar{J}^{(j,i)}]$$

Type	Description	Symbol
INPUT	Wavelength of the incident radiation	λ
	Index of refraction (real part only) of the surrounding medium	n_0
	All the N-Particles Centered T-Matrices	$\bar{T}^{(i,j)}$
OUTPUT	All the N-Particles Centered T-Matrices	C_{ext}^T

Annex 1

Input parameters for the H and J matrices

```
double x1, y1, z1 ;

for (int i=1; i<=k; i++)
    for (int j=1; j<=k; j++)    {
        if (i != j) {
            x1 = vobjet[j-1].g_x() - vobjet[i-1].g_x() ;
            y1 = vobjet[j-1].g_y() - vobjet[i-1].g_y() ;
            z1 = vobjet[j-1].g_z() - vobjet[i-1].g_z() ;
            math1::transformCartesianToSphericalCoordinate
            (x1, y1, z1, dij(i,j), thetaij(i,j), phiiij(i,j)) ;
        }
    }

void math1::transformCartesianToSphericalCoordinate
(double x, double y, double z, double& r, double& theta, double& phi)
{
    // Etape 1: evaluation of dij
    r = pow (x*x+y*y+z*z,0.5) ;

    // Etape 2 : evaluation of thetaij and phiiij special cases
    // =====
    if (r==0.0)    {
        theta = 0.0 ;
        phi = 0.0 ;
        return ;
    }

    if (x==0.0 && y==0.0)    {
        if (z>=0.0) theta=0.0 ;
        if (z<0.0) theta=pi ;
        phi = 0.0 ;
        return ;
    }
    // Etape 3: evaluation of thetaij and phiiij general cases
    // =====
    theta = acos(z / r) ;

    if (x==0.0) {
        if (y>0.0)
            phi = pi/2.0 ;

        if (y<0.0)
            phi = 3.0*pi/2.0 ;
    }
    else    {
        phi = atan2(y,x) ;
    }
}
```

Annex 2

Orientation average extinction cross-sections

```
Cext = 0.0 ;

for (int i=1; i<=nbp; i++) {
    for (int j=1; j<=nbp; j++) {
        if (i==j) {
            Cext = Cext + real (tMatij_np1[findice(i,j)].trace()) ;

        }
        else {
            Cext = Cext +
                real(tMatij_np1[findice(i,j)].traceDeAfoisB(tMatij_n[findice(j,i)])) ;
        }
    }
}

double k0m = incidentRadiation.g_k0m() ;
Cext = Cext * 2.0*PI / k0m / k0m
```

Note : the tMatij_n matrices now contain the J matrices.