User Guide for the Discrete Dipole Approximation Code DDSCAT 7.1

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Abstract

DDSCAT 7.1 is a freely available open-source Fortran-90 software package applying the "discrete dipole approximation" (DDA) to calculate scattering and absorption of electromagnetic waves by targets with arbitrary geometries and complex refractive index. The targets may be isolated entities (e.g., dust particles), but may also be 1-d or 2-d periodic arrays of "target unit cells", which can be used to study absorption, scattering, and electric fields around arrays of nanostructures.

The DDA approximates the target by an array of polarizable points. The theory of the DDA and its implementation in **DDSCAT** is presented in Draine (1988) and Draine & Flatau (1994), and its extension to periodic structures (and near-field calculations) in Draine & Flatau (2008). **DDSCAT 7.1** allows accurate calculations of electromagnetic scattering from targets with "size parameters" $2\pi a_{\rm eff}/\lambda \lesssim 25$ provided the refractive index m is not large compared to unity ($|m-1| \lesssim 2$). **DDSCAT 7.1** includes support for MPI, OpenMP, and the Intel® Math Kernel Library (MKL).

DDSCAT supports calculations for a variety of target geometries (e.g., ellipsoids, regular tetrahedra, rectangular solids, finite cylinders, hexagonal prisms, etc.). Target materials may be both inhomogeneous and anisotropic. It is straightforward for the user to "import" arbitrary target geometries into the code. **DDSCAT** automatically calculates total cross sections for absorption and scattering and selected elements of the Mueller scattering intensity matrix for specified orientation of the target relative to the incident wave, and for specified scattering directions. **DDSCAT 7.1** can calculate scattering and absorption by targets that are periodic in one or two dimensions. **DDSCAT 7.1** also supports postprocessing to calculate **E** and **B** at user-selected locations in or near the target; a Fortran-90 code **DDfield** for this purpose is included in the distribution.

This User Guide explains how to use **DDSCAT 7.1** (release 7.1.0) to carry out electromagnetic scattering calculations.

Contents

1   Introduction

DDSCAT is a software package to calculate scattering and absorption of electromagnetic waves by targets with arbitrary geometries using the "discrete dipole approximation" (DDA). In this approximation the target is replaced by an array of point dipoles (or, more precisely, polarizable points); the electromagnetic scattering problem for an incident periodic wave interacting with this array of point dipoles is then solved essentially exactly. The DDA (sometimes referred to as the "coupled dipole approximation") was apparently first proposed by Purcell & Pennypacker (1973). DDA theory was reviewed and developed further by Draine (1988), Draine & Goodman (1993), reviewed by Draine & Flatau (1994) and Draine (2000), and recently extended to periodic structures by Draine & Flatau (2008).

DDSCAT 7.1, the current release of DDSCAT, is an open-source Fortran 90 implementation of the DDA developed by the authors.[1] It extends DDSCAT to treat structures that are periodic in one or two dimensions, using methods described by Draine & Flatau (2008).

DDSCAT is intended to be a versatile tool, suitable for a wide variety of applications including studies of interstellar dust, atmospheric aerosols, blood cells, marine microorganisms, and nanostructure arrays. As provided, **DDSCAT 7.1** should be usable for many applications without modification, but the program is written in a modular form, so that modifications, if required, should be fairly straightforward.

The authors make this code openly available to others, in the hope that it will prove a useful tool. We ask only that:

- If you publish results obtained using **DDSCAT**, please acknowledge the source of the code, and cite relevant papers, such as Draine & Flatau (1994), Draine & Flatau (2008), and this UserGuide (Draine & Flatau 2010).

- If you discover any errors in the code or documentation, please promptly communicate them to the authors.

- You comply with the "copyleft" agreement (more formally, the GNU General Public License) of the Free Software Foundation: you may copy, distribute, and/or modify the software identified as coming under this agreement. If you distribute copies of this software, you must give the recipients all the rights which you have. See the file `doc/copyleft.txt` distributed with the DDSCAT software.

We also strongly encourage you to send email to `draine@astro.princeton.edu` identifying yourself as a user of DDSCAT; this will enable the authors to notify you of any bugs, corrections, or improvements in DDSCAT. Up-to-date information on DDSCAT can be found at

   `http://www.astro.princeton.edu/∼draine/DDSCAT.html`

Information is also available at `http://ddscat.wikidot.com/start`

The current version, **DDSCAT 7.1**, uses the DDA formulae from Draine (1988), with dipole polarizabilities determined from the Lattice Dispersion Relation (Draine & Goodman 1993, Gutkowicz-Krusin & Draine 2004). The code incorporates Fast Fourier Transform (FFT) methods (Goodman, Draine, & Flatau 1991). **DDSCAT 7.1** includes capability to calculate scattering and absorption by targets that are

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[1] The release history of **DDSCAT** is as follows:

- **DDSCAT 4b**: Released 1993 March 12
- **DDSCAT 4b1**: Released 1993 July 9
- **DDSCAT 4c**: Although never announced, `DDSCAT.4c` was made available to a number of interested users beginning 1994 December 18
- **DDSCAT 5a7**: Released 1996
- **DDSCAT 5a8**: Released 1997 April 24
- **DDSCAT 5a9**: Released 1998 December 15
- **DDSCAT 5a10**: Released 2000 June 15
- **DDSCAT 6.0**: Released 2003 September 2
- **DDSCAT 6.1**: Released 2004 September 10
- **DDSCAT 7.0**: Released 2008 September 1
- **DDSCAT 7.1**: Released 2010 February 7

periodic in one or two dimensions – arrays of nanostructures, for example. The theoretical basis for application of the DDA to periodic structures is developed in Draine & Flatau (2008).

We refer you to the list of references at the end of this document for discussions of the theory and accuracy of the DDA [in particular, reviews by Draine and Flatau (1994) and Draine (2000), and recent extension to 1-d and 2-d arrays by Draine & Flatau (2008).]. In §4 we describe the principal changes between **DDSCAT 7.1** and the previous releases. The succeeding sections contain instructions for:

- compiling and linking the code;
- running a sample calculation;
- understanding the output from the sample calculation;
- modifying the parameter file to do your desired calculations;
- specifying target orientation;
- changing the DIMENSIONing of the source code to accommodate your desired calculations.

The instructions for compiling, linking, and running will be appropriate for a Linux system; slight changes will be necessary for non-Linux sites, but they are quite minor and should present no difficulty.

Finally, the current version of this User Guide can be obtained from http://arxiv.org/abs/1002.1505 – you will be offered the options of downloading either Postscript or PDF versions of the User Guide.

2   Applicability of the DDA

The principal advantage of the DDA is that it is completely flexible regarding the geometry of the target, being limited only by the need to use an interdipole separation d small compared to (1) any structural lengths in the target, and (2) the wavelength λ. Numerical studies (Draine & Goodman 1993; Draine & Flatau 1994; Draine 2000) indicate that the second criterion is adequately satisfied if

$$|m|kd < 1 \quad , \tag{1}$$

where m is the complex refractive index of the target material, and $k \equiv 2\pi/\lambda$, where λ is the wavelength *in vacuo*. This criterion is valid provide $|m-1| \lesssim 3$ or so. When $\text{Im}(m)$ becomes large, the DDA solution tends to overestimate the absorption cross section C_{abs}, and it may be necessary to use interdipole separations d smaller than indicated by eq. (1) to reduce the errors in C_{abs} to acceptable values.

If accurate calculations of the scattering phase function (e.g., radar or lidar cross sections) are desired, a more conservative criterion

$$|m|kd < 0.5 \tag{2}$$

will usually ensure that differential scattering cross sections $dC_{\text{sca}}/d\Omega$ are accurate to within a few percent of the average differential scattering cross section $C_{\text{sca}}/4\pi$ (see Draine 2000).

Let V be the actual volume of solid material in the target.[2] If the target is represented by an array of N dipoles, located on a cubic lattice with lattice spacing d, then

$$V = Nd^3 \quad . \tag{3}$$

We characterize the size of the target by the "effective radius"

$$a_{\text{eff}} \equiv (3V/4\pi)^{1/3} \quad , \tag{4}$$

the radius of an equal volume sphere. A given scattering problem is then characterized by the dimensionless "size parameter"

$$x \equiv ka_{\text{eff}} = \frac{2\pi a_{\text{eff}}}{\lambda} \quad . \tag{5}$$

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[2] In the case of an infinite periodic target, V is the volue of solid material in one "Target Unit Cell".

The size parameter can be related to N and $|m|kd$:

$$x \equiv \frac{2\pi a_{\text{eff}}}{\lambda} = \frac{62.04}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \cdot |m|kd \quad . \tag{6}$$

Equivalently, the target size can be written

$$a_{\text{eff}} = 9.873 \frac{\lambda}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \cdot |m|kd \quad . \tag{7}$$

Practical considerations of CPU speed and computer memory currently available on scientific worksta-tions typically limit the number of dipoles employed to $N < 10^6$ (see §16 for limitations on N due to available RAM); for a given N, the limitations on $|m|kd$ translate into limitations on the ratio of target size to wavelength.

For calculations of total cross sections C_{abs} and C_{sca}, we require $|m|kd < 1$:

$$a_{\text{eff}} < 9.88 \frac{\lambda}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \quad \text{or} \quad x < \frac{62.04}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \quad . \tag{8}$$

For scattering phase function calculations, we require $|m|kd < 0.5$:

$$a_{\text{eff}} < 4.94 \frac{\lambda}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \quad \text{or} \quad x < \frac{31.02}{|m|} \left(\frac{N}{10^6} \right)^{1/3} \quad . \tag{9}$$

It is therefore clear that the DDA is not suitable for very large values of the size parameter x, or very large values of the refractive index m. The primary utility of the DDA is for scattering by dielectric targets with sizes comparable to the wavelength. As discussed by Draine & Goodman (1993), Draine & Flatau (1994), and Draine (2000), total cross sections calculated with the DDA are accurate to a few percent provided $N > 10^4$ dipoles are used, criterion (1) is satisfied, and the refractive index is not too large.

For fixed $|m|kd$, the accuracy of the approximation degrades with increasing $|m - 1|$, for reasons having to do with the surface polarization of the target as discussed by Collinge & Draine (2004). With the present code, good accuracy can be achieved for $|m - 1| < 2$.

Examples illustrating the accuracy of the DDA are shown in Figs. 1–2 which show overall scattering and absorption efficiencies as a function of wavelength for different discrete dipole approximations to a sphere, with N ranging from 304 to 59728. The DDA calculations assumed radiation incident along the (1,1,1) direction in the "target frame". Figs. 3–4 show the scattering properties calculated with the DDA for $x = ka = 7$. Additional examples can be found in Draine & Flatau (1994) and Draine (2000).

As discussed below, **DDSCAT 7.1** can also calculate scattering and absorption by targets that are periodic in one or two directions – for examples, see Draine & Flatau (2008).

3   DDSCAT 7.1

3.1   What Does It Calculate?

3.1.1   Absorption and Scattering by Finite Targets

DDSCAT 7.1, like previous versions of **DDSCAT**, solves the problem of scattering and absorption by a finite target, represented by an array of polarizable point dipoles, interacting with a monochromatic plane wave incident from infinity. **DDSCAT 7.1** has the capability of automatically generating dipole array representations for a variety of target geometries (see §19) and can also accept dipole array repre-sentations of targets supplied by the user (although the dipoles must be located on a cubic lattice). The incident plane wave can have arbitrary elliptical polarization (see §22), and the target can be arbitrarily oriented relative to the incident radiation (see §17). The following quantities are calculated by **DDSCAT 7.1** :
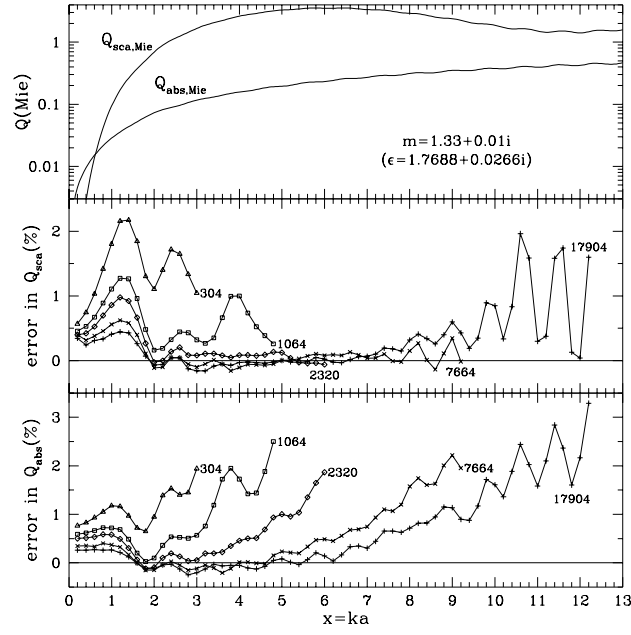
Figure 1: Scattering and absorption for a sphere with $m = 1.33 + 0.01i$. The upper panel shows the exact values of Q_{sca} and Q_{abs}, obtained with Mie theory, as functions of $x = ka$. The middle and lower panels show fractional errors in Q_{sca} and Q_{abs}, obtained using **DDSCAT** with polarizabilities obtained from the Lattice Dispersion Relation, and labelled by the number N of dipoles in each pseudosphere. After Fig. 1 of Draine & Flatau (1994).
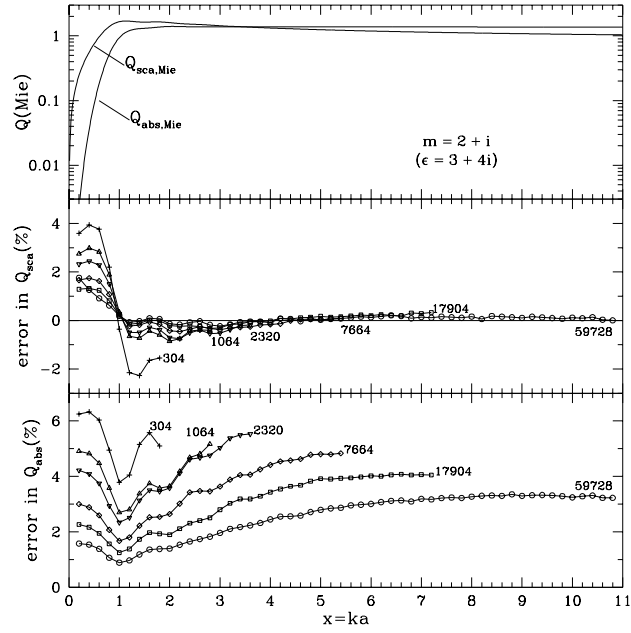
Figure 2: Same as Fig. 1, but for $m = 2 + i$. After Fig. 2 of Draine & Flatau (1994).
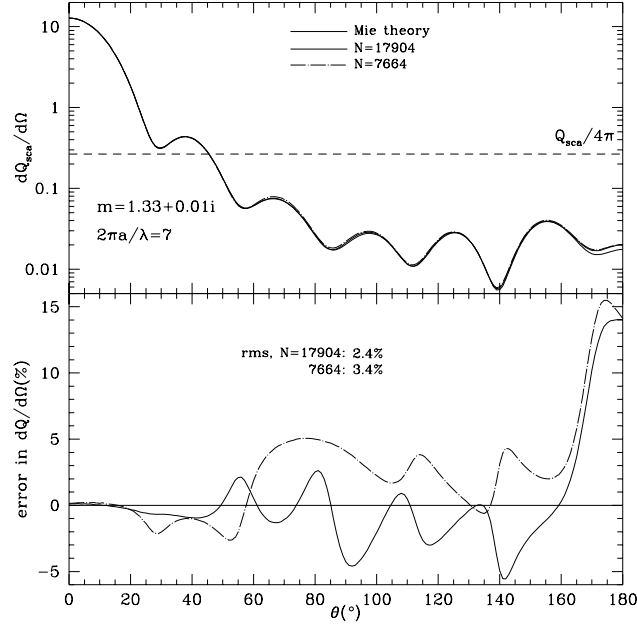
Figure 3: Differential scattering cross section for $m = 1.33 + 0.01i$ pseudosphere and $ka = 7$. Lower panel shows fractional error compared to exact Mie theory result. The $N = 17904$ pseudosphere has $|m|kd = 0.57$, and an rms fractional error in $d\sigma/d\Omega$ of 2.4%. After Fig. 5 of Draine & Flatau (1994).
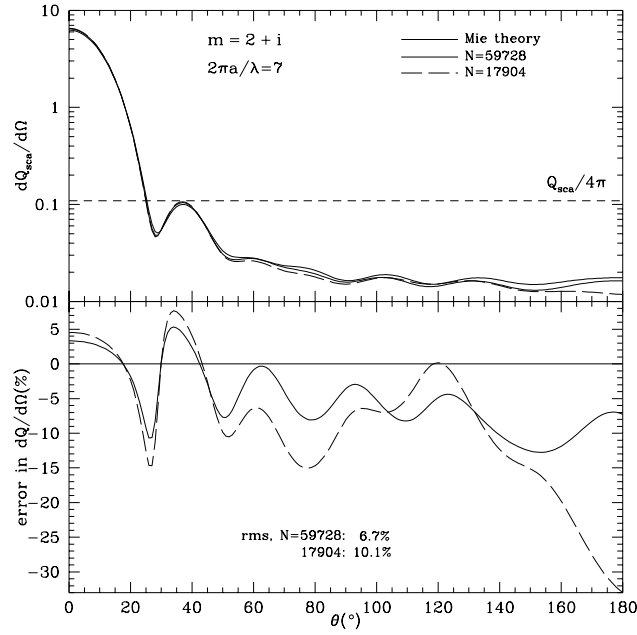
Figure 4: Same as Fig. 3 but for $m = 2 + i$. The $N = 59728$ pseudosphere has $|m|kd = 0.65$, and an rms fractional error in $d\sigma/d\Omega$ of 6.7%. After Fig. 8 of Draine & Flatau (1994).

- Absorption efficiency factor $Q_{\rm abs} \equiv C_{\rm abs}/\pi a_{\rm eff}^2$, where $C_{\rm abs}$ is the absorption cross section;
- Scattering efficiency factor $Q_{\rm sca} \equiv C_{\rm sca}/\pi a_{\rm eff}^2$, where $C_{\rm sca}$ is the scattering cross section;
- Extinction efficiency factor $Q_{\rm ext} \equiv Q_{\rm sca} + Q_{\rm abs}$;
- Phase lag efficiency factor $Q_{\rm pha}$, defined so that the phase-lag (in radians) of a plane wave after propagating a distance L is just $n_t Q_{\rm pha} \pi a_{\rm eff}^2 L$, where n_t is the number density of targets.
- The 4×4 Mueller scattering intensity matrix S_{ij} describing the complete scattering properties of the target for scattering directions specified by the user (see §24).
- Radiation force efficiency vector $\mathbf{Q}_{\rm rad}$ (see §15).
- Radiation torque efficiency vector $\mathbf{Q}_\Gamma$ (see §15).

In addition, the user can choose to have **DDSCAT 7.1** store the solution for post-processing. A separate Fortran-90 program **DDfield** (see §27) is provided that can readily calculate **E** and **B** at user-selected locations.

3.1.2 Absorption and Scattering by Periodic Arrays of Finite Structures

DDSCAT 7.1 includes the capability to solve the problem of scattering and absorption by an infinite target consisting of a 1-d or 2-d periodic array of finite structures, illuminated by an incident plane wave. The finite structures are themselves represented by arrays of point dipoles.

The electromagnetic scattering problem is formulated by Draine & Flatau (2008), who show how the problem can be reduced to a finite system of linear equations, and solved by the same methods used for scattering by finite targets.

The far-field scattering properties of the 1-d and 2-d periodic arrays can be conveniently represented by a generalization of the Mueller scattering matrix to the 1-d or 2-d periodic geometry – see Draine & Flatau (2008) for definition of $S_{ij}^{(1d)}(M, \zeta)$ and $S_{ij}^{(2d)}(M, N)$. For targets with 1-d periodicity, **DDSCAT 7.1** calculates $S_{ij}^{(1d)}(M, \zeta)$ for user-specified M and ζ. For targets with 2-d periodicity, **DDSCAT 7.1** calculates $S_{ij}^{(2d)}(M, N)$ for both transmission and reflection, for user-specified (M, N).

As for finite targets, the user can choose to have **DDSCAT 7.1** store the calculated polarization field for post-processing. A separate Fortran-90 program **DDfield** is provided to calculate **E** and **B** at user-selected locations, which can be located anywhere (including within the target).

3.2 Application to Targets in Dielectric Media

Let ω be the angular frequency of the incident radiation. For many applications, the target is essentially *in vacuo*, in which case the dielectric function ϵ which the user should supply to DDSCAT is the actual complex dielectric function $\epsilon_{\rm target}(\omega)$, or complex refractive index $m_{\rm target}(\omega) = \sqrt{\epsilon_{\rm target}}$ of the target material.

However, for many applications of interest (e.g., marine optics, or biological optics) the "target" body is embedded in a (nonabsorbing) dielectric medium (e.g., water at visible wavelengths) with (real) dielectric function $\epsilon_{\rm medium}(\omega)$, or (real) refractive index $m_{\rm medium}(\omega) = \sqrt{\epsilon_{\rm medium}}$. **DDSCAT** is fully applicable to these scattering problems, except that:

- The complex "dielectric function" or complex "refractive index" supplied to **DDSCAT** should be the *relative* dielectric function

$$\epsilon(\omega) = \frac{\epsilon_{\rm target}(\omega)}{\epsilon_{\rm medium}(\omega)} \tag{10}$$

  or *relative* refractive index:

$$m(\omega) = \frac{m_{\rm target}(\omega)}{m_{\rm medium}(\omega)}. \tag{11}$$

- The wavelength λ specified in ddscat.par should be the wavelength *in the medium*:

$$\lambda = \frac{\lambda_{\rm vac}}{m_{\rm medium}}, \tag{12}$$

  where $\lambda_{\rm vac} = 2\pi c/\omega$ is the wavelength *in vacuo*.

Because **DDSCAT** will be using the *relative refractive index* $m(\omega)$ and the wavelength *in the medium*, the file supplying the refractive index as a function of wavelength should give the *relative refractive index* or *relative dielectric function* as a function of *wavelength in the medium.* Those using **DDSCAT** for targets that are not *in vacuo* must be attentive to this when preparing the input table(s) giving the *relative* dielectric function or refractive index of the target material(s).

The absorption, scattering, extinction, and phase lag efficiency factors Q_{abs}, Q_{sca}, and Q_{ext} calculated by **DDSCAT** will then be equal to the physical cross sections for absorption, scattering, and extinction divided by πa_{eff}^2. For example, the attenuation coefficient for radiation propagating through a medium with a number density n_t of scatterers will be just $\alpha = n_t Q_{\mathrm{ext}} \pi a_{\mathrm{eff}}^2$. Similarly, the phase lag (in radians) after propagating a distance L will be $n_t Q_{\mathrm{pha}} \pi a_{\mathrm{eff}}^2 L$.

The elements S_{ij} of the 4×4 Mueller scattering matrix $\mathbf{S}$ calculated by **DDSCAT** for finite targets will be correct for scattering in the medium:

$$\mathbf{I}_{\mathrm{sca}} = \left(\frac{\lambda}{2\pi r}\right)^2 \mathbf{S} \cdot \mathbf{I}_{\mathrm{in}}, \tag{13}$$

where $\mathbf{I}_{\mathrm{in}}$ and $\mathbf{I}_{\mathrm{sca}}$ are the Stokes vectors for the incident and scattered light (in the medium), r is the distance from the target, and λ is the wavelength in the medium (eq. 12). See §24 for a detailed discussion of the Mueller scattering matrix.

The time-averaged radiative force and torque (see §15) on a finite target in a dielectric medium are

$$\mathbf{F}_{\mathrm{rad}} = \mathbf{Q}_{pr} \pi a_{\mathrm{eff}}^2 u_{\mathrm{rad}} \quad, \tag{14}$$

$$\mathbf{\Gamma}_{\mathrm{rad}} = \mathbf{Q}_{\Gamma} \pi a_{\mathrm{eff}}^2 u_{\mathrm{rad}} \frac{\lambda}{2\pi} \quad, \tag{15}$$

where the time-averaged energy density is

$$u_{\mathrm{rad}} = \epsilon_{\mathrm{medium}} \frac{E_0^2}{8\pi} \quad, \tag{16}$$

where $E_0 \cos(\omega t + \phi)$ is the electric field of the incident plane wave in the medium.

4   What's New?

DDSCAT 7.1 differs from **DDSCAT 6.1** in a number of ways, including:

1. N.B.: The structure of the parameter file ddscat.par has been changed: ddscat.par files that were used with DDSCAT 6.1 will need to be modified. See §8 and Appendix A.

2. **DDSCAT 7.0** can calculate scattering by targets consisting of anisotropic materials with arbitrary orientation. Two new target options ANIFRMFIL and SPH_ANI_N are provided that make use of this capability.
   ANIFRMFIL reads an input file with a list of dipoles for a general anisotropic target. For each dipole, the input file gives the dipole location, composition for each of three principal axes of the local dielectric tensor, and the orientation of the local "Dielectric Frame" (DF) relative to the "Target Frame" (TF).
   Target option SPH_ANI_N creates target consisting of N anisotropic spheres. An input file lists, for each sphere, the location, radius, composition corresponding to each of three principal axes of dielectric tensor, and the orientation of the DF for this sphere relative to the TF.

3. The user now has the option of specifying the scattering directions either relative to the *Lab Frame* (as in DDSCAT 6.1) or relative to the *Target Frame*. This is selected by providing a new character variable, either LFRAME or TFRAME in the parameter file ddscat.par. Note that this choice *must* be specified in ddscat.par.

4. The user must now specify the value of parameter IWRPOL in the parameter file ddscat.par. See §8 and Appendix A.

5. A separate Fortran-90 code **DDfield** is provided that can read the stored polarization array that is written if IWRPOL = 1 and use this data to calculate **E** and **B** at user-specified positions in or near the target.

6. **DDSCAT 7.0** can solve the problem of scattering and absorption by a target that is periodic in one dimension (and finite in the other two dimensions) or periodic in two dimensions (and finite in the third) and illuminated by a monochromatic plane wave, using periodic boundary conditions (PBC). The theory is described in Draine & Flatau (2008). A number of built-in target options are provided (see §20), including BISLINPBC, CYLNDRPBC, DSKLYRPBC, HEXGONPBC, LYRSLBPBC, RCTGL_PBC, SPHRN_PBC,

7. **DDSCAT 7.0** uses dynamic memory allocation. An additional line is now required in the ddscat.par file to inform **DDSCAT 7.1** how much memory should initially be allocated to safely generate the requested target. Once the target has been generated, **DDSCAT 7.1** reevaluates the memory requirements, and then allocates only the memory required to carry out the scattering calculation for the chosen target.

8. The user can choose to compile **DDSCAT 7.0** in either single- or double-precision.

9. **DDSCAT 7.0** includes built-in support for OpenMP; if this is enabled, certain parts of the calculation can be distributed over available cpu cores. This can speed execution on multi-core systems.

10. **DDSCAT 7.0** includes built-in support to use the Intel® Math Kernel Library (MKL) for calculation of FFTs.

11. **DDSCAT 7.1** is distributed with a set of examples, including both ddscat.par files and selected output files. These should be useful to new users.

12. **DDSCAT 7.1** (version 7.1.0) allows the user to study periodic targets with the target unit cell (TUC) geometry (i.e., dipole locations) and composition provided via an input file [new target options FRMFILPBC (§20.1) and ANIFILPBC (§20.2)].

13. **DDSCAT 7.1** (version 7.1.0) supports new target options SLAB_HOLE (rectangular block with cylindrical hole) and SLBHOLPBC periodic array of rectangular blocks with cylindrical holes. SLBHOLPBC can be used to create a uniform slab with uniformly-spaced cylindrical holes in a rectangular pattern.

14. **DDSCAT 7.1** (version 7.1.0) includes a new version of **DDfield**, with modification to the structure of the input file ddfield.in to facilitate sampling the **E** and **B** fields at many points.

5 Obtaining and Installing the Source Code

DDSCAT 7.1 is written in standard Fortran-90 with a single extension: it uses the Fortran-95 standard library call CPU_TIME to obtain timing information. **DDSCAT 7.1** is therefore portable to any system having a f90 or f95 compiler. It has been successfully compiled with many different compilers, including gfortran, g95, ifort, pgf77, and NAG® f95.

It is possible to use **DDSCAT 7.1** on PCs running Microsoft Windows operating systems, including Vista and Windows 7. More information on how to do this can be found at

    http://code.google.com/p/ddscat

The remainder of this section will assume that the installation is taking place on a Unix, Linux or Mac OSX system with the standard developer tools (e.g., tar, make, and a f90 or f95 compiler) installed.

The complete source code for **DDSCAT 7.1** is provided in a single gzipped tarfile.

There are 4 ways to obtain the source code:

- Point your browser to the **DDSCAT** home page:
  http://www.astro.princeton.edu/~draine/DDSCAT.html
  and right=click on the link to ddscat7.1.0.tgz.

- Point your browser to
  http://code.google.com/p/ddscat/ and download the latest release.

- Point your browser to
  `ftp://ftp.astro.princeton.edu/draine/scat/ddscat/7.1.0`
  right-click on `ddscat7.1.0.tgz`.

- Use anonymous `ftp` to `ftp.astro.princeton.edu`.
  In response to "Name:" enter `anonymous`.
  In response to "Password:" enter your full email address.
  `cd draine/scat/ddscat/ver7.1.0`
  `binary` *(to enable transfer of binary data)*
  `get ddscat7.1.0.tgz`

After downloading `ddscat7.1.0.tgz` into the directory where you would like **DDSCAT 7.1** to reside (you should have at least 10 Mbytes of disk space available), the source code can be installed as follows:

If you are on a Linux system, you should be able to type
  `tar xvzf ddscat7.1.0.tgz`
which will"extract" the files from the gzipped tarfile. If your version of "tar" doesn't support the "z" option (e.g., you are running Solaris) then try
  `zcat ddscat7.1.0.tgz | tar xvf -`
If neither of the above work on your system, try the two-stage procedure
  `gunzip ddscat7.1.0.tgz`
  `tar xvf ddscat7.1.0.tar`
A disadvantage of this two-stage procedure is that it uses more disk space, since after the second step you will have the uncompressed tarfile `ddscat7.1.0.tar` – about 3.8 Mbytes – in addition to all the files you have extracted from the tarfile – another 4.6 Mbytes.

Any of the above approaches should create subdirectories `src`, `doc`, and `examples_exp`. The source code will be in subdirectory `src`, and documentation in subdirectory `doc`. The `examples_exp` subdirectory contains sample `ddscat.par` files as well as output files for various target options, including both isolated targets and infinite periodic targets.

6 Compiling and Linking

In the discussion below, it is assumed that the **DDSCAT 7.1** source code has been installed in a directory `DDA/src`. The instructions below assume that you are on a Unix, Linux, or Mac OSX system.

6.1 The default Makefile

It is assumed that the system has the following already installed:

- a Fortran-90 compiler (e.g., `gfortran`, `g95`, Intel® `ifort`, or NAG® `f95`).

- `cpp` – the "C preprocessor".

There are a number of different ways to create an executable, depending on what options the user wants:

- what compiler and compiler flags?

- single- or double-precision?

- enable OpenMP?

- enable MKL?

- enable MPI?

Each of the above choices needs requires setting of appropriate "flags" in the Makefile.
The default Makefile has the following "vanilla" settings:

- `gfortran -O2`

- single-precision arithmetic

- OpenMP not used

- MKL not used
- MPI not used.

To compile the code with the default settings, simply position yourself in the directory `DDA/src`, and type

```
make ddscat
```

If you have `gfortran` and `cpp` installed on your system, the above should work. You will get some warnings from the compiler, but the code will compile and create an executable `ddscat`.

If you wish to use a different compiler (or compiler options) you will need to edit the file `Makefile` to change the choice of compiler (variable `FC`), compilation options (variable `FFLAGS`), and possibly and loader options (variable `LDFLAGS`). The file `Makefile` as provided includes examples for compilers other than `gfortran`; you may be able to simply "comment out" the section of `Makefile` that was designed for `gfortran`, and "uncomment" a section designed for another compiler (e.g., Intel® `ifort`).

6.2 Optimization

The performance of **DDSCAT 7.1** will benefit from optimization during compilation and the user should enable the appropriate compiler flags.

6.3 Single vs. Double Precision

DDSCAT 7.1 is written to allow the user to easily generate either single- or double-precision versions of the executable. For most purposes, the single-precision precision version of **DDSCAT 7.1** should work fine, but if you encounter a scattering problem where the single-precision version of **DDSCAT 7.1** seems to be having trouble converging to a solution, you may wish to try using the double-precision version – this can be beneficial in the event that round-off error is compromising the performance of the conjugate-gradient solver. Of course, the double precision version will demand about twice as much memory as the single-precision version, and will take somewhat longer per iteration.

The only change required is in the Makefile: for single-precision, set

```
PRECISION = sp
```

or for double-precision, set

```
PRECISION = dp
```

After changing the `PRECISION` variable in the Makefile (either sp → dp, or dp → sp), it is necessary to recompile the entire code. Simply type

```
make clean
make ddscat
```

to create `ddscat` with the appropriate precision.

6.4 OpenMP

OpenMP is a standard for support of shared-memory parallel programming, and can provide a performance advantage when using **DDSCAT 7.1** on platforms with multiple cpus or multiple cores. OpenMP is supported by many common compilers, such as `gfortran` and Intel® `ifort`.

If you are using a multi-cpu (or multi-core) system with OpenMP (`www.openmp.org`) installed, you can compile **DDSCAT 7.1** with OpenMP directives to parallelize some of the calculations. To do so, simply change

```
DOMP =
OPENMP =
```

to

```
DOMP = -Dopenmp
OPENMP = -openmp
```

Note: `OPENMP` is compiler-dependent: `gfortran`, for instance, requires

```
OPENMP = -fopenmp
```

6.5 MKL: the Intel® Math Kernel Library

Intel® offers the Math Kernel Library (MKL) with the ifort compiler. This library includes `DFTI` for computing FFTs. At least on some systems, `DFTI` offers better performance than the GPFA package.

To use the MKL library routine `DFTI`:

- You must obtain the routine `mkl_dfti.f90` and place a copy in the directory where you are compiling **DDSCAT 7.1**. `mkl_dfti.f90` is Intel® proprietary software, so we cannot distribute it with the **DDSCAT 7.1** source code, but it should be available on any system with a license for the Intel® MKL library. If you cannot find it, ask your system administrator.

- Edit the Makefile: define variables `CXFFTMKL.f` and `CXFFTMKL.o` to:
  ```
  CXFFTMFKL.f = $(MKL_f)
  CXFFTMKL.f = $(MKL_o)
  ```

- Successful linking will require that the appropriate MKL libraries be available, and that the string `LFLAGS` in the Makefile be defined so as to include these libraries.
  ```
  -lmkl_em64t -lmkl_intel_thread -lmkl_core -lguide -lpthread -lmkl_intel_lp64
  ```
  appears to work on at least one installation. The Makefile contains examples.

- type
  ```
  make clean
  make ddscat
  ```

- The parameter file `ddscat.par` should have `FFTMKL` as the value of `CMETHD`.

6.6 MPI: Message Passing Interface

DDSCAT 7.1 includes support for parallelization under MPI. MPI (Message Passing Interface) is a standard for communication between processes. More than one implementation of `MPI` exists (e.g., `mpich` and `openmpi`). `MPI` support within **DDSCAT 7.1** is compliant with the MPI-1.2 and MPI-2 standards[3], and should be usable under any implementation of `MPI` that is compatible with those standards.

Many scattering calculations will require multiple orientations of the target relative to the incident radiation. For **DDSCAT 7.1**, such calculations are "embarassingly parallel", because they are carried out essentially independently. **DDSCAT 7.1** uses MPI so that scattering calculations at a single wavelength but for multiple orientations can be carried out in parallel, with the information for different orientations gathered together for averaging etc. by the master process.

If you intend to use **DDSCAT 7.1** for only a single orientation, MPI offers no advantage for **DDSCAT 7.1** so you should compile with MPI disabled. However, if you intend to carry out calculations for multiple orientations, *and* would like to do so in parallel over more than one cpu, *and* you have MPI installed on your platform, then you will want to compile **DDSCAT 7.1** with MPI enabled.

To compile with MPI disabled: in the Makefile, set
```
DMPI =
MIP.f = mpi_fake.f90
MPI.o = mpi_fake.o
```
To compile with MPI enabled: in the Makefile, set
```
DMPI = -Dmpi
MIP.f = $(MPI_f)
MPI.o = $(MPI_o)
```
and edit `LFLAGS` as needed to make sure that you link to the appropriate MPI library (if in doubt, consult your systems administrator). The `Makefile` in the distribution includes some examples, but library names and locations are often system-dependent. Please do *not* direct questions regarding `LFLAGS` to the authors – ask your sys-admin or other experts familiar with your installation.

Note that the MPI-capable executable can also be used for ordinary serial calculations using a single cpu.

---

[3]`http://www.mpi-forum.org/`

6.7 Device Numbers `IDVOUT` and `IDVERR`

So far as we know, there are only one operating-system-dependent aspect of **DDSCAT 7.1**: the device number to use for "standard output".

The variables `IDVOUT` and `IDVERR` specify device numbers for "running output" and "error messages", respectively. Normally these would both be set to the device number for "standard output" (e.g., writing to the screen if running interactively). Variables `IDVERR` are set by `DATA` statements in the "main" program `DDSCAT.f90` and in the output routine `WRIMSG` (file `wrimsg.f90`). The executable statement `IDVOUT=0` initializes `IDVOUT` to 0. In the as-distributed version of `DDSCAT.f90`, the statement

```
OPEN(UNIT=IDVOUT,FILE=CFLLOG)
```

causes the output to `UNIT=IDVOUT` to be buffered and written to the file `ddscat.log_nnn`, where `nnn=000` for the first cpu, 001 for the second cpu, etc. If it is desirable to have this output unbuffered for debugging purposes, (so that the output will contain up-to-the-moment information) simply comment out this `OPEN` statement.

7 Moving the Executable

Now reposition yourself into the directory `DDA` (e.g., type `cd ..`), and copy the executable from `src/ddscat` to the `DDA` directory by typing

```
cp src/ddscat ddscat
```

This should copy the file `DDA/src/ddscat` to `DDA/ddscat` (you could, alternatively, create a symbolic link). Similarly, copy the sample parameter file `ddscat.par` and the file `diel.tab` to the `DDA` directory by typing

```
cp doc/ddscat.par ddscat.par
cp doc/diel.tab diel.tab
```

8 The Parameter File `ddscat.par`

When the tarfile is unpacked, it will create four directories: `src`, `doc`, `diel`, and `examples_exp`. The `examples_exp` directory has a number of subdirectories, each with files for a sample calculation. Here we focus on the files in the subdirectory `RCTGLPRSM`.

The file `ddscat.par` (see also Appendix A) provides parameters to the program `ddscat`:

```
' ========= Parameter file for v7.1 ==================='
'**** Preliminaries ****'
'NOTORQ' = CMTORQ*6 (NOTORQ, DOTORQ) -- either do or skip torque calculations
'PBCGS2' = CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT' = CMDFFT*6 (GPFAFT, FFTMKL) -- select FFT method
'GKDLDR' = CALPHA*6 (GKDLDR, LATTDR) -- select prescription for polarizabilities
'NOTBIN' = CBINFLAG (NOTBIN, ORIBIN, ALLBIN) -- specify binary output
'**** Initial Memory Allocation ****'
100 100 100 = dimensioning allowance for target generation
'**** Target Geometry and Composition ****'
'RCTGLPRSM' = CSHAPE*9 shape directive
32 64 64  = shape parameters 1 - 3
1         = NCOMP = number of dielectric materials
'../diel/Au_evap' = file with refractive index 1
'**** Error Tolerance ****'
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
1.00e-2 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
0.5 = ETASCA (number of angles is proportional to [(3+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
0.5000 0.5000 1 'LIN' = wavelengths (first,last,how many,how=LIN,INV,LOG)
'**** Effective Radii (micron) **** '
0.49237 0.49237 1 'LIN' = aeff (first,last,how many,how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
```

```
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
'**** Specify which output files to write ****'
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA)
'**** Prescribe Target Rotations ****'
0.    0.   1  = BETAMI, BETAMX, NBETA  (beta=rotation around a1)
0.    0.   1  = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
0.    0.   1  = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0   0   0   = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6 = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41 = indices ij of elements to print
'**** Specify Scattered Directions ****'
'LFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
2 = NPLANES = number of scattering planes
0.  0. 180.  5 = phi, thetan_min, thetan_max, dtheta (in deg) for plane 1
90.  0. 180. 5 = phi, thetan_min, thetan_max, dtheta (in deg) for plane 2
```

Here we discuss the general structure of `ddscat.par` (see also Appendix A).

8.1   Preliminaries

`ddscat.par` starts by setting the values of five strings:

- CMDTRQ specifying whether or not radiative torques are to be calculated (e.g., NOTORQ)
- CMDSOL specifying the solution method (e.g., PBCGS2) (see section §11).
- CMDFFT specifying the FFT method (e.g., GPFAFT) (see section §12).
- CALPHA specifying the polarizability prescription (e.g., GKDLDR) (see §13).
- CBINFLAG specifying whether to write out binary files (e.g., NOTBIN)

8.2   Initial Memory Allocation

Three integers
        MXNX MXNY MXNZ
are given that need to be equal to or larger than the anticipated target size (in lattice units) in the $\hat{\mathbf{x}}_{TF}$, $\hat{\mathbf{y}}_{TF}$, and $\hat{\mathbf{z}}_{TF}$ directions. This is required for initial memory allocation. A value like
        100 100 100
would require initial memory allocation of only ~ 100 MBytes. Note that after the target geometry has been determined, **DDSCAT 7.1** will proceed to reallocate only as much memory as is actually required for the calculation.

8.3   Target Geometry and Composition

- CSHAPE specifies the target geometry (e.g., RCTGLPRSM)

As provided, the file `ddscat.par` is set up to calculate scattering by a $32\times64\times64$ rectangular array of 131072 dipoles.

The user must specify NCOMP, which specifies how many different dielectric functions will be used. This is then followed by NCOMP lines, with each line giving the name (in quotes) of each dielectric function file. In our example, NCOMP is set to 1. The dielectric function of the target material is provided in the file `../diel/Au_evap`, which is gives the refractive index of evaporated Au over a range of wavelengths.

8.4   Error Tolerance

`TOL` = the error tolerance. Conjugate gradient iteration will proceed until the linear equations are solved to a fractional error `TOL`. The sample calculation has `TOL`=10^{-5}.

8.5 Interaction Cutoff Parameter for PBC Calculations

GAMMA = parameter limiting certain summations that are required for periodic targets (see Draine & Flatau 2008). **The value of** GAMMA **has no effect on computations for finite targets** – it can be set to any value, including 0).

For targets that are periodic in 1 or 2 dimensions, GAMMA needs to be small for high accuracy, but the required cpu time increases as GAMMA becomes smaller. GAMMA $= 10^{-2}$ is reasonable for initial calculations, but you may want to experiment to see if the results you are interested in are sensitive to the value of GAMMA. Draine & Flatau (2008) show examples of how computed results for scattering can depend on the value of γ.

8.6 Angular Resolution for Computation of $\langle \cos\theta \rangle$, etc.

The parameter ETASCA determines the selection of scattering angles used for computation of certain angular averages, such as $\langle \cos\theta \rangle$ and $\langle \cos^2\theta \rangle$, and the radiation pressure force (see §15) and radiative torque (if CMDTRQ=DOTORQ). Small values of ETASCA result in increased accuracy but also cost additional computation time. ETASCA=0.5 generally gives accurate results.

If accurate computation of $\langle \cos\theta \rangle$ or the radiation pressure force is not required, the user can set ETASCA to some large number, e.g. 10, to minimize unnecessary computation.

8.7 Wavelength

Wavelengths λ are specified one line in ddscat.par consisting of values for 4 variables:
    WAVINI WAVEND NWAV CDIVID
where WAVINI and WAVEND are real numbers, NWAV is an integer, and CDIVID is a character variable.

- If CDIVID = 'LIN', the λ will be uniformly spaced beween WAVINI and WAVEND.

- If CDIVID = 'INV', the λ will be uniformly spaced in $1/\lambda$ between WAVINI and WAVEND

- If CDIVID = 'LOG', the λ will be uniformly spaced in $\log(\lambda)$ between WAVINI and WAVEND

- If CDIVID = 'TAB', the λ will be read from a user-supplied file wave.tab, with one wavelength per line. For this case, the values of WAVINI, WAVEND, and NWAV will be disregarded.

The sample ddscat.par file specifies that the calculations be done for a single ($\lambda = 0.50$). The units must be the same as the wavelength units used in the file specifying the refractive index. In this case, we are using μm.

8.8 Target Size a_{eff}

Note that in **DDSCAT** the "effective radius" a_{eff} is the radius of a sphere of equal volume – i.e., a sphere of volume Nd^3, where d is the lattice spacing and N is the number of occupied (i.e., non-vacuum) lattice sites in the target. Thus the effective radius $a_{\text{eff}} = (3N/4\pi)^{1/3}d$. Our target should have a thickness $a = 0.5\mu$m in the $\hat{\mathbf{x}}_{\text{TF}}$ direction. If the rectangular solid is $a \times b \times c$, with $a : b : c :: 32 : 64 : 64$, then $V = abc = 4a^3$. Thus $a_{\text{eff}} = (3V/4\pi)^{1/3} = (3/\pi)^{1/3}a = 0.49237\mu$m.

8.9 Incident Polarization

The incident radiation is always assumed to propagate along the x axis in the "Lab Frame". The sample ddscat.par file specifies incident polarization state $\hat{\mathbf{e}}_{01}$ to be along the y axis (and consequently polarization state $\hat{\mathbf{e}}_{02}$ will automatically be taken to be along the z axis). IORTH=2 in ddscat.par calls for calculations to be carried out for both incident polarization states ($\hat{\mathbf{e}}_{01}$ and $\hat{\mathbf{e}}_{02}$ – see §22).

8.10   Output Files to Write

The sample `ddscat.par` file sets `1=IWRKSC`, so that ".sca" files will be written out with scattering information for each orientation.

The sample `ddscat.par` file sets `1=IWRPOL`, so that a ".pol" file will be writtten out for each incident polarization and each orientation. Note that each such file has a size that is proportional to the number of dipoles, and can be quite large. For this modest test problem, with $N = 131072$ dipoles, the .pol files are each 11.8 MBytes. These files are only useful if post-processing of the solution is desired, such as evaluation of the electromagnetic field near the target using the `DDfield` program as described in §27.

8.11   Target Orientation

The target is assumed to have two vectors $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ embedded in it; $\hat{\mathbf{a}}_2$ is perpendicular to $\hat{\mathbf{a}}_1$. For the present target shape RCTGLPRSM, the vector $\hat{\mathbf{a}}_1$ is along the $\hat{\mathbf{x}}_{\rm TF}$ axis of the target, and the vector $\hat{\mathbf{a}}_2$ is along the $\hat{\mathbf{y}}_{\rm TF}$ axis (see §19.18). The target orientation in the Lab Frame is set by three angles: β, Θ, and Φ, defined and discussed below in §17. Briefly, the polar angles Θ and Φ specify the direction of $\hat{\mathbf{a}}_1$ in the Lab Frame. The target is assumed to be rotated around $\hat{\mathbf{a}}_1$ by an angle β. The sample `ddscat.par` file specifies $\beta = 0$ and $\Phi = 0$ (see lines in `ddscat.par` specifying variables BETA and PHI), and calls for three values of the angle Θ (see line in `ddscat.par` specifying variable THETA). **DDSCAT** chooses Θ values uniformly spaced in $\cos \Theta$; thus, asking for three values of Θ between 0 and 90° yields $\Theta = 0, 60°$, and 90°.

8.12   Starting Values of `IWAV`, `IRAD`, `IORI`

Normally we begin the calculation with `IWAVE=0`, `IRAD=0`, and `IORI=0`. However, under some circumstances, a prior calculation may have completed some of the cases. If so, the user can specify starting values of `IWAV`, `IRAD`, `IORI`; the computations will begin with this case, and continue.

8.13   Which Mueller Matrix Elements?

The sample parameter file specifies that **DDSCAT** should calculate 6 distinct Mueller scattering matrix elements S_{ij}, with 11, 12, 21, 22, 31, 41 being the chosen values of ij.

8.14   What Scattering Directions?

8.14.1   Isolated Finite Targets

For finite targets, the user may specify the scattering directions in either the Lab Frame ('LFRAME') or the Target Frame ('TFRAME').

For finite targets, such as specified in this sample `ddscat.par`, the S_{ij} are to be calculated for scattering directions specified by angles (θ, ϕ).

The sample `ddscat.par` specifies that 2 scattering planes are to be specified: the first has $\phi = 0$ and the second has $\phi = 90°$; for each scattering plane θ values run from 0 to 180° in increments of 10°.

8.14.2   1-D Periodic Targets

For periodic targets, the scattering directions `must` be specified in the Target Frame: 'TFRAME' = CMDFRM .

Scattering from 1-d periodic targets is discussed in detail by Draine & Flatau (2008). For periodic targets, the user does not specify scattering planes. For 1-dimensional targets, the user specifies scattering cones, corresponding to different scattering orders M. For each scattering cone M, the user specifies $\zeta_{\rm min}$, $\zeta_{\rm max}$, $\Delta\zeta$ (in degrees); the azimuthal angle ζ will run from $\zeta_{\rm min}$ to ζ_{max}, in increments of $\Delta\zeta$. For example:

```
'TFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
1 = number of scattering cones
0.  0. 180. 0.05  = OrderM zetamin zetamax dzeta for scattering cone 1
```

8.14.3 2-D Periodic Targets

For targets that are periodic in 2 dimensions, the scattering directions must be specified in the Target
Frame: 'TFRAME' = CMDFRM.

   Scattering from targets that are periodic in 2 dimensions is discussed in detail by Draine & Flatau
(2008). For 2-D periodic targets, the user specifies the diffraction orders (M, N) for transmitted radi-
ation: the code will automatically calculate the scattering matrix elements $S_{ij}^{(2d)}(M, N)$ for both trans-
mitted and reflected radiation for each (M, N) specified by the user. For example:

```
'TFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
1 = number of scattering orders
0.  0. = OrderM OrderN for scattered radiation
```

9   Running DDSCAT 7.1 Using the Sample `ddscat.par` File

9.1   Single-Process Execution

To execute the program on a UNIX system (running either sh or csh), simply type
       ./ddscat >& ddscat.out &
which will redirect the "standard output" to the file ddscat.out, and run the calculation in the back-
ground. The sample calculation [32x24x16=12288 dipole target, 3 orientations, two incident polar-
izations, with scattering (Mueller matrix elements S_{ij}) calculated for 38 distinct scattering directions],
requires 27.9 cpu seconds to complete on a 2.0 GHz single-core Xeon workstation.

9.2   Code Execution Under MPI

Local installations of MPI will vary – you should consult with someone familiar with way MPI is in-
stalled and used on your system.

   At Princeton University Dept. of Astrophysical Sciences we use PBS (Portable Batch System)[4] to
schedule jobs. MPI jobs are submitted using PBS by first creating a shell script such as the following
example file pbs.submit:

```
#!/bin/bash
#PBS -l nodes=2:ppn=1
#PBS -l mem=1200MB,pmem=300MB
#PBS -m bea
#PBS -j oe
cd $PBS_O_WORKDIR
/usr/local/bin/mpiexec ddscat
```

The lines beginning with #PBS -l specify the required resources:
#PBS -l nodes=2:ppn=1 specifies that 2 nodes are to be used, with 1 processor per node.
#PBS -l mem=1200MB,pmem=300MB specifies that the total memory required (mem) is 1200MB,
and the maximum physical memory used by any single process (pmem) is 300MB. The actual definition
of mem is not clear, but in practice it seems that it should be set equal to $2 \times (nodes) \times (ppn) \times (pmem)$.
#PBS -m bea specifies that PBS should send email when the job begins (b), and when it ends (e) or
aborts (a).
#PBS -j oe specifies that the output from stdout and stderr will be merged, intermixed, as stdout.

---

[4]http://www.openpbs.org

This example assumes that the executable `dscat` is located in the same directory where the code is to execute and write its output. If `ddscat` is located in another directory, simply give the full pathname. to it. The `qsub` command is used to submit the `PBS` job:

   `qsub pbs.submit`

As the calculation proceeds, the usual output files will be written to this directory: for each wavelength, target size, and target orientation, there will be a file w*aaa*r*bbb*k*ccc*`.sca`, where *aaa=000, 001, 002, ...* specifies the wavelength, *bbb=000, 001, 002, ...* specifies the target size, and *cc=000, 001, 002, ...* specifies the orientation. For each wavelength and target size there will also be a file w*aaa*r*bbb*ori`.avg` with orientationally-averaged quantities. Finally, there will also be tables `qtable`, and `qtable2` with orientationally-averaged cross sections for each wavelength and target size.

In addition, each processor employed will write to its own log file `ddscat.log_`*nnn*, where *nnn=000, 001, 002, ...*. These files contain information concerning cpu time consumed by different parts of the calculation, convergence to the specified error tolerance, etc. If you are uncertain about how the calculation proceeded, examination of these log files is recommended.

10   Output Files

10.1   ASCII files

If you run DDSCAT using the command
    `ddscat >& ddscat.out &`
you will have various types of ASCII files when the computation is complete:

- a file `ddscat.out`;
- a file `ddscat.log_000`;
- a file `mtable`;
- a file `qtable`;
- a file `qtable2`;
- files w*xxx*r*yyy*ori`.avg` (one, w000r000ori`.avg`, for the sample calculation);
- if `ddscat.par` specified `IWRKSC=1`, there will also be files w*xxx*r*yyy*k*zzz*`.sca` (3 for the sample calculation: `w000r000k000.sca`, `w000r000k001.sca`, `w000r000k002.sca`).
- if `ddscat.par` specified `IWRPOL=1`, there will also be files w*xxx*r*yyy*k*zzz*`.pol`*n* for *n*=1 and (if `IORTH=2`) *n*=2

The file `ddscat.out` will contain minimal information (it may in fact be empty).

The file `ddscat.log_000` will contain any error messages generated as well as a running report on the progress of the calculation, including creation of the target dipole array. During the iterative calculations, Q_{ext}, Q_{abs}, and Q_{pha} are printed after each iteration; you will be able to judge the degree to which convergence has been achieved. Unless `TIMEIT` has been disabled, there will also be timing information. If the `MPI` option is used to run the code on multiple cpus, there will be one file of the form `ddscat.log_`*nnn* for each of the cpus, with `nnn=000,001,002,...`.

The file `mtable` contains a summary of the dielectric constant used in the calculations.

The file `qtable` contains a summary of the orientationally-averaged values of Q_{ext}, Q_{abs}, Q_{sca}, $g(1) = \langle \cos(\theta_s) \rangle$, $\langle \cos^2(\theta_s) \rangle$, Q_{bk}, and N_{sca}. Here Q_{ext}, Q_{abs}, and Q_{sca} are the extinction, absorption, and scattering cross sections divided by πa_{eff}^2. Q_{bk} is the differential cross section for backscattering (area per sr) divided by πa_{eff}^2. N_{sca} is the number of scattering directions used for averaging over scattering directions (to obtain $\langle \cos \theta \rangle$, etc.) (see §23).

The file `qtable2` contains a summary of the orientationally-averaged values of Q_{pha}, Q_{pol}, and Q_{cpol}. Here Q_{pha} is the "phase shift" cross section divided by πa_{eff}^2 (see definition in Draine 1988). Q_{pol} is the "polarization efficiency factor", equal to the difference between Q_{ext} for the two orthogonal polarization states. We define a "circular polarization efficiency factor" $Q_{cpol} \equiv Q_{pol} Q_{pha}$, since an

optically-thin medium with a small twist in the alignment direction will produce circular polarization in initially unpolarized light in proportion to Q_{cpol}.

For each wavelength and size, **DDSCAT 7.1** produces a file with a name of the form w*xxx*r*yyy*ori.avg, where index *xxx* (=000, 001, 002....) designates the wavelength and index *yyy* (=000, 001, 002...) designates the "radius"; this file contains Q values and scattering information averaged over however many target orientations have been specified (see §17. The file w000r000ori.avg produced by the sample calculation is provided below in Appendix B.

In addition, if ddscat.par has specified IWRKSC=1 (as for the sample calculation), **DDSCAT 7.1** will generate files with names of the form w*xxx*r*yyy*k*zzz*.avg, where *xxx* and *yyy* are as before, and index *zzz* =(000,001,002...) designates the target orientation; these files contain Q values and scattering information for *each* of the target orientations. The structure of each of these files is very similar to that of the w*xxx*r*yyy*ori.avg files. Because these files may not be of particular interest, and take up disk space, you may choose to set IWRKSC=0 in future work. However, it is suggested that you run the sample calculation with IWRKSC=1.

The sample ddscat.par file specifies IWRKSC=1 and calls for use of 1 wavelength, 1 target size, and averaging over 3 target orientations. Running **DDSCAT 7.1** with the sample ddscat.par file will therefore generate files w000r000k000.sca, w000r000k001.sca, and w000r000k002.sca. To understand the information contained in one of these files, please consult Appendix C, which contains an example of the file w000r000k000.sca produced in the sample calculation.

10.2 Binary Option

It is possible to output an "unformatted" or "binary" file (dd.bin) with fairly complete information, including header and data sections. This is accomplished by specifying either ALLBIN or ORIBIN in ddscat.par.

Subroutine writebin.f90 provides an example of how this can be done. The "header" section contains dimensioning and other variables which do not change with wavelength, particle geometry, and target orientation. The header section contains data defining the particle shape, wavelengths, particle sizes, and target orientations. If ALLBIN has been specified, the "data" section contains, for each orientation, Mueller matrix results for each scattering direction. The data output is limited to actual dimensions of arrays; e.g. nscat, 4, 4 elements of Muller matrix are written rather than mxscat, 4, 4. This is an important consideration when writing postprocessing codes.

11 Choice of Iterative Algorithm

As discussed elsewhere (e.g., Draine 1988), the problem of electromagnetic scattering of an incident wave $\mathbf{E}_{\mathrm{inc}}$ by an array of N point dipoles can be cast in the form

$$\mathbf{AP} = \mathbf{E} \tag{17}$$

where $\mathbf{E}$ is a $3N$-dimensional (complex) vector of the incident electric field $\mathbf{E}_{\mathrm{inc}}$ at the N lattice sites, $\mathbf{P}$ is a $3N$-dimensional (complex) vector of the (unknown) dipole polarizations, and $\mathbf{A}$ is a $3N \times 3N$ complex matrix.

Because $3N$ is a large number, direct methods for solving this system of equations for the unknown vector $\mathbf{P}$ are impractical, but iterative methods are useful: we begin with a guess (typically, $\mathbf{P} = 0$) for the unknown polarization vector, and then iteratively improve the estimate for $\mathbf{P}$ until equation (17) is solved to some error criterion. The error tolerance may be specified as

$$\frac{|\mathbf{A}^\dagger \mathbf{AP} - \mathbf{A}^\dagger \mathbf{E}|}{|\mathbf{A}^\dagger \mathbf{E}|} < h \quad , \tag{18}$$

where $\mathbf{A}^\dagger$ is the Hermitian conjugate of $\mathbf{A}$ [$(A^\dagger)_{ij} \equiv (A_{ji})^*$], and h is the error tolerance. We typically use $h = 10^{-5}$ in order to satisfy eq.(17) to high accuracy. The error tolerance h can be specified by the user through the parameter TOL in the parameter file ddscat.par (see Appendix A).

A major change in going from **DDSCAT.4b** to **5a** (and subsequent versions) was the implementation of several different algorithms for iterative solution of the system of complex linear equations. **DDSCAT 7.1** is now structured to permit solution algorithms to be treated in a fairly "modular" fashion, facilitating the testing of different algorithms. A number of algorithms were compared by Flatau (1997)[5]; two of them (PBCGST and PETRKP) performed well and are made available to the user in **DDSCAT**. **DDSCAT 7.1** now also offers a third option, PBCGS2. The choice of algorithm is made by specifying one of the options:

- PBCGS2 – BiConjugate Gradient with Stabilization as implemented in the routine ZBCG2 by M.A. Botchev, University of Twente. This is based on the PhD thesis of D.R. Fokkema, and on work by Sleijpen & vanderVorst (1995,1996).

- PBCGST – Preconditioned BiConjugate Gradient with STabilitization method from the Parallel Iterative Methods (PIM) package created by R. Dias da Cunha and T. Hopkins.

- PETRKP – the complex conjugate gradient algorithm of Petravic & Kuo-Petravic (1979), as coded in the Complex Conjugate Gradient package (CCGPACK) created by P.J. Flatau. This is the algorithm discussed by Draine (1988) and used in previous versions of **DDSCAT**.

All three methods work fairly well. Our experience suggests that PBCGS2 is generally fastest and best-behaved, and we recommend that the user try it first. However, in case it runs into numerical difficulties, PBCGST and PETRKP are available as alternatives.[6]

12 Choice of FFT Algorithm

DDSCAT 7.1 offers two FFT options: (1) the GPFA FFT algorithm developed by Dr. Clive Temperton (1992), [7] and (2) the Intel® MKL routine DFTI.

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[5] A postscript copy of this report – file cg.ps – is distributed with the **DDSCAT 7.1** documentation.

[6] The Parallel Iterative Methods (PIM) by Rudnei Dias da Cunha (rdd@ukc.ac.uk) and Tim Hopkins (trh@ukc.ac.uk) is a collection of Fortran 77 routines designed to solve systems of linear equations on parallel and scalar computers using a variety of iterative methods (available at
http://www.mat.ufrgs.br/pim-e.html). PIM offers a number of iterative methods, including

- Conjugate-Gradients, CG (Hestenes 1952),
- Bi-Conjugate-Gradients, BICG (Fletcher 1976),
- Conjugate-Gradients squared, CGS (Sonneveld 1989),
- the stabilised version of Bi-Conjugate-Gradients, BICGSTAB (van der Vorst 1991),
- the restarted version of BICGSTAB, RBICGSTAB (Sleijpen & Fokkema 1992)
- the restarted generalized minimal residual, RGMRES (Saad 1986),
- the restarted generalized conjugate residual, RGCR (Eisenstat 1983),
- the normal equation solvers, CGNR (Hestenes 1952 and CGNE (Craig 1955),
- the quasi-minimal residual, QMR (highly parallel version due to Bucker & Sauren 1996),
- transpose-free quasi-minimal residual, TFQMR (Freund 1992),
- the Chebyshev acceleration, CHEBYSHEV (Young 1981).

The source code for these methods is distributed with DDSCAT but only PBCGST and PETRKP can be called directly via ddscat.par. It is possible to add other options by changing the code in getfml.f90. Flatau (1997) has compared the convergence rates of a number of different methods. A helpful introduction to conjugate gradient methods is provided by the report "Conjugate Gradient Method Without Agonizing Pain" by Jonathan R. Shewchuk, available as a postscript file: ftp://REPORTS.ADM.CS.CMU.EDU/usr0/anon/1994/CMU-CS-94-125.ps.

[7]The GPFA code contains a parameter LVR which is set in data statements in the routines gpfa2f, gpfa3f, and gpfa5f. LVR is supposed to be optimized to correspond to the "length of a vector register" on vector machines. As delivered, this parameter is set to 64, which is supposed to be appropriate for Crays other than the C90. For the C90, 128 is supposed to be preferable (and perhaps "preferable" should be read as "necessary" – there is some basis for fearing that results computed on a C90 with LVR other than 128 run the risk of being incorrect!) The value of LVR is not critical for scalar machines, as long as it is fairly large. We found
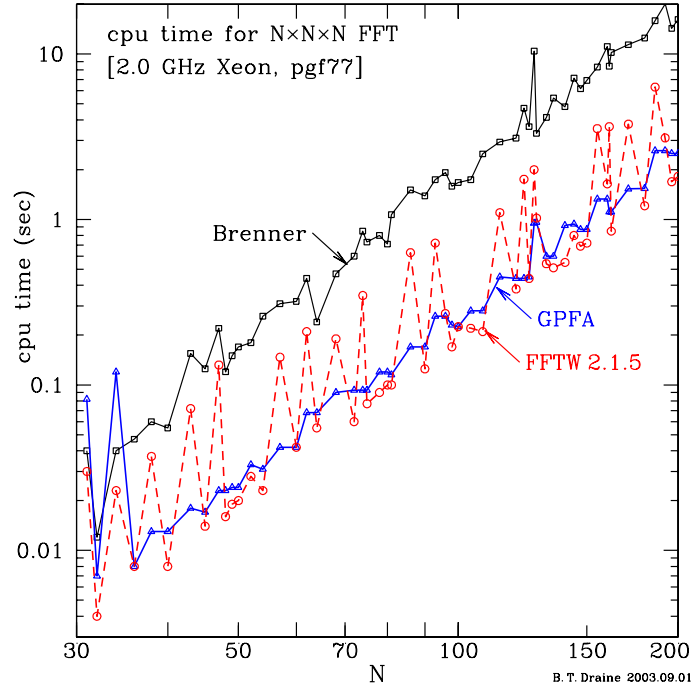
Figure 5: Comparison of cpu time required by 3 different FFT implementations. It is seen that the GPFA and FFTW implementations have comparable speeds, much faster than Brenner's FFT implementation.

The GPFA routine is portable and quite fast: Figure 5 compares the speed of three FFT implementations: Brenner's, GPFA, and FFTW (`http://www.fftw.org`). We see that while for some cases FFTW 2.1.5 is faster than the GPFA algorithm, the difference is only marginal. The FFTW code and GPFA code are quite comparable in performance – for some cases the GPFA code is faster, for other cases the FFTW code is faster. For target dimensions which are factorizable as $2^i 3^j 5^k$ (for integer i, j, k), the GPFA and FFTW codes have the same memory requirements. For targets with extents N_x, N_y, N_z which are not factorizable as $2^i 3^j 5^k$, the GPFA code needs to "extend" the computational volume to have values of N_x, N_y, and N_z which are factorizable by 2, 3, and 5. For these cases, GPFA requires somewhat more memory than FFTW. However, the fractional difference in required memory is not large, since integers factorizable as $2^i 3^j 5^k$ occur fairly frequently.[8] [Note: This "extension" of the target volume occurs automatically and is transparent to the user.]

DDSCAT 7.1 offers a new FFT option: the Intel® Math Kernel Library `DFTI`. This is tuned for optimum performance, and appears to offer real performance advantages on modern multi-core cpus. With this now available, the FFTW option, which had been included in **DDSCAT 6.1**, has been removed from **DDSCAT 7.1**.

The choice of FFT implementation is obtained by specifying one of:

- `FFTMKL` to use the Intel® MKL routine `DFTI` (see §6.5). **This is recommended, but requires that the Intel® Math Kernel Library be installed on your system**.

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little difference between `LVR`=64 and 128 on a Sparc 10/51, on an Ultrasparc 170, and on an Intel® Xeon cpu. You may wish to experiment with different `LVR` values on your computer architecture. To change `LVR`, you need to edit `gpfa.f90` and change the three `data` statements where `LVR` is set.

[8] 2, 3, 4, 5, 6, 8, 9, 10, 12, 15, 16, 18, 20, 24, 25, 27, 30, 32, 36, 40, 45, 48, 50, 54, 60, 64, 72, 75, 80, 81, 90, 96, 100, 108, 120, 125, 128, 135, 144, 150, 160, 162, 180, 192, 200 216, 225, 240, 243, 250, 256, 270, 288, 300, 320, 324, 360, 375, 384, 400, 405, 432, 450, 480, 486, 500, 512, 540, 576, 600, 625, 640, 648, 675, 720, 729, 750, 768, 800, 810, 864, 900, 960, 972, 1000, 1024, 1080, 1125, 1152, 1200, 1215, 1250, 1280, 1296, 1350, 1440, 1458, 1500, 1536, 1600, 1620, 1728, 1800, 1875, 1920, 1944, 2000, 2025, 2048, 2160, 2187, 2250, 2304, 2400, 2430, 2500, 2560, 2592, 2700, 2880, 2916, 3000, 3072, 3125, 3200, 3240, 3375, 3456, 3600, 3645, 3750, 3840, 3888, 4000, 4050, 4096 are the integers ≤ 4096 which are of the form $2^i 3^j 5^k$.
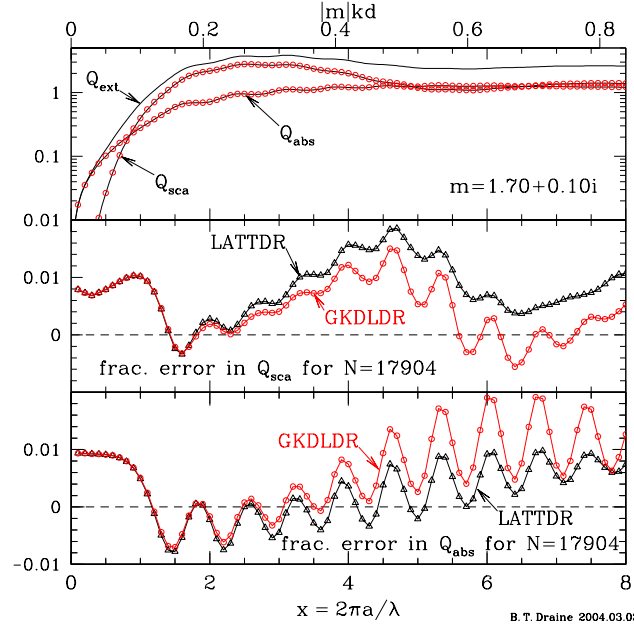
Figure 6: Scattering and absorption for a $m = 1.7 + 0.1i$ sphere, calculated using two prescriptions for the polarizability: LATTDR is the lattice dispersion relation result of Draine & Goodman (1993). GKDLDR is the lattice dispersion relation result of Gutkowicz-Krusin & Draine (2004). Results are shown as a function of scattering parameter $x = 2\pi a/\lambda$; the upper scale gives values of $|m|kd$. We see that the cross sections calculated with these two prescriptions are quite similar for $|m|kd \lesssim 0.5$. For other examples see Gutkowicz-Krusin & Draine (2004).

- `GPFAFT` to use the GPFA algorithm (Temperton 1992).**This is is not quite as fast as FFTMKL, but is written in plain Fortran-90.**

13 Dipole Polarizabilities

Option `GKDLDR` specifies that the polarizability be prescribed by the "Lattice Dispersion Relation", with the polarizability found by Gutkowicz-Krusin & Draine (2004), who corrected a subtle error in the analysis of Draine & Goodman (1993). For $|m|kd \lesssim 1$, the `GKDLDR` polarizability differs slightly from the `LATTDR` polarizability, but the differences in calculated scattering cross sections are relatively small, as can be seen from Figure 6. We recommend option `GKDLDR`.

Users wishing to compare can invoke option `LATTDR` to specify that the "Lattice Dispersion Relation" of Draine & Goodman (1993) be employed to determine the dipole polarizabilities. This polarizability also works well.

14 Dielectric Functions

In order to assign the appropriate dipole polarizabilities, **DDSCAT 7.1** must be given the dielectric constant of the material (or materials) of which the target of interest is composed *relative to the dielectric constant of the ambient medium*. This information is supplied to **DDSCAT 7.1** through a table (or tables), read by subroutine `DIELEC` in file `dielec.f90`, and providing either the complex refractive index $m = n + ik$ or complex dielectric function $\epsilon = \epsilon_1 + i\epsilon_2$ as a function of wavelength λ. Since $m = \epsilon^{1/2}$, or $\epsilon = m^2$, the user must supply either m or ϵ.

DDSCAT 7.1 can calculate scattering and absorption by targets with anisotropic dielectric functions, with arbitrary orientation of the optical axes relative to the target shape. See §26.

As discussed in §3.2, **DDSCAT** calculates scattering for targets embedded in dielectric media using the *relative* dielectric constant $\epsilon = \epsilon_{\text{target}}(\omega)/\epsilon_{\text{medium}}(\omega)$ or the *relative* refractive index $m =$

$m_{\text{target}}(\omega)/m_{\text{medium}}(\omega)$ and the wavelength *in the medium* $\lambda = (2\pi c/\omega)/m_{\text{medium}}$, where c is the speed of light *in vacuo*.

It is therefore important that the table containing the dielectric function information give the *relative* dielectric function or refractive index as a function of the *wavelength in the ambient medium*.

The table formatting is intended to be quite flexible. The first line of the table consists of text, up to 80 characters of which will be read and included in the output to identify the choice of dielectric function. (For the sample problem, it consists of simply the statement `m = 1.33 + 0.01i`.) The second line consists of 5 integers; either the second and third *or* the fourth and fifth should be zero.

- The first integer specifies which column the wavelength is stored in.
- The second integer specifies which column $\text{Re}(m)$ is stored in.
- The third integer specifies which column $\text{Im}(m)$ is stored in.
- The fourth integer specifies which column $\text{Re}(\epsilon)$ is stored in.
- The fifth integer specifies which column $\text{Im}(\epsilon)$ is stored in.

If the second and third integers are zeros, then `DIELEC` will read $\text{Re}(\epsilon)$ and $\text{Im}(\epsilon)$ from the file; if the fourth and fifth integers are zeros, then $\text{Re}(m)$ and $\text{Im}(m)$ will be read from the file.

The third line of the file is used for column headers, and the data begins in line 4. *There must be at least 3 lines of data:* even if ϵ is required at only one wavelength, please supply two additional "dummy" wavelength entries in the table so that the interpolation apparatus will not be confused.

15 Calculation of ⟨cos θ⟩, Radiative Force, and Radiation Torque

In addition to solving the scattering problem for a dipole array, **DDSCAT** can compute the three-dimensional force $\mathbf{F}_{\text{rad}}$ and torque $\mathbf{\Gamma}_{\text{rad}}$ exerted on this array by the incident and scattered radiation fields. The radiation torque calculation is carried out, after solving the scattering problem, only if `DOTORQ` has been specified in `ddscat.par`. For each incident polarization mode, the results are given in terms of dimensionless efficiency vectors $\mathbf{Q}_{pr}$ and $\mathbf{Q}_{\Gamma}$, defined by

$$\mathbf{Q}_{\text{pr}} \equiv \frac{\mathbf{F}_{\text{rad}}}{\pi a_{\text{eff}}^2 u_{\text{rad}}} \quad , \tag{19}$$

$$\mathbf{Q}_{\Gamma} \equiv \frac{k\mathbf{\Gamma}_{\text{rad}}}{\pi a_{\text{eff}}^2 u_{\text{rad}}} \quad , \tag{20}$$

where $\mathbf{F}_{\text{rad}}$ and $\mathbf{\Gamma}_{\text{rad}}$ are the time-averaged force and torque on the dipole array, $k = 2\pi/\lambda$ is the wavenumber *in vacuo*, and $u_{\text{rad}} = E_0^2/8\pi$ is the time-averaged energy density for an incident plane wave with amplitude $E_0 \cos(\omega t + \phi)$. The radiation pressure efficiency vector can be written

$$\mathbf{Q}_{\text{pr}} = Q_{\text{ext}}\hat{\mathbf{k}} - Q_{\text{sca}}\mathbf{g} \quad , \tag{21}$$

where $\hat{\mathbf{k}}$ is the direction of propagation of the incident radiation, and the vector $\mathbf{g}$ is the mean direction of propagation of the scattered radiation:

$$\mathbf{g} = \frac{1}{C_{\text{sca}}} \int d\Omega \frac{dC_{\text{sca}}(\hat{\mathbf{n}}, \hat{\mathbf{k}})}{d\Omega}\hat{\mathbf{n}} \quad , \tag{22}$$

where $d\Omega$ is the element of solid angle in scattering direction $\hat{\mathbf{n}}$, and $dC_{\text{sca}}/d\Omega$ is the differential scattering cross section. The components of $\mathbf{Q}_{\text{pr}}$ are reported in the Target Frame: $Q_{\text{pr},1} \equiv \mathbf{F}_{\text{rad}} \cdot \hat{\mathbf{x}}_{\text{TF}}$, $Q_{\text{pr},2} \equiv \mathbf{F}_{\text{rad}} \cdot \hat{\mathbf{y}}_{\text{TF}}$, $Q_{\text{pr},3} \equiv \mathbf{F}_{\text{rad}} \cdot \hat{\mathbf{z}}_{\text{TF}}$.

Equations for the evaluation of the radiative force and torque are derived by Draine & Weingartner (1996). It is important to note that evaluation of $\mathbf{Q}_{\text{pr}}$ and $\mathbf{Q}_{\Gamma}$ involves averaging over scattering directions to evaluate the linear and angular momentum transport by the scattered wave. This evaluation requires appropriate choices of the parameter `ETASCA` – see §23.

In addition, **DDSCAT** calculates $\langle \cos\theta \rangle$ [the first component of the vector g in eq. (22)] and the second moment $\langle \cos^2\theta \rangle$. These two moments are useful measures of the anisotropy of the scattering. For example, Draine (2003) gives an analytic approximation to the scattering phase function of dust mixtures that is parameterized by the two moments $\langle \cos\theta \rangle$ and $\langle \cos^2\theta \rangle$.

16 Memory Requirements

The memory requirements are determined by the size of the "computational volume" – this is a rectangular region, of size NX×NY×NZ that is large enough to contain the target. If using the GPFAFT option, then NX, NY, NZ are also required to have only 2,3, and 5 as prime factors (see footnote 8).

In single precision, the memory requirement for **DDSCAT 7.1** is approximately

$$(35. + 0.0010 \times \text{NX} \times \text{NY} \times \text{NZ}) \text{ Mbytes} \quad \text{for single precision} \tag{23}$$

$$(42 + 0.0020 \times \text{NX} \times \text{NY} \times \text{NZ}) \text{ Mbytes} \quad \text{for double precision} \tag{24}$$

Thus, in single precision, a 48×48×48 calculation requires ∼146 MBytes.

The memory is allocated dynamically – once the target has been created, **DDSCAT 7.1** will determine just how much overall memory is needed, and will allocate it. However, the user must provide information (via ddscat.par) to allow **DDSCAT 7.1** to allocate sufficiently large arrays to carry out the initial target creation. Initially, the only arrays that will be allocated are those related to the target geometry, so it is OK to be quite generous in this initial allowance, as the memory required for the target generation step is small compared to the memory required to carry out the full scattering calculation.

17 Target Orientation

Recall that we define a "Lab Frame" (LF) in which the incident radiation propagates in the $+x$ direction. For purposes of discussion we will always let unit vectors $\hat{\mathbf{x}}_{\text{LF}}$, $\hat{\mathbf{y}}_{\text{LF}}$, $\hat{\mathbf{z}}_{\text{LF}} = \hat{\mathbf{x}}_{\text{LF}} \times \hat{\mathbf{y}}_{\text{LF}}$ be the three coordinate axes of the LF.

In ddscat.par one specifies the first polarization state $\hat{\mathbf{e}}_{01}$ (which obviously must lie in the y, z plane in the LF); **DDSCAT** automatically constructs a second polarization state $\hat{\mathbf{e}}_{02} = \hat{\mathbf{x}}_{\text{LF}} \times \hat{\mathbf{e}}_{01}^*$ orthogonal to $\hat{\mathbf{e}}_{01}$. Users will often find it convenient to let polarization vectors $\hat{\mathbf{e}}_{01} = \hat{\mathbf{y}}$, $\hat{\mathbf{e}}_{02} = \hat{\mathbf{z}}$ (although this is not mandatory – see §22).

Recall that definition of a target involves specifying two unit vectors, $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$, which are imagined to be "frozen" into the target. We require $\hat{\mathbf{a}}_2$ to be orthogonal to $\hat{\mathbf{a}}_1$. Therefore we may define a "Target Frame" (TF) defined by the three unit vectors $\hat{\mathbf{a}}_1$, $\hat{\mathbf{a}}_2$, and $\hat{\mathbf{a}}_3 = \hat{\mathbf{a}}_1 \times \hat{\mathbf{a}}_2$.

For example, when **DDSCAT** creates a 32×24×16 rectangular solid, it fixes $\hat{\mathbf{a}}_1$ to be along the longest dimension of the solid, and $\hat{\mathbf{a}}_2$ to be along the next-longest dimension.

Important Note: for periodic targets, **DDSCAT 7.1** requires that the periodic target have $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{\text{TF}}$.

Orientation of the target relative to the incident radiation can in principle be determined two ways:

1. specifying the direction of $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ in the LF, or

2. specifying the directions of $\hat{\mathbf{x}}_{\text{LF}}$ (incidence direction) and $\hat{\mathbf{y}}_{\text{LF}}$ in the TF.

DDSCAT uses method 1.: the angles Θ, Φ, and β are specified in the file ddscat.par. The target is oriented such that the polar angles Θ and Φ specify the direction of $\hat{\mathbf{a}}_1$ relative to the incident direction $\hat{\mathbf{x}}_{\text{LF}}$, where the $\hat{\mathbf{x}}_{\text{LF}}$,$\hat{\mathbf{y}}_{\text{LF}}$ plane has $\Phi = 0$. Once the direction of $\hat{\mathbf{a}}_1$ is specified, the angle β then specifies how the target is to rotated around the axis $\hat{\mathbf{a}}_1$ to fully specify its orientation. A more extended and precise explanation follows:

17.1 Orientation of the Target in the Lab Frame

DDSCAT uses three angles, Θ, Φ, and β, to specify the directions of unit vectors $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ in the LF (see Fig. 7).

Θ is the angle between $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{x}}_{\text{LF}}$.

When $\Phi = 0$, $\hat{\mathbf{a}}_1$ will lie in the $\hat{\mathbf{x}}_{\text{LF}}$, $\hat{\mathbf{y}}_{\text{LF}}$ plane. When Φ is nonzero, it will refer to the rotation of $\hat{\mathbf{a}}_1$ around $\hat{\mathbf{x}}_{\text{LF}}$: e.g., $\Phi = 90°$ puts $\hat{\mathbf{a}}_1$ in the $\hat{\mathbf{x}}_{\text{LF}}$, $\hat{\mathbf{z}}_{\text{LF}}$ plane.

When $\beta = 0$, $\hat{\mathbf{a}}_2$ will lie in the $\hat{\mathbf{x}}_{\text{LF}}$, $\hat{\mathbf{a}}_1$ plane, in such a way that when $\Theta = 0$ and $\Phi = 0$, $\hat{\mathbf{a}}_2$ is in the $\hat{\mathbf{y}}_{\text{LF}}$ direction: e.g, $\Theta = 90°$, $\Phi = 0$, $\beta = 0$ has $\hat{\mathbf{a}}_1 = \hat{\mathbf{y}}_{\text{LF}}$ and $\hat{\mathbf{a}}_2 = -\hat{\mathbf{x}}_{\text{LF}}$. Nonzero β introduces an additional rotation of $\hat{\mathbf{a}}_2$ around $\hat{\mathbf{a}}_1$: e.g., $\Theta = 90°$, $\Phi = 0$, $\beta = 90°$ has $\hat{\mathbf{a}}_1 = \hat{\mathbf{y}}_{\text{LF}}$ and $\hat{\mathbf{a}}_2 = \hat{\mathbf{z}}_{\text{LF}}$.
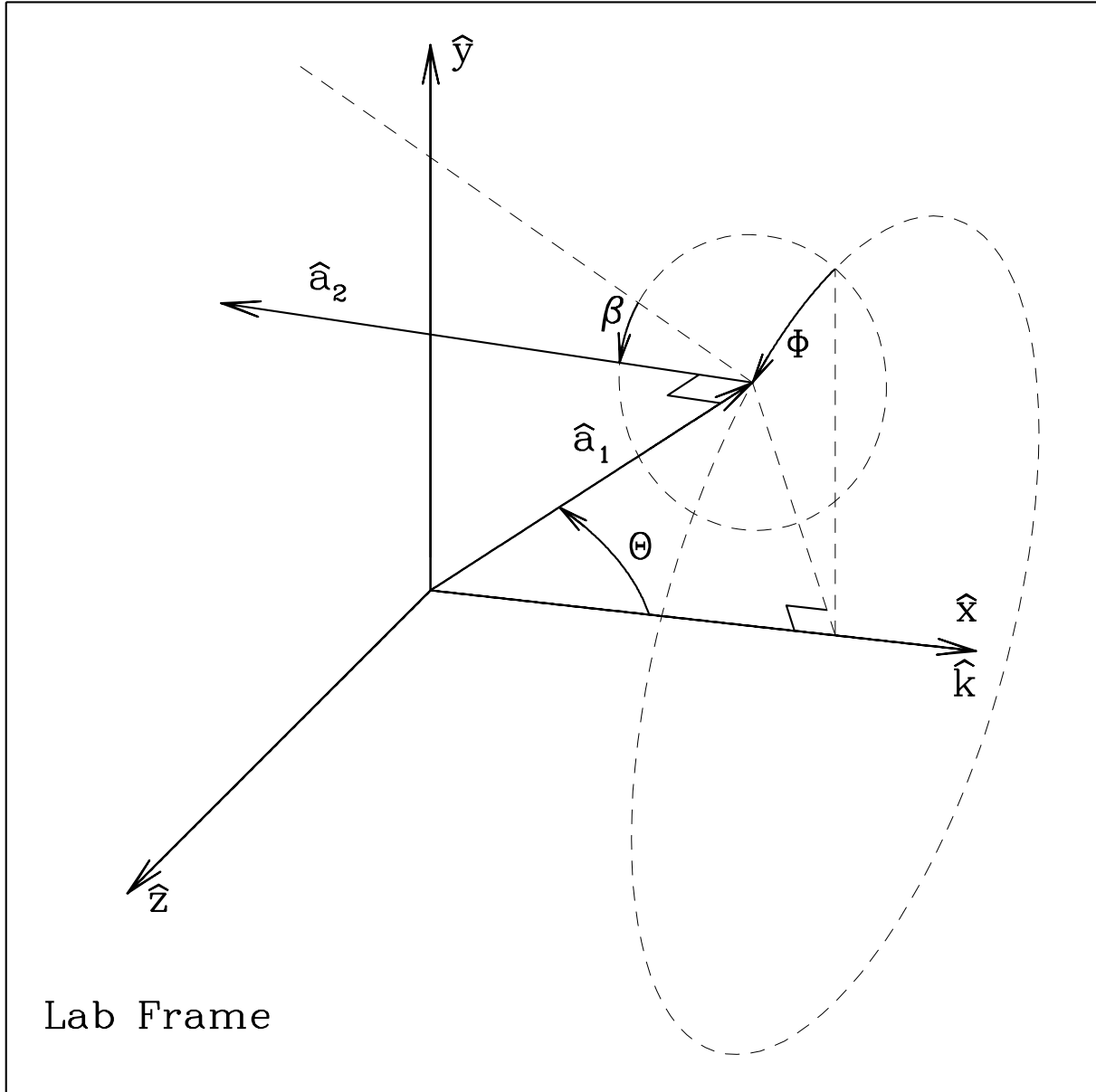
Figure 7: Target orientation in the Lab Frame. $\hat{\mathbf{x}} = \hat{\mathbf{x}}_{\mathrm{LF}}$ is the direction of propagation of the incident radiation, and $\hat{\mathbf{y}} = \hat{\mathbf{y}}_{\mathrm{LF}}$ is the direction of the real component (at $x_{\mathrm{LF}} = 0$, $t = 0$) of the first incident polarization mode. In this coordinate system, the orientation of target axis $\hat{\mathbf{a}}_1$ is specified by angles Θ and Φ. With target axis $\hat{\mathbf{a}}_1$ fixed, the orientation of target axis $\hat{\mathbf{a}}_2$ is then determined by angle β specifying rotation of the target around $\hat{\mathbf{a}}_1$. When $\beta = 0$, $\hat{\mathbf{a}}_2$ lies in the $\hat{\mathbf{a}}_1$,$\hat{\mathbf{x}}_{\mathrm{LF}}$ plane.

Mathematically:

$$\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\mathrm{LF}} \cos\Theta + \hat{\mathbf{y}}_{\mathrm{LF}} \sin\Theta \cos\Phi + \hat{\mathbf{z}}_{\mathrm{LF}} \sin\Theta \sin\Phi \tag{25}$$

$$\hat{\mathbf{a}}_2 = -\hat{\mathbf{x}}_{\mathrm{LF}} \sin\Theta \cos\beta + \hat{\mathbf{y}}_{\mathrm{LF}}[\cos\Theta \cos\beta \cos\Phi - \sin\beta \sin\Phi]$$
$$+\hat{\mathbf{z}}_{\mathrm{LF}}[\cos\Theta \cos\beta \sin\Phi + \sin\beta \cos\Phi] \tag{26}$$

$$\hat{\mathbf{a}}_3 = \hat{\mathbf{x}}_{\mathrm{LF}} \sin\Theta \sin\beta - \hat{\mathbf{y}}_{\mathrm{LF}}[\cos\Theta \sin\beta \cos\Phi + \cos\beta \sin\Phi]$$
$$-\hat{\mathbf{z}}_{\mathrm{LF}}[\cos\Theta \sin\beta \sin\Phi - \cos\beta \cos\Phi] \tag{27}$$

or, equivalently:

$$\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1 \cos\Theta - \hat{\mathbf{a}}_2 \sin\Theta \cos\beta + \hat{\mathbf{a}}_3 \sin\Theta \sin\beta \tag{28}$$

$$\hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1 \sin\Theta \cos\Phi + \hat{\mathbf{a}}_2[\cos\Theta \cos\beta \cos\Phi - \sin\beta \sin\Phi]$$
$$-\hat{\mathbf{a}}_3[\cos\Theta \sin\beta \cos\Phi + \cos\beta \sin\Phi] \tag{29}$$

$$\hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1 \sin\Theta \sin\Phi + \hat{\mathbf{a}}_2[\cos\Theta \cos\beta \sin\Phi + \sin\beta \cos\Phi]$$
$$-\hat{\mathbf{a}}_3[\cos\Theta \sin\beta \sin\Phi - \cos\beta \cos\Phi] \tag{30}$$

17.2 Orientation of the Incident Beam in the Target Frame

Under some circumstances, one may wish to specify the target orientation such that $\hat{\mathbf{x}}_{\mathrm{LF}}$ (the direction of propagation of the radiation) and $\hat{\mathbf{y}}_{\mathrm{LF}}$ (usually the first polarization direction) and $\hat{\mathbf{z}}_{\mathrm{LF}}$ ($= \hat{\mathbf{x}}_{\mathrm{LF}} \times \hat{\mathbf{y}}_{\mathrm{LF}}$) refer to certain directions in the TF. Given the definitions of the LF and TF above, this is simply an exercise in coordinate transformation. For example, one might wish to have the incident radiation propagating along the (1,1,1) direction in the TF (example 14 below). Here we provide some selected examples:

1. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3 : \Theta = 0, \Phi + \beta = 0$
2. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_2 : \Theta = 0, \Phi + \beta = 90°$
3. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_3 : \Theta = 90°, \beta = 180°, \Phi = 0$
4. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1 : \Theta = 90°, \beta = 180°, \Phi = 90°$
5. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2 : \Theta = 90°, \beta = -90°, \Phi = 0$
6. $\hat{\mathbf{x}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_1 : \Theta = 90°, \beta = -90°, \Phi = -90°$
7. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_1, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_3 : \Theta = 180°, \beta + \Phi = 180°$
8. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_1, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2 : \Theta = 180°, \beta + \Phi = 90°$
9. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_2, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3 : \Theta = 90°, \beta = 0, \Phi = 0$
10. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_2, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_1 : \Theta = 90°, \beta = 0, \Phi = -90°$
11. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_3, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1, \hat{\mathbf{z}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_2 : \Theta = 90°, \beta = -90°, \Phi = 0$
12. $\hat{\mathbf{x}}_{\mathrm{LF}} = -\hat{\mathbf{a}}_3, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_2, \hat{\mathbf{z}}_{\mathrm{LF}} = \hat{\mathbf{a}}_1 : \Theta = 90°, \beta = -90°, \Phi = 90°$
13. $\hat{\mathbf{x}}_{\mathrm{LF}} = (\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2)/\sqrt{2}, \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{a}}_3, \hat{\mathbf{z}}_{\mathrm{LF}} = (\hat{\mathbf{a}}_1 - \hat{\mathbf{a}}_2)/\sqrt{2} : \Theta = 45°, \beta = 180°, \Phi = 90°$
14. $\hat{\mathbf{x}}_{\mathrm{LF}} = (\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2 + \hat{\mathbf{a}}_3)/\sqrt{3}, \hat{\mathbf{y}}_{\mathrm{LF}} = (\hat{\mathbf{a}}_1 - \hat{\mathbf{a}}_2)/\sqrt{2}, \hat{\mathbf{z}}_{\mathrm{LF}} = (\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2 - 2\hat{\mathbf{a}}_3)/\sqrt{6} :$
    $\Theta = 54.7356°, \beta = 135°, \Phi = 30°$.

17.3 Sampling in Θ, Φ, and β

The present version, **DDSCAT 7.1**, chooses the angles β, Θ, and Φ to sample the intervals (BETAMI, BETAMX), (THETMI, THETMX), (PHIMIN, PHIMAX), where BETAMI, BETAMX, THETMI, THETMX, PHIMIN, PHIMAX are specified in ddscat.par. The prescription for choosing the angles is to:

- uniformly sample in β;
- uniformly sample in Φ;

- uniformly sample in $\cos \Theta$.

This prescription is appropriate for random orientation of the target, within the specified limits of β, Φ, and Θ.

Note that when **DDSCAT 7.1** chooses angles it handles β and Φ differently from Θ. The range for β is divided into NBETA intervals, and the midpoint of each interval is taken. Thus, if you take BETAMI=0, BETAMX=90, NBETA=2 you will get $\beta = 22.5°$ and $67.5°$. Similarly, if you take PHIMIN=0, PHIMAX=180, NPHI=2 you will get $\Phi = 45°$ and $135°$.

Sampling in Θ is done quite differently from sampling in β and Φ. First, as already mentioned above, **DDSCAT 7.1** samples uniformly in $\cos \Theta$, not Θ. Secondly, the sampling depends on whether NTHETA is even or odd.

- If NTHETA is odd, then the values of Θ selected include the extreme values THETMI and THETMX; thus, THETMI=0, THETMX=90, NTHETA=3 will give you $\Theta = 0, 60°, 90°$.

- If NTHETA is even, then the range of $\cos \Theta$ will be divided into NTHETA intervals, and the midpoint of each interval will be taken; thus, THETMI=0, THETMX=90, NTHETA=2 will give you $\Theta = 41.41°$ and $75.52°$ [$\cos \Theta = 0.25$ and 0.75].

The reason for this is that if odd NTHETA is specified, then the "integration" over $\cos \Theta$ is performed using Simpson's rule for greater accuracy. If even NTHETA is specified, then the integration over $\cos \Theta$ is performed by simply taking the average of the results for the different Θ values.

If averaging over orientations is desired, it is recommended that the user specify an *odd* value of NTHETA so that Simpson's rule will be employed.

18 Orientational Averaging

DDSCAT has been constructed to facilitate the computation of orientational averages. How to go about this depends on the distribution of orientations which is applicable.

18.1 Randomly-Oriented Targets

For randomly-oriented targets, we wish to compute the orientational average of a quantity $Q(\beta, \Theta, \Phi)$:

$$\langle Q \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\beta \int_{-1}^1 d\cos\Theta \int_0^{2\pi} d\Phi \, Q(\beta, \Theta, \Phi) \quad . \tag{31}$$

To compute such averages, all you need to do is edit the file ddscat.par so that DDSCAT knows what ranges of the angles β, Θ, and Φ are of interest. For a randomly-oriented target with no symmetry, you would need to let β run from 0 to $360°$, Θ from 0 to $180°$, and Φ from 0 to $360°$.

For targets with symmetry, on the other hand, the ranges of β, Θ, and Φ may be reduced. First of all, remember that averaging over Φ is relatively "inexpensive", so when in doubt average over 0 to $360°$; most of the computational "cost" is associated with the number of different values of (β, Θ) which are used. Consider a cube, for example, with axis $\hat{a}_1$ normal to one of the cube faces; for this cube β need run only from 0 to $90°$, since the cube has fourfold symmetry for rotations around the axis $\hat{a}_1$. Furthermore, the angle Θ need run only from 0 to $90°$, since the orientation (β, Θ, Φ) is indistinguishable from $(\beta, 180° - \Theta, 360° - \Phi)$.

For targets with symmetry, the user is encouraged to test the significance of β, Θ, Φ on targets with small numbers of dipoles (say, of the order of 100 or so) but having the desired symmetry.

18.2 Nonrandomly-Oriented Targets

Some special cases (where the target orientation distribution is uniform for rotations around the x axis = direction of propagation of the incident radiation), one may be able to use **DDSCAT 7.1** with appropriate choices of input parameters. More generally, however, you will need to modify subroutine ORIENT to generate a list of NBETA values of β, NTHETA values of Θ, and NPHI values of Φ, plus two weighting arrays WGTA(1-NTHETA,1-NPHI) and WGTB(1-NBETA). Here WGTA gives the weights which

should be attached to each (Θ,Φ) orientation, and WGTB gives the weight to be attached to each β orientation. Thus each orientation of the target is to be weighted by the factor WGTA×WGTB. For the case of random orientations, **DDSCAT** chooses Θ values which are uniformly spaced in $\cos\Theta$, and β and Φ values which are uniformly spaced, and therefore uses uniform weights

> WGTB=1./NBETA

When NTHETA is even, **DDSCAT** sets

> WGTA=1./(NTHETA×NPHI)

but when NTHETA is odd, **DDSCAT** uses Simpson's rule when integrating over Θ and

> WGTA= (1/3 or 4/3 or 2/3)/(NTHETA×NPHI)

Note that the program structure of **DDSCAT** may not be ideally suited for certain highly oriented cases. If, for example, the orientation is such that for a given Φ value only one Θ value is possible (this situation might describe ice needles oriented with the long axis perpendicular to the vertical in the Earth's atmosphere, illuminated by the Sun at other than the zenith) then it is foolish to consider all the combinations of Θ and Φ which the present version of **DDSCAT** is set up to do. We hope to improve this in a future version of **DDSCAT**.

19   Target Generation: Isolated Finite Targets

DDSCAT contains routines to generate dipole arrays representing finite targets of various geometries, including spheres, ellipsoids, rectangular solids, cylinders, hexagonal prisms, tetrahedra, two touching ellipsoids, and three touching ellipsoids. The target type is specified by variable CSHAPE on line 9 of ddscat.par, up to 12 target shape parameters (SHPAR$_1$, SHPAR$_2$, SHPAR$_3$, ...) on line 10.   The target geometry is most conveniently described in a coordinate system attached to the target which we refer to as the "Target Frame" (TF), with orthonormal unit vectors $\hat{\mathbf{x}}_{\mathrm{TF}}$, $\hat{\mathbf{y}}_{\mathrm{TF}}$, $\hat{\mathbf{z}}_{\mathrm{TF}} \equiv \hat{\mathbf{x}}_{\mathrm{TF}} \times \hat{\mathbf{y}}_{\mathrm{TF}}$. Once the target is generated, the orientation of the target in the Lab Frame is accomplished as described in §17.

Every target generation routine will specify

- The "occupied" lattice sites;
- The composition associated with each occupied lattice site;
- Two "target axes" $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ that are used as references when specifying the target orientation; and
- The location of the Target Frame origin of coordinates.

Target geometries currently supported include:

19.1   FROM_FILE = Target composed of possibly anisotropic material, defined by list of dipole locations and "compositions" obtained from a file

If anisotropic, the "microcrystals" in the target are assumed to be aligned with the principal axes of the dielectric tensor parallel to $\hat{\mathbf{x}}_{\mathrm{TF}}$, $\hat{\mathbf{y}}_{\mathrm{TF}}$, and $\hat{\mathbf{z}}_{\mathrm{TF}}$. This option causes **DDSCAT** to read the target geometry and composition information from a file shape.dat instead of automatically generating one of the geometries for which DDSCAT has built-in target generation capability. The shape.dat file is read by routine REASHP (file reashp.f90). The file shape.dat gives the number N of dipoles in the target, the components of the "target axes" $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ in the Target Frame (TF), the vector $x_0(1-3)$ determining the correspondence between the integers IXYZ and actual coordinates in the TF, and specifications for the location and "composition" of each dipole. The user can customize REASHP as needed to conform to the manner in which the target description is stored in file shape.dat. However, as supplied, REASHP expects the file shape.dat to have the following structure:

- one line containing a description; the first 67 characters will be read and printed in various output statements
- N = number of dipoles in target
- a_{1x} a_{1y} a_{1z} = x,y,z components (in TF) of $\mathbf{a_1}$

- $a_{2x}\ a_{2y}\ a_{2z}$ = x,y,z components (in TF) of $\mathbf{a_2}$
- $d_x/d\ \ d_y/d\ \ d_z/d = 1.\ 1.\ 1.$ = relative spacing of dipoles in $\hat{\mathbf{x}}_{TF}$, $\hat{\mathbf{y}}_{TF}$, $\hat{\mathbf{z}}_{TF}$ directions
- $x_{0x}\ \ x_{0y}\ \ x_{0z}$ = TF coordinates $x_{TF}/d\ \ y_{TF}/d\ \ z_{TF}/d$ corresponding to lattice site `IXYZ`= 0 0 0
- (line containing comments)
- *dummy* `IXYZ(1,1) IXYZ(1,2) IXYZ(1,3) ICOMP(1,1) ICOMP(1,2) ICOMP(1,3)`
- *dummy* `IXYZ(2,1) IXYZ(2,2) IXYZ(2,3) ICOMP(2,1) ICOMP(2,2) ICOMP(2,3)`
- *dummy* `IXYZ(3,1) IXYZ(3,2) IXYZ(3,3) ICOMP(3,1) ICOMP(3,2) ICOMP(3,3)`
- ...
- *dummy* `IXYZ(J,1) IXYZ(J,2) IXYZ(J,3) ICOMP(J,1) ICOMP(J,2) ICOMP(J,3)`
- ...
- *dummy* `IXYZ(N,1) IXYZ(N,2) IXYZ(N,3) ICOMP(N,1) ICOMP(N,2) ICOMP(N,3)`

where *dummy* is a number (integer or floating point)that might, for example, identify the dipole. This number will *not* be used in any calculations.

If the target material at location `J` is isotropic, `ICOMP(J,1)`, `ICOMP(J,2)`, and `ICOMP(J,3)` have the same value.

```
--- demo file for target option FROM_FILE (homogeneous,isotropic target) ---
8        = NAT
1.000    0.000    0.000    = target vector a1 (in TF)
0.000    1.000    0.000    = target vector a2 (in TF)
1.       1.       1.       = d_x/d  d_y/d  d_z/d  (normally 1 1 1)
0.5      0.5      0.5       = X0(1-3) = location in lattice of "target origin"
J    JX   JY   JZ   ICOMPX,ICOMPY,ICOMPZ
1     0    0    0    1  1  1
2     0    0    1    1  1  1
3     0    1    0    1  1  1
4     0    1    1    1  1  1
5     1    0    0    1  1  1
6     1    0    1    1  1  1
7     1    1    0    1  1  1
8     1    1    1    1  1  1
```

The above sample target consists of 8 dipoles arranged to represent a cube.
This example is homogeneous: All sites have composition 1
The target origin `X0` is set to be at the center of the target
Note that ICOMPX,ICOMPY,ICOMPZ could differ, allowing treatment of anisotropic targets, provided the dielectric tensor at each location is diagonal in the TF.

```
--- demo file for target option FROM_FILE (inhomogeneous, isotropic target) ---
8        = NAT
1.000    0.000    0.000    = target vector a1 (in TF)
0.000    1.000    0.000    = target vector a2 (in TF)
1.       1.       1.       = d_x/d  d_y/d  d_z/d  (normally 1 1 1)
0.5      0.5      0.5       = X0(1-3) = location in lattice of "target origin"
J    JX   JY   JZ   ICOMPX,ICOMPY,ICOMPZ
1     0    0    0    1  1  1
2     0    0    1    1  1  1
3     0    1    0    1  1  1
4     0    1    1    1  1  1
5     1    0    0    2  2  2
6     1    0    1    2  2  2
7     1    1    0    2  2  2
8     1    1    1    2  2  2
```

This sample target consists of 8 dipoles arranged to represent a cube.
This example is inhomogeneous: The lower half of the cube (JX=0) has isotropic composition 1
The upper half of the cube (JX=1) has isotropic composition 2
The target origin X0 is set to be at the center of the target.
Note that ICOMPX, ICOMPY, ICOMPZ can be different, allowing treatment of anisotropic targets, provided the dielectric tensor at each location is diagonal in the TF.

Sample calculation: The directory examples_exp/FROM_FILE contains files for calculation of scattering by a $0.5\mu m \times 1\mu m \times 1\mu m$ Au block, represented by a $32 \times 64 \times 64$ dipole array.

19.2 ANIFRMFIL = General anistropic target defined by list of dipole locations,"compositions", and material orientations obtained from a file

This option causes **DDSCAT** to read the target geometry information from a file shape.dat instead of automatically generating one of the geometries listed below. The file shape.dat gives the number N of dipoles in the target, the components of the "target axes" $\hat{a}_1$ and $\hat{a}_2$ in the Target Frame (TF), the vector $x_0(1-3)$ determining the correspondence between the integers IXYZ and actual coordinates in the TF, and specifications for the location and "composition" of each dipole. For each dipole J, the file shape.dat provides the location IXYZ(J,1-3), the composition identifier integer ICOMP(J,1-3) specifying the dielectric function corresponding to the three principal axes of the dielectric tensor, and angles Θ_{DF}, Φ_{DF}, and β_{DF} specifying the orientation of the local "Dielectric Frame" (DF) relative to the "Target Frame" (TF) (see §26). The DF is the reference frame in which the dielectric tensor is diagonalized. The Target Frame is the reference frame in which we specify the dipole locations.

The shape.dat file is read by routine REASHP (file reshp.f90). The user can customize REASHP as needed to conform to the manner in which the target geometry is stored in file shape.dat. However, as supplied, REASHP expects the file shape.dat to have the following structure:

- one line containing a description; the first 67 characters will be read and printed in various output statements.
- N = number of dipoles in target
- a_{1x} a_{1y} a_{1z} = x,y,z components (in Target Frame) of $\mathbf{a_1}$
- a_{2x} a_{2y} a_{2z} = x,y,z components (in Target Frame) of $\mathbf{a_2}$
- d_x/d d_y/d d_z/d = 1. 1. 1. = relative spacing of dipoles in $\hat{x}_{TF}$, $\hat{y}_{TF}$, $\hat{z}_{TF}$ directions
- x_{0x} x_{0y} x_{0z} = TF coordinates x_{TF}/d y_{TF}/d z_{TF}/d corresponding to lattice site IXYZ= 0 0 0
- (line containing comments)
- *dummy* IXYZ(1,1-3) ICOMP(1,1-3) THETADF(1) PHIDF(1) BETADF(1)
- *dummy* IXYZ(2,1-3) ICOMP(2,1-3) THETADF(2) PHIDF(2) BETADF(2)
- *dummy* IXYZ(3,1-3) ICOMP(3,1-3) THETADF(3) PHIDF(3) BETADF(3)
- ...
- *dummy* IXYZ(J,1-3) ICOMP(J,1-3) THETADF(J) PHIDF(J) BETADF(J)
- ...
- *dummy* IXYZ(N,1-3) ICOMP(N,1-3) THETADF(N) PHIDF(N) BETADF(N)

Where *dummy* is a number (either integer or floating point) that might, for example, give the number identifying the dipole. This number will *not* be used in any calculations.
THETADF PHIDF BETADF should be given in **radians**.

Here is an example of the first few lines of a target description file suitable for target option ANIFRMFIL:

```
--- demo file for target option ANIFRMFIL (this line is for comments) ---
8       = NAT
1.000   0.000   0.000   = target vector a1 (in TF)
0.000   1.000   0.000   = target vector a2 (in TF)
```

```
1.      1.      1.       = d_x/d  d_y/d  d_z/d  (normally 1 1 1)
0.      0.      0.       = X0(1-3) = location in lattice of "target origin"
J    JX   JY   JZ   ICOMP(J,1-3) THETADF PHIDF BETADF
1    0    0    0    1  1  1    0.     0.     0.
2    0    0    1    1  1  1    0.     0.     0.
3    0    1    0    1  1  1    0.     0.     0.
4    0    1    1    1  1  1    0.     0.     0.
5    1    0    0    2  3  3    0.5236 1.5708 0.
6    1    0    1    2  3  3    0.5236 1.5708 0.
7    1    1    0    2  3  3    0.5236 1.5708 0.
8    1    1    1    2  3  3    0.5236 1.5708 0.
```

This sample target consists of 8 dipoles arranged to represent a cube.
Half of the cube (dipoles with JX=0) has isotropic composition 1. For this case, the angles THETADF, PHIDF, BETADF do not matter, and it convenient to set them all to zero.
The other half of the cube (dipoles with JX=1) consists of a uniaxial material, with dielectric function 2 for E fields parallel to one axis (the "c-axis"), and dielectric function 3 for E fields perpendicular to the c-axis. The c-axis is 30° (0.5236 radians) away from $\hat{\mathbf{x}}_{\mathrm{TF}}$, and lies in the $\hat{\mathbf{x}}_{\mathrm{TF}}$-$\hat{\mathbf{z}}_{\mathrm{TF}}$ plane (having been rotated by 1.5708 radians around $\hat{\mathbf{x}}_{\mathrm{TF}}$).
Note that ICOMP(J,K) can be different for K=1,3, allowing treatment of anisotropic targets, provided the dielectric tensor at each location is diagonal in the TF.

19.3   ANIELLIPS = Homogeneous, anisotropic ellipsoid.

SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ define the ellipsoidal boundary:

$$\left(\frac{x_{\mathrm{TF}}/d}{\mathrm{SHPAR_1}}\right)^2 + \left(\frac{y_{\mathrm{TF}}/d}{\mathrm{SHPAR_2}}\right)^2 + \left(\frac{z_{\mathrm{TF}}/d}{\mathrm{SHPAR_3}}\right)^2 = \frac{1}{4} \quad , \tag{32}$$

The TF origin is located at the centroid of the ellipsoid.

19.4   ANI_ELL_2 = Two touching, homogeneous, anisotropic ellipsoids, with distinct compositions

Geometry as for ELLIPSO_2; SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ have same meanings as for ELLIPSO_2.
Target axes $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$.
Line connecting ellipsoid centers is $\parallel \hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\mathrm{TF}}$.
TF origin is located between ellipsoids, at point of contact.
It is assumed that (for both ellipsoids) the dielectric tensor is diagonal in the TF. User must set NCOMP=6 and provide xx, yy, zz components of dielectric tensor for first ellipsoid, and xx, yy, zz components of dielectric tensor for second ellipsoid (ellipsoids are in order of increasing x_{TF}).

19.5   ANI_ELL_3 = Three touching homogeneous, anisotropic ellipsoids with same size and orientation but distinct dielectric tensors

SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ have same meanings as for ELLIPSO_3.
Target axis $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ (along line of ellipsoid centers), and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$.
TF origin is located at center of middle ellipsoid.
It is assumed that dielectric tensors are all diagonal in the TF. User must set NCOMP=9 and provide xx, yy, zz elements of dielectric tensor for first ellipsoid, xx, yy, zz elements for second ellipsoid, and xx, yy, zz elements for third ellipsoid (ellipsoids are in order of increasing x_{TF}).

19.6   ANIRCTNGL = Homogeneous, anisotropic, rectangular solid

x, y, z lengths/d = SHPAR$_1$, SHPAR$_2$, SHPAR$_3$.
Target axes $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$ in the TF.

$(x_{\mathrm{TF}}, y_{\mathrm{TF}}, z_{\mathrm{TF}}) = (0,0,0)$ at middle of upper target surface, (where "up" = $\hat{\mathbf{x}}_{\mathrm{TF}}$). (The target surface is taken to be $d/2$ about the upper dipole layer.)

Dielectric tensor is assumed to be diagonal in the target frame.

User must set NCOMP=3 and supply names of three files for ϵ as a function of wavelength or energy: first for ϵ_{xx}, second for ϵ_{yy}, and third for ϵ_{zz}, as in the following sample ddscat.par file:

```
' ============ Parameter file for v7.1.0 ==================='
'**** PRELIMINARIES ****'
'NOTORQ'= CMTORQ*6 (DOTORQ, NOTORQ) -- either do or skip torque calculations
'PBCGS2'= CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT'= CMETHD*6 (GPFAFT, FFTMKL)
'GKDLDR'= CALPHA*6 (GKDLDR, LATTDR)
'NOTBIN'= CBINFLAG (ALLBIN, ORIBIN, NOTBIN)
'ANIRCTNGL'= CSHAPE*9 shape directive
'**** Initial Memory Allocation ****'
10 25 50 = upper bound on target extent
'**** Target Geometry and Composition ****'
'ANIRCTNGL'= CSHAPE*9 shape directive
10 25 50 = shape parameters SHPAR1, SHPAR2, SHPAR3
3         = NCOMP = number of dielectric materials
'/u/draine/DDA/diel/m2.00_0.10' = name of file containing dielectric function
'/u/draine/DDA/diel/m1.50_0.00'
'/u/draine/DDA/diel/m1.50_0.00'
'**** Error Tolerance ****'
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
5.00e-3 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
2.0     = ETASCA (number of angles is proportional to [(2+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
500. 500. 1 'INV' = wavelengths (first,last,how many,how=LIN,INV,LOG)
'**** Effective Radii (micron) **** '
30.60 30.60 1  'LIN' = eff. radii (first, last, how many, how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
'**** Specify which output files to write ****'
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA)
'**** Prescribe Target Rotations ****'
 0.   0.  1 = BETAMI, BETAMX, NBETA (beta=rotation around a1)
 0.  90.  3 = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
 0.   0.  1 = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0   0   0   = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6       = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41       = indices ij of elements to print
'**** Specify Scattered Directions ****'
'LFRAME' = CMDFRM*6 ('LFRAME' or 'TFRAME' for Lab Frame or Target Frame)
2 = number of scattering planes
0.  0. 180. 30 = phi, thetan_min, thetan_max, dtheta (in degrees) for plane A
90. 0. 180. 30 = phi, ... for plane B
```

19.7 CONELLIPS = Two concentric ellipsoids

SHPAR_1, SHPAR_2, SHPAR_3 = lengths/d of the *outer* ellipsoid along the $\hat{\mathbf{x}}_{\mathrm{TF}}$, $\hat{\mathbf{y}}_{\mathrm{TF}}$, $\hat{\mathbf{z}}_{\mathrm{TF}}$ axes;

SHPAR_4, SHPAR_5, SHPAR_6 = lengths/d of the *inner* ellipsoid along the $\hat{\mathbf{x}}_{\mathrm{TF}}$, $\hat{\mathbf{y}}_{\mathrm{TF}}$, $\hat{\mathbf{z}}_{\mathrm{TF}}$ axes.

Target axes $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$, $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$.

TF origin is located at centroids of ellipsoids.

The "core" within the inner ellipsoid is composed of isotropic material 1; the "mantle" between inner and outer ellipsoids is composed of isotropic material 2.

User must set NCOMP=2 and provide dielectric functions for "core" and "mantle" materials.

19.8   CYLINDER1 = Homogeneous, isotropic finite cylinder

$\text{SHPAR}_1 = \text{length}/d$, $\text{SHPAR}_2 = \text{diameter}/d$, with
$\text{SHPAR}_3 = 1$ for cylinder axis $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{x}}_{\text{TF}}$: $\hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$;
$\text{SHPAR}_3 = 2$ for cylinder axis $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{y}}_{\text{TF}}$: $\hat{\mathbf{a}}_1 = (0,1,0)_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = (0,0,1)_{\text{TF}}$;
$\text{SHPAR}_3 = 3$ for cylinder axis $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{z}}_{\text{TF}}$: $\hat{\mathbf{a}}_1 = (0,0,1)_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = (1,0,0)_{\text{TF}}$ in the TF.
TF origin is located at centroid of cylinder.
User must set NCOMP=1.

19.9   CYLNDRCAP = Homogeneous, isotropic finite cylinder with hemispherical endcaps.

$\text{SHPAR}_1 = \text{cylinder length}/d$ (*not* including end-caps!) and $\text{SHPAR}_2 = \text{cylinder diameter}/d$, with cylinder axis $= \hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$. The total length along the target axis (including the endcaps) is $(\text{SHPAR}_1+\text{SHPAR}_2)d$.
TF origin is located at centroid of cylinder.
User must set NCOMP=1.

19.10   DSKRCTNGL = Disk on top of a homogeneous rectangular slab

This option causes **DDSCAT** to create a target consisting of a disk of composition 1 resting on top of a rectangular block of composition 2. Materials 1 and 2 are assumed to be homogeneous and isotropic. ddscat.par should set NCOMP to 2 .
The cylindrical disk has thickness $\text{SHPAR}_1 \times d$ in the x-direction, and diameter $\text{SHPAR}_2 \times d$. The rectangular block is assumed to have thickness $\text{SHPAR}_3 \times d$ in the x-direction, length $\text{SHPAR}_4 \times d$ in the y-direction, and length $\text{SHPAR}_5 \times d$ in the z-direction. The lower surface of the cylindrical disk is in the $x = 0$ plane. The upper surface of the slab is also in the $x = 0$ plane.

The Target Frame origin $(0,0,0)$ is located where the symmetry axis of the disk intersects the $x = 0$ plane (the upper surface of the slab, and the lower surface of the disk). In the Target Frame, dipoles representing the rectangular block are located at $(x/d, y/d, z/d) = (j_x + 0.5, j_y + \Delta_y, j_z + \Delta_z)$, where j_x, j_y, and j_z are integers. $\Delta_y = 0$ or 0.5 depending on whether SHPAR_4 is even or odd. $\Delta_z = 0$ or 0.5 depending on whether SHPAR_5 is even or odd.

Dipoles representing the disk are located at
$$x/d = 0.5, 1.5, ..., [\text{int}(\text{SHPAR}_4 + 0.5) - 0.5]$$
As always, the physical size of the target is fixed by specifying the value of the effective radius $a_{\text{eff}} \equiv (3V_{\text{T}}/4\pi)^{1/3}$, where V_{T} is the total volume of solid material in the target. For this geometry, the number of dipoles in the target will be approximately $N = [\text{SHPAR}_1 \times \text{SHPAR}_2 \times \text{SHPAR}_3 + (\pi/4)((\text{SHPAR}_4)^2 \times \text{SHPAR}_5)]$, although the exact number may differ because of the dipoles are required to be located on a rectangular lattice. The dipole spacing d in physical units is determined from the specified value of a_{eff} and the number N of dipoles in the target: $d = (4\pi/3N)^{1/3}a_{\text{eff}}$. This option requires 5 shape parameters:
The pertinent line in ddscat.par should read

```
SHPAR1 SHPAR₂ SHPAR3 SHPAR4 SHPAR₅
```

where
$\text{SHPAR}_1 = [\text{disk thickness (in } \hat{\mathbf{x}}_{\text{TF}} \text{ direction)}]/d$ [material 1]
$\text{SHPAR}_2 = (\text{disk diameter})/d$
$\text{SHPAR}_3 = (\text{brick thickness in } \hat{\mathbf{x}}_{\text{TF}} \text{ direction})/d$ [material 2]
$\text{SHPAR}_4 = (\text{brick thickness in } \hat{\mathbf{y}}_{\text{TF}} \text{ direction})/d$
$\text{SHPAR}_5 = (\text{brick thickness in } \hat{\mathbf{z}}_{\text{TF}} \text{ direction})/d$

The overall size of the target (in terms of numbers of dipoles) is determined by parameters (SHPAR1+SHPAR4), SHPAR_2, and SHPAR_3. The periodicity in the TF y and z directions is determined by parameters SHPAR_4

and SHPAR$_5$.

The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file ddscat.par.

The "computational volume" is determined by (SHPAR$_1$+SHPAR$_4$)×SHPAR$_2$×SHPAR$_3$.

The target axes (in the TF) are set to $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\text{TF}} = (1,0,0)_{\text{TF}}$ – i.e., normal to the "slab" – and $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{\text{TF}} = (0,1,0)_{\text{TF}}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles Θ, Φ, and β (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the slab.

19.11   DW1996TAR = 13 block target used by Draine & Weingartner (1996).

Single, isotropic material. Target geometry was used in study by Draine & Weingartner (1996) of radiative torques on irregular grains. $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are principal axes with largest and second-largest moments of inertia. User must set NCOMP=1. Target size is controlled by shape parameter SHPAR(1) = width of one block in lattice units.

TF origin is located at centroid of target.

19.12   ELLIPSOID = Homogeneous, isotropic ellipsoid.

"Lengths" SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ in the x, y, z directions in the TF:

$$\left(\frac{x_{\text{TF}}}{\text{SHPAR}_1 d}\right)^2 + \left(\frac{y_{\text{TF}}}{\text{SHPAR}_2 d}\right)^2 + \left(\frac{z_{\text{TF}}}{\text{SHPAR}_3 d}\right)^2 = \frac{1}{4} \quad , \tag{33}$$

where d is the interdipole spacing.

The target axes are set to $\hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$.

Target Frame origin = centroid of ellipsoid.

User must set NCOMP=1 on line 9 of ddscat.par.

A **homogeneous, isotropic sphere** is obtained by setting SHPAR$_1$ = SHPAR$_2$ = SHPAR$_3$ = diameter/d.

19.13   ELLIPSO_2 = Two touching, homogeneous, isotropic ellipsoids, with distinct compositions

SHPAR$_1$, SHPAR$_2$, SHPAR$_3$=x-length/d, y-length/d, z-length/d of one ellipsoid. The two ellipsoids have identical shape, size, and orientation, but distinct dielectric functions. The line connecting ellipsoid centers is along the $\hat{\mathbf{x}}_{\text{TF}}$-axis. Target axes $\hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ [along line connecting ellipsoids] and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$.

Target Frame origin = midpoint between ellipsoids (where ellipsoids touch).

User must set NCOMP=2 and provide dielectric function file names for both ellipsoids. Ellipsoids are in order of increasing x_{TF}: first dielectric function is for ellipsoid with center at negative x_{TF}, second dielectric function for ellipsoid with center at positive x_{TF}.

19.14   ELLIPSO_3 = Three touching homogeneous, isotropic ellipsoids of equal size and orientation, but distinct compositions

SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ have same meaning as for ELLIPSO_2. Line connecting ellipsoid centers is parallel to $\hat{\mathbf{x}}_{\text{TF}}$ axis. Target axis $\hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ (along line of ellipsoid centers), and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$.

Target Frame origin = centroid of middle ellipsoid.

User must set NCOMP=3 and provide (isotropic) dielectric functions for first, second, and third ellipsoid.

Sample calculation: The directory examples_exp/ELLIPSOID contains ddscat.par for calculation of scattering by a sphere with refractive index $m = 1.5 + 0.01i$ and $2\pi a/\lambda = 5$, represented by a $N = 110592$ dipole pseudosphere just fitting within a $48 \times 48 \times 48$ computational volume.

19.15   HEX_PRISM = Homogeneous, isotropic hexagonal prism

SHPAR$_1$ = (Length of prism)/d = (distance between hexagonal faces)/d,
SHPAR$_2$ = (distance between opposite vertices of one hexagonal face)/d = 2×hexagon side/d.
SHPAR$_3$ selects one of 6 orientations of the prism in the Target Frame (TF).
Target axis $\hat{\mathbf{a}}_1$ is along the prism axis (i.e., normal to the hexagonal faces), and target axis $\hat{\mathbf{a}}_2$ is normal to one of the rectangular faces. There are 6 options for SHPAR$_3$:
SHPAR$_3$ = 1 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{y}}_{\mathrm{TF}}$;   SHPAR$_3$ = 2 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$;
SHPAR$_3$ = 3 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{y}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$;   SHPAR$_3$ = 4 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{y}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$;
SHPAR$_3$ = 5 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$;   SHPAR$_3$ = 6 for $\hat{\mathbf{a}}_1 \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 \parallel \hat{\mathbf{y}}_{\mathrm{TF}}$
TF origin is located at the centroid of the target.
User must set NCOMP=1.

19.16   LAYRDSLAB = Multilayer rectangular slab

Multilayer rectangular slab with overall x, y, z lengths $a_x =$ SHPAR$_1 \times d$
$a_y =$ SHPAR$_2 \times d$,
$a_z =$ SHPAR$_3 \times d$.
Upper surface is at $x_{\mathrm{TF}} = 0$, lower surface at $x_{\mathrm{TF}} = -$SHPAR$_1 \times d$
SHPAR$_4$ = fraction which is composition 1 (top layer).
SHPAR$_5$ = fraction which is composition 2 (layer below top)
SHPAR$_6$ = fraction which is composition 3 (layer below comp 2)
$1 - ($SHPAR$_4 +$ SHPAR$_5 +$ SHPAR$_6) =$ fraction which is composition 4 (bottom layer).
To create a bilayer slab, just set SHPAR$_5 =$ SHPAR$_6 = 0$
To create a trilayer slab, just set SHPAR$_6 = 0$
User must set NCOMP=2,3, or 4 and provide dielectric function files for each of the two layers. Top dipole layer is at $x_{\mathrm{TF}} = -d/2$. Origin of TF is at center of top surface.

19.17   MLTBLOCKS = Homogeneous target constructed from cubic "blocks"

Number and location of blocks are specified in separate file blocks.par with following structure:
   one line of comments (may be blank)
   PRIN (= 0 or 1 – see below)
   N (= number of blocks)
   B (= width/d of one block)
   x_{TF} y_{TF} z_{TF} (= position of 1st block in units of Bd)
   x_{TF} y_{TF} z_{TF} (= position of 2nd block in units of Bd))
   ...
   x_{TF} y_{TF} z_{TF} (= position of Nth block in units of Bd)
If PRIN=0, then $\hat{\mathbf{a}}_1 = (1, 0, 0)_{\mathrm{TF}}$, $\hat{\mathbf{a}}_2 = (0, 1, 0)_{\mathrm{TF}}$. If PRIN=1, then $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are set to principal axes with largest and second largest moments of inertia, assuming target to be of uniform density. User must set NCOMP=1.

19.18   RCTGLPRSM = Homogeneous, isotropic, rectangular solid

x, y, z lengths/$d =$ SHPAR$_1$, SHPAR$_2$, SHPAR$_3$.
Target axes $\hat{\mathbf{a}}_1 = (1, 0, 0)_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 = (0, 1, 0)_{\mathrm{TF}}$.
TF origin at center of upper surface of solid: target extends from $x_{\mathrm{TF}}/d = -$SHPAR$_1$ to 0,
y_{TF}/d from $-0.5 \times$ SHPAR$_2$ to $+0.5 \times$ SHPAR$_2$
z_{TF}/d from $-0.5 \times$ SHPAR$_3$ to $+0.5 \times$ SHPAR$_3$
User must set NCOMP=1.
    The directory examples_exp/RCTGLPRSM contains ddscat.par for calculation of scattering by a 0.5μm $\times 1\mu$m $\times 1\mu$m Au block, represented by a $32 \times 64 \times 64$ dipole array.

19.19   RCTGLBLK3 = Stack of 3 rectangular blocks, with centers on the $\hat{\mathbf{x}}_{\mathrm{TF}}$ axis.

Each block consists of a distinct material. There are 9 shape parameters:
$\mathtt{SHPAR_1}$ = (upper solid thickness in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)$/d$ [material 1]
$\mathtt{SHPAR_2}$ = (upper solid width in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction)$/d$
$\mathtt{SHPAR_3}$ = (upper solid width in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction)$/d$
$\mathtt{SHPAR_4}$ = (middle solid thickness in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)$/d$ [material 2]
$\mathtt{SHPAR_5}$ = (middle solid width in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction)$/d$
$\mathtt{SHPAR_6}$ = (middle solid width in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction)$/d$
$\mathtt{SHPAR_7}$ = (lower solid thickness in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)$/d$ [material 3]
$\mathtt{SHPAR_8}$ = (lower solid width in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction)$/d$
$\mathtt{SHPAR_9}$ = (lower solid width in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction)$/d$
TF origin is at center of top surface of material 1.

19.20   SLAB_HOLE = Rectangular slab with a cylindrical hole.

The target consists of a rectangular block with a cylindrical hole with the axis passing through the centroid and aligned with the $\hat{\mathbf{x}}_{\mathrm{TF}}$ axis. The block dimensions are $a \times b \times c$. The cylindrical hole has radius r. The pertinent line in `ddscat.par` should read
$\mathtt{SHPAR_1}$ $\mathtt{SHPAR_2}$ $\mathtt{SHPAR_3}$ $\mathtt{SHPAR_4}$
where
$\mathtt{SHPAR_1} = a/d$ (d is the interdipole spacing)
$\mathtt{SHPAR_2} = b/a$
$\mathtt{SHPAR_3} = c/a$
$\mathtt{SHPAR_4} = r/a$
Ideally, $\mathtt{SHPAR_1}$, $\mathtt{SHPAR_2}{\times}\mathtt{SHPAR_1}$, $\mathtt{SHPAR_3}{\times}\mathtt{SHPAR_1}$ will be integers (so that the cubic lattice can accurately approximate the desired target geometry), and $\mathtt{SHPAR_4}{\times}\mathtt{SHPAR_1}$ will be large enough for the circular cross section to be well-approximated.
The TF origin is at the center of the top surface (the top surface lies in the $\hat{\mathbf{y}}_{\mathrm{TF}} - \hat{\mathbf{z}}_{\mathrm{TF}}$ plane, and extends from $y_{\mathrm{TF}} = -b/2$ to $+b/2$, and $z_{\mathrm{TF}} = -c/2$ to $+c/2$). The cylindrical hole axis runs from $(x_{\mathrm{TF}} = 0, y_{\mathrm{TF}} = 0, z_{\mathrm{TF}} = 0)$ to $(x_{\mathrm{TF}} = -a, y_{\mathrm{TF}} = 0, z_{\mathrm{TF}} = 0)$.

19.21   SPHERES_N = Multisphere target = union of N spheres of single isotropic material

Spheres may overlap if desired. The relative locations and sizes of these spheres are defined in an external file, whose name (enclosed in single quotes) is passed through `ddscat.par`. The length of the file name should not exceed 80 characters. The pertinent line in `ddscat.par` should read
$\mathtt{SHPAR_1}$ $\mathtt{SHPAR_2}$ *'filename'* (quotes must be used)
where $\mathtt{SHPAR_1}$ = target diameter in x direction (in Target Frame) in units of d
$\mathtt{SHPAR_2}$= 0 to have $a_1 = (1, 0, 0)_{\mathrm{TF}}$, $a_2 = (0, 1, 0)_{\mathrm{TF}}$.
$\mathtt{SHPAR_2}$= 1 to use principal axes of moment of inertia tensor for a_1 (largest I) and a_2 (intermediate I).
filename is the name of the file specifying the locations and relative sizes of the spheres.
The overall size of the multisphere target (in terms of numbers of dipoles) is determined by parameter $\mathtt{SHPAR_1}$, which is the extent of the multisphere target in the x-direction, in units of the lattice spacing d. The file '*filename*' should have the following structure:

N (= number of spheres)
line of comments (may be blank)
line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
x_1 y_1 z_1 a_1 (arb. units)

$x_2\ y_2\ z_2\ a_2$ (arb. units)

...

$x_N\ y_N\ z_N\ a_N$ (arb. units)

where x_j, y_j, z_j are the coordinates (in the TF) of the center of sphere j, and a_j is the radius of sphere j. Note that x_j, y_j, z_j, a_j $(j = 1, ..., N)$ establish only the *shape* of the $N-$sphere target. For instance, a target consisting of two touching spheres with the line between centers parallel to the x axis could equally well be described by lines 6 and 7 being

    0 0 0 0.5

    1 0 0 0.5

or

    0 0 0 1

    2 0 0 1

The actual size (in physical units) is set by the value of a_{eff} specified in `ddscat.par`, where, as always, $a_{\mathrm{eff}} \equiv (3V/4\pi)^{1/3}$, where V is the total volume of material in the target.

Target axes $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are set to be principal axes of moment of inertia tensor (for uniform density), where $\hat{\mathbf{a}}_1$ corresponds to the largest eigenvalue, and $\hat{\mathbf{a}}_2$ to the intermediate eigenvalue.

The TF origin is taken to be located at the volume-weighted centroid.

User must set `NCOMP=1`.

19.22 SPHROID_2 = Two touching homogeneous, isotropic spheroids, with distinct compositions

First spheroid has length SHPAR_1 along symmetry axis, diameter SHPAR_2 perpendicular to symmetry axis. Second spheroid has length SHPAR_3 along symmetry axis, diameter SHPAR_4 perpendicular to symmetry axis. Contact point is on line connecting centroids. Line connecting centroids is in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction. Symmetry axis of first spheroid is in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction. Symmetry axis of second spheroid is in direction $\hat{\mathbf{y}}_{\mathrm{TF}} \cos(\mathrm{SHPAR}_5) + \hat{\mathbf{z}}_{\mathrm{TF}} \sin(\mathrm{SHPAR}_5)$, and SHPAR_5 is in degrees. If $\mathrm{SHPAR}_6 = 0.$, then target axes $\hat{\mathbf{a}}_1 = (1, 0, 0)_{\mathrm{TF}}$, $\hat{\mathbf{a}}_2 = (0, 1, 0)_{\mathrm{TF}}$. If $\mathrm{SHPAR}_6 = 1.$, then axes $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are set to principal axes with largest and 2nd largest moments of inertia assuming spheroids to be of uniform density.

Origin of TF is located between spheroids, at point of contact.

User must set `NCOMP=2` and provide dielectric function files for each spheroid.

19.23 SPH_ANI_N = Multisphere target consisting of the union of N spheres of various materials, possibly anisotropic

Spheres may NOT overlap. The relative locations and sizes of these spheres are defined in an external file, whose name (enclosed in single quotes) is passed through `ddscat.par`. The length of the file name should not exceed 80 characters. Target axes $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are set to be principal axes of moment of inertia tensor (for uniform density), where $\hat{\mathbf{a}}_1$ corresponds to the largest eigenvalue, and $\hat{\mathbf{a}}_2$ to the intermediate eigenvalue.

The TF origin is taken to be located at the volume-weighted centroid.

The pertinent line in `ddscat.par` should read

SHPAR_1 SHPAR_2 *'filename'* (quotes must be used)

where SHPAR_1 = target diameter in x direction (in Target Frame) in units of d

$\mathrm{SHPAR}_2 = 0$ to have $a_1 = (1, 0, 0)_{\mathrm{TF}}$, $a_2 = (0, 1, 0)_{\mathrm{TF}}$ in Target Frame.

$\mathrm{SHPAR}_2 = 1$ to use principal axes of moment of inertia tensor for a_1 (largest I) and a_2 (intermediate I).

filename is the name of the file specifying the locations and relative sizes of the spheres.

The overall size of the multisphere target (in terms of numbers of dipoles) is determined by parameter SHPAR_1, which is the extent of the multisphere target in the x-direction, in units of the lattice spacing d. The file *'filename'* should have the following structure:

    N (= number of spheres)

    line of comments (may be blank)

line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
x_1 y_1 z_1 r_1 Cx_1 Cy_1 Cz_1 $\Theta_{\mathrm{DF},1}$ $\Phi_{\mathrm{DF},1}$ $\beta_{\mathrm{DF},1}$
x_2 y_2 z_2 r_2 Cx_2 Cy_2 Cz_2 $\Theta_{\mathrm{DF},2}$ $\Phi_{\mathrm{DF},2}$ $\beta_{\mathrm{DF},2}$
...
x_N y_N z_N r_N Cx_N Cy_N Cz_N $\Theta_{\mathrm{DF},N}$ $\Phi_{\mathrm{DF},N}$ $\beta_{\mathrm{DF},N}$

where x_j, y_j, z_j are the coordinates of the center, and r_j is the radius of sphere j (arbitrary units), Cx_j, Cy_j, Cz_j are integers specifying the "composition" of sphere j in the x, y, z directions in the "Dielectric Frame" (see §26) of sphere j, and $\Theta_{\mathrm{DF},j}$ $\Phi_{\mathrm{DF},j}$ $\beta_{\mathrm{DF},j}$ are angles (in radians) specifying orientation of the dielectric frame (DF) of sphere j relative to the Target Frame. Note that x_j, y_j, z_j, r_j ($j = 1, ..., N$) establish only the *shape* of the $N-$sphere target, just as for target option NSPHER. The actual size (in physical units) is set by the value of a_{eff} specified in ddscat.par, where, as always, $a_{\mathrm{eff}} \equiv (3V/4\pi)^{1/3}$, where V is the volume of material in the target.
User must set NCOMP to the number of different dielectric functions being invoked (i.e., the range of $\{Cx_j, Cy_j, Cz_j\}$.

Note that while the spheres can be anisotropic and of differing composition, they can of course also be isotropic and of a single composition, in which case the relevant lines in the file '*filename*' would be simply

N (= number of spheres)
line of comments (may be blank)
line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
line of comments (may be blank) [N.B.: changed from v7.0.7]
x_1 y_1 z_1 r_1 1 1 1 0 0 0
x_2 y_2 z_2 r_2 1 1 1 0 0 0
...
x_N y_N z_N r_N 1 1 1 0 0 0

Subdirectory examples_exp/SPH_ANI_N contains ddscat.par for calculating scattering by a random aggregate of 64 spheres [aggregated according following the "BAM2" aggregation process described by Shen, Draine & Johnson (2008)]. 32 of the spheres are assumed to consist of "astrosilicate", and 32 of crystalline graphite, with random orientations for each of the 32 graphite spheres. Each sphere is assumed to have a radius 0.050μm. The entire cluster is represented by $N = 7947$ dipoles, or about 124 dipoles per sphere. Scattering and absorption are calculated for $\lambda = 0.55\mu$m.

19.24   TETRAHDRN = Homogeneous, isotropic tetrahedron

SHPAR$_1$=length/d of one edge. Orientation: one face parallel to $\hat{\mathbf{y}}_{\mathrm{TF}}, \hat{\mathbf{z}}_{\mathrm{TF}}$ plane, opposite "vertex" is in $+\hat{\mathbf{x}}_{\mathrm{TF}}$ direction, and one edge is parallel to $\hat{\mathbf{z}}_{\mathrm{TF}}$. Target axes $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ [emerging from one vertex] and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$ [emerging from an edge] in the TF. User must set NCOMP=1.

19.25   TRNGLPRSM = Triangular prism of homogeneous, isotropic material

SHPAR$_1$, SHPAR$_2$, SHPAR$_3$, SHPAR$_4$ = $a/d, b/a, c/a, L/a$
The triangular cross section has sides of width a, b, c. L is the length of the prism. d is the lattice spacing. The triangular cross-section has interior angles α, β, γ (opposite sides a, b, c) given by $\cos\alpha = (b^2 + c^2 - a^2)/2bc$, $\cos\beta = (a^2 + c^2 - b^2)/2ac$, $\cos\gamma = (a^2 + b^2 - c^2)/2ab$. In the Target Frame, the prism axis is in the $\hat{\mathbf{x}}$ direction, the normal to the rectangular face of width a is (0,1,0), the normal to the rectangular face of width b is $(0, -\cos\gamma, \sin\gamma)$, and the normal to the rectangular face of width c is $(0, -\cos\gamma, -\sin\gamma)$.

19.26   UNIAXICYL = Homogeneous finite cylinder with uniaxial anisotropic dielectric tensor

SHPAR_1, SHPAR_2 have same meaning as for CYLINDER1. Cylinder axis $= \hat{\mathbf{a}}_1 = (1, 0, 0)_{\text{TF}}$, $\hat{\mathbf{a}}_2 = (0, 1, 0)_{\text{TF}}$. It is assumed that the dielectric tensor ϵ is diagonal in the TF, with $\epsilon_{yy} = \epsilon_{zz}$. User must set NCOMP=2. Dielectric function 1 is for $\mathbf{E} \parallel \hat{\mathbf{a}}_1$ (cylinder axis), dielectric function 2 is for $\mathbf{E} \perp \hat{\mathbf{a}}_1$.

19.27   Modifying Existing Routines or Writing New Ones

The user should be able to easily modify these routines, or write new routines, to generate targets with other geometries. The user should first examine the routine `target.f90` and modify it to call any new target generation routines desired. Alternatively, targets may be generated separately, and the target description (locations of dipoles and "composition" corresponding to x,y,z dielectric properties at each dipole site) read in from a file by invoking the option FROM_FILE in ddscat.f90.

Note that it will also be necessary to modify the routine `reapar.f90` so that it will accept whatever new target option is added to the target generation code .

19.28   Testing Target Generation using CALLTARGET

It is often desirable to be able to run the target generation routines without running the entire **DDSCAT** code. We have therefore provided a program CALLTARGET which allows the user to generate targets interactively; to create this executable just type[9]

    make calltarget.

The program `calltarget` is to be run interactively; the prompts are self-explanatory. You may need to edit the code to change the device number IDVOUT as for DDSCAT (see §6.7 above).

After running, `calltarget` will leave behind an ASCII file `target.out` which is a list of the occupied lattice sites in the last target generated. The format of `target.out` is the same as the format of the `shape.dat` files read if option FROM_FILE is used (see above). Therefore you can simply

    mv target.out shape.dat

and then use DDSCAT with the option FROM_FILE (or option ANIFRMFIL in the case of anisotropic target materials with arbitrary orientation relative to the Target Frame) in order to input a target shape generated by CALLTARGET.

Note that CALLTARGET – designed to generate finite targets – can be used with some of the "PBC" target options (see §20 below) to generate a list of dipoles in the TUC. At the moment, CALLTARGET has support for target options BISLINPBC, DSKBLYPBC, and DSKRCTPBC.

20   Target Generation: Periodic Targets

A periodic target consists of a "Target Unit Cell" (TUC) which is then repeated in either the $\hat{\mathbf{y}}_{\text{TF}}$ direction, the $\hat{\mathbf{z}}_{\text{TF}}$ direction, or both. Please see Draine & Flatau (2008) for illustration of how periodic targets are assembled out of TUCs, and how the scattering from these targets in different diffraction orders M or (M, N) is constrained by the periodicity.

The following options are included in **DDSCAT**:

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[9] Non-Linux sites: The source code for CALLTARGET is in the file CALLTARGET.f90. You must compile and link CALLTARGET.f90, ddcommon.f90, dsyevj3.f90, errmsg.f90, gasdev.f90, p_lm.f90, prinaxis.f90, ran3.f90, reashp.f90, sizer.f90, tar2el.f90, tar2sp.f90, tar3el.f90, taranirec.f90, tarblocks.f90, tarcel.f90, tarcyl.f90, tarcylcap.f90, tarell.f90, target.f90, targspher.f90, tarhex.f90, tarnas.f90, tarnsp.f90, tarpbxn.f90, tarprsm.f90, tarrctblk3.f90, tarrecrec.f90, tarslblin.f90, tartet.f90, and wrimsg.f90.

20.1   FRMFILPBC = periodic target with TUC geometry and composition input from a file

The TUC can have arbitrary geometry and inhomogeneous composition, and is assumed to repeat periodically in either 1-d (y or z) or 2-d (y and z).

The pertinent line in `ddscat.par` should read

SHPAR$_1$ SHPAR$_2$ *'filename'* (quotes must be used)

SHPAR$_1$ = P_y/d (P_y = periodicity in $\hat{\mathbf{y}}_{\rm TF}$ direction)

SHPAR$_2$ = P_z/d (P_z = periodicity in $\hat{\mathbf{z}}_{\rm TF}$ direction)

filename is the name of the file specifying the locations of the dipoles, and the "composition" at each dipole location. The composition can be anisotropic, but the dielectric tensor must be diagonal in the TF. The shape and composition of the TUC are provided *exactly* as for target option FROM_FILE – see §19.1

If SHPAR$_1$ = 0 then the target does *not* repeat in the $\hat{\mathbf{y}}_{\rm TF}$ direction.

If SHPAR$_2$ = 0 then the target does *not* repeat in the $\hat{\mathbf{z}}_{\rm TF}$ direction.

20.2   ANIFILPBC = general anisotropic periodic target with TUC geometry and composition input from a file

The TUC can have arbitrary geometry and inhomogeneous composition, and is assumed to repeat periodically in either 1-d (y or z) or 2-d (y and z).

The pertinent line in `ddscat.par` should read

SHPAR$_1$ SHPAR$_2$ *'filename'* (quotes must be used)

SHPAR$_1$ = P_y/d (P_y = periodicity in $\hat{\mathbf{y}}_{\rm TF}$ direction)

SHPAR$_2$ = P_z/d (P_z = periodicity in $\hat{\mathbf{z}}_{\rm TF}$ direction)

filename is the name of the file specifying the locations of the dipoles, and the "composition" at each dipole location. The composition can be anisotropic, and the dielectric tensor need not be diagonal in the TF. The shape and composition of the TUC are provided *exactly* as for target option ANIFRMFIL – see §19.2

If SHPAR$_1$ = 0 then the target does *not* repeat in the $\hat{\mathbf{y}}_{\rm TF}$ direction.

If SHPAR$_2$ = 0 then the target does *not* repeat in the $\hat{\mathbf{z}}_{\rm TF}$ direction.

20.3   BISLINPBC = Bi-Layer Slab with Parallel Lines

The target consists of a bi-layer slab, on top of which there is a "line" with rectangular cross-section.

The "line" on top is composed of material 1, has height X_1 (in the $\hat{\mathbf{x}}_{\rm TF}$ direction), width Y_1 (in the $\hat{\mathbf{y}}_{\rm TF}$ direction), and is infinite in extent in the $\hat{\mathbf{z}}_{\rm TF}$ direction.

The bilayer slab has width Y_2 (in the $\hat{\mathbf{y}}_{\rm TF}$ direction). It is consists of a layer of thickness X_2 of material 2, on top of a layer of material 3 with thickness X_3.

SHPAR$_1$ = X_1/d (X_1 = thickness of line)

SHPAR$_2$ = Y_1/d (Y_1 = width of line)

SHPAR$_3$ = X_2/d (X_2 = thickness of upper layer of slab)

SHPAR$_4$ = X_3/d (X_3 = thickness of lower layer of slab)

SHPAR$_5$ = Y_2/d (Y_2 = width of slab)

SHPAR$_6$ = P_y/d (P_y = periodicity in $\hat{\mathbf{y}}_{\rm TF}$ direction).

If SHPAR$_6$ = 0, the target is NOT periodic in the $\hat{\mathbf{y}}_{\rm TF}$ direction, consisting of a single column, infinite in the $\hat{\mathbf{z}}_{\rm TF}$ direction.

20.4   CYLNDRPBC = Target consisting of homogeneous cylinder repeated in target y and/or z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of an infinite array of cylinders. The individual cylinders are assumed to be homogeneous and isotropic, just as for option RCTNGL (see §19.18).

Let us refer to a single cylinder as the Target Unit Cell (TUC). The TUC is then repeated in the target y- and/or z-directions, with periodicities PYD$\times d$ and PZD$\times d$, where d is the lattice spacing. To repeat in only one direction, set either PYD or PZD to zero.

This option requires 5 shape parameters: The pertinent line in ddscat.par should read

SHPAR$_1$ SHPAR$_2$ SHPAR$_3$ SHPAR$_4$ SHPAR$_5$

where SHPAR$_1$, SHPAR$_2$, SHPAR$_3$, SHPAR$_4$, SHPAR$_5$ are numbers:
SHPAR$_1$ = cylinder length along axis (in units of d) in units of d
SHPAR$_2$ = cylinder diameter/d
SHPAR$_3$ = 1 for cylinder axis $\parallel \hat{\mathbf{x}}_{\mathrm{TF}}$
     = 2 for cylinder axis $\parallel \hat{\mathbf{y}}_{\mathrm{TF}}$
     = 3 for cylinder axis $\parallel \hat{\mathbf{z}}_{\mathrm{TF}}$ (see below)
SHPAR$_4$ = PYD = periodicity/d in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction (= 0 to suppress repetition)
SHPAR$_5$ = PZD = periodicity/d in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction (= 0 to suppress repetition)

The overall size of the TUC (in terms of numbers of dipoles) is determined by parameters SHPAR1 and SHPAR$_2$. The orientation of a single cylinder is determined by SHPAR$_3$. The periodicity in the TF y and z directions is determined by parameters SHPAR$_4$ and SHPAR$_5$.

The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file ddscat.par, with the usual correspondence $d = (4\pi/3N)^{1/3}a_{\mathrm{eff}}$, where N is the number of dipoles in the TUC.

With target option CYLNDRPBC, the target becomes a periodic structure, of infinite extent.

- If NPY > 0 and NPZ > 0, then the target cylindrical TUC repeats in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction, with periodicity NPY $\times d$.

- If NPY $= 0$ and NPZ > 0 then the target cylindrical TUC repeats in the $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction, with periodicity NPZ $\times d$.

- If NPY > 0 and NPZ > 0 then the target cylindrical TUC repeats in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction, with periodicity NPY $\times d$, and in the $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction, with periodicity NPZ $\times d$.

Target Orientation: The target axes (in the TF) are set to $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$. Note that $\hat{\mathbf{a}}_1$ does **not** necessarily coincide with the cylinder axis: individual cylinders may have any of 3 different orientations in the TF.

Example 1: One could construct a single infinite cylinder with the following two lines in ddscat.par:

100 1 100
1.0   100.49   2   1.0   0.

The first line ensures that there will be enough memory allocated to generate the target. The TUC would be a thin circular "slice" containing just one layer of dipoles. The diameter of the circular slice would be about 100.49d in extent, so the TUC would have approximately $(\pi/4) \times (100.49)^2 = 7931$ dipoles (7932 in the actual realization) within a $100 \times 1 \times 100$ "extended target volume". The TUC would be oriented with the cylinder axis in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction (SHPAR3=2) and the structure would repeat in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction with a period of $1.0 \times d$. SHPAR$_5$=0 means that there will be no repetition in the z direction. As noted above, the "target axis" vector $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\mathrm{TF}}$.

Note that SHPAR$_1$, SHPAR$_2$, SHPAR$_4$, and SHPAR$_5$ need not be integers. However, SHPAR$_3$, determining the orientation of the cylinders in the TF, can only take on the values 1,2,3.

The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the periodic structure.

Sample calculation: The subdirectory `examples_exp/CYLNDRPBC` contains `ddscat.par` for calculating scattering by an infinite cylinder with $m = 1.33 + 0.01i$ for $2\pi R/\lambda = 10$, where R is the cylinder radius.

20.5 DSKBLYPBC = Target consisting of a periodic array of disks on top of a two-layer rectangular slabs.

This option causes **DDSCAT** to create a target consisting of a periodic or biperiodic array of Target Unit Cells (TUCs), each TUC consisting of a disk of composition 1 resting on top of a rectangular block consisting of two layers: composition 2 on top and composition 3 below. Materials 1, 2, and 3 are assumed to be homogeneous and isotropic.
This option requires 8 shape parameters:
The pertinent line in `ddscat.par` should read

SHPAR_1 SHPAR_2 SHPAR_3 SHPAR_4 SHPAR_5 SHPAR_6 SHPAR_7 SHPAR_8

where
SHPAR_1 = disk thickness in x direction (in Target Frame) in units of d
SHPAR_2 = (disk diameter)/d
SHPAR_3 = (upper slab thickness)/d
SHPAR_4 = (lower slab thickness)/d
SHPAR_5 = (slab extent in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction)/d
SHPAR_6 = (slab extent in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction)/d
SHPAR_7 = period in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction/d
SHPAR_8 = period in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction/d

The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file `ddscat.par`.

The "computational volume" is determined by
$(\mathrm{SHPAR}_1 + \mathrm{SHPAR}_3 + \mathrm{SHPAR}_4) \times \mathrm{SHPAR}_5 \times \mathrm{SHPAR}_6$.

The lower surface of the cylindrical disk is in the $x = 0$ plane. The upper surface of the slab is also in the $x = 0$ plane. It is required that $\mathrm{SHPAR}_2 \leq \min(\mathrm{SHPAR}_4, \mathrm{SHPAR}_5)$.

The Target Frame origin (0,0,0) is located where the symmetry axis of the disk intersects the $x = 0$ plane (the upper surface of the slab, and the lower surface of the disk).
In the Target Frame, dipoles representing the disk are located at
$\qquad x/d = 0.5, 1.5, ..., [\mathrm{int}(\mathrm{SHPAR}_1 + 0.5) - 0.5]$
and at (y, z) values
$\qquad y/d = \pm 0.5, \pm 1.5, ...$ and
$\qquad z/d = \pm 0.5, \pm 1.5, ...$ satisfying
$\qquad (y^2 + z^2) \leq (\mathrm{SHPAR}_2/2)^2 d^2$.
Dipoles representing the rectangular slab are located at $(x/d, y/d, z/d) = (j_x + 0.5, j_y + \Delta y, j_z + \Delta z)$, where j_x, j_y, and j_z are integers. $\Delta y = 0$ or 0.5 depending on whether SHPAR_5 is even or odd. $\Delta z = 0$ or 0.5 depending on whether SHPAR_6 is even or odd.

The TUC is repeated in the target y- and z-directions, with periodicities $\mathrm{SHPAR}_7 \times d$ and $\mathrm{SHPAR}_8 \times d$.
As always, the physical size of the target is fixed by specifying the value of the effective radius $a_{\mathrm{eff}} \equiv (3V_{\mathrm{TUC}}/4\pi)^{1/3}$, where V_{TUC} is the total volume of solid material in one TUC. For this geometry,

the number of dipoles in the target will be approximately

$$N = (\pi/4) \times \mathtt{SHPAR}_1 \times (\mathtt{SHPAR}_2)^2 + [\mathtt{SHPAR}_3 + \mathtt{SHPAR}_4] \times \mathtt{SHPAR}_5 \times \mathtt{SHPAR}_6$$

although the exact number may differ because of the dipoles are required to be located on a rectangular lattice. The dipole spacing d in physical units is determined from the specified value of a_{eff} and the number N of dipoles in the target: $d = (4\pi/3N)^{1/3}a_{\mathrm{eff}}$.

The target axes (in the TF) are set to $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\mathrm{TF}} = (1,0,0)_{\mathrm{TF}}$ – i.e., normal to the "slab" – and $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{\mathrm{TF}} = (0,1,0)_{\mathrm{TF}}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the slab.

20.6   DSKRCTPBC = Target consisting of homogeneous rectangular brick plus a disk, extended in target y and z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of a biperiodic array of Target Unit Cells. Each Target Unit Cell (TUC) consists of a disk of composition 1 resting on top of a rectangular block of composition 2. Materials 1 and 2 are assumed to be homogeneous and isotropic.

The cylindrical disk has thickness $\mathtt{SHPAR}_1 \times d$ in the x-direction, and diameter $\mathtt{SHPAR}_2 \times d$. The rectangular block is assumed to have thickness $\mathtt{SHPAR}_3 \times d$ in the x-direction, extent $\mathtt{SHPAR}_4 \times d$ in the y-direction, and extent $\mathtt{SHPAR}_5 \times d$ in the z-direction. The lower surface of the cylindrical disk is in the $x = 0$ plane. The upper surface of the slab is also in the $x = 0$ plane. It is required that $\mathtt{SHPAR}_2 \leq \min(\mathtt{SHPAR4}, \mathtt{SHPAR}_5)$.

The Target Frame origin (0,0,0) is located where the symmetry axis of the disk intersects the $x = 0$ plane (the upper surface of the slab, and the lower surface of the disk). In the Target Frame, dipoles representing the rectangular block are located at $(x/d, y/d, z/d) = (j_x + 0.5, j_y + \Delta y, j_z + \Delta z)$, where j_x, j_y, and j_z are integers. $\Delta y = 0$ or 0.5 depending on whether $\mathtt{SHPAR}_4$ is even or odd. $\Delta z = 0$ or 0.5 depending on whether $\mathtt{SHPAR}_5$ is even or odd.

     $j_x = -[\mathrm{int}(\mathtt{SHPAR}_3 + 0.5)], ..., -1.$
     $j_y = -[\mathrm{int}(0.5 \times \mathtt{SHPAR}_4 - 0.5) + 1], ... , j_z = -[\mathrm{int}(\mathtt{SHPAR}_4 + 0.5) - 0.5]$
     $y/d = -[\mathrm{int}(0.5 \times \mathtt{SHPAR}_4 + 0.5) - 0.5], ..., [\mathrm{int}(0.5 \times \mathtt{SHPAR}_4 + 0.5) - 0.5]$
     $z/d = -[\mathrm{int}(0.5 \times \mathtt{SHPAR}_5 + 0.5) - 0.5], ..., [\mathrm{int}(0.5 \times \mathtt{SHPAR}_5 + 0.5) - 0.5]$

where $\mathrm{int}(x)$ is the greatest integer less than or equal to x. Dipoles representing the disk are located at

     $x/d = 0.5, 1.5, ..., [\mathrm{int}(\mathtt{SHPAR}_4 + 0.5) - 0.5]$

and at (y, z) values

     $y/d = \pm 0.5, \pm 1.5, ...$ and
     $z/d = \pm 0.5, \pm 1.5, ...$ satisfying
     $(y^2 + z^2) \leq (\mathtt{SHPAR}_5/2)^2 d^2$.

The TUC is repeated in the target y- and z-directions, with periodicities $\mathtt{SHPAR}_6 \times d$ and $\mathtt{SHPAR}_7 \times d$. As always, the physical size of the target is fixed by specifying the value of the effective radius $a_{\mathrm{eff}} \equiv (3V_{\mathrm{TUC}}/4\pi)^{1/3}$, where V_{TUC} is the total volume of solid material in one TUC. For this geometry, the number of dipoles in the target will be approximately $N = [\mathtt{SHPAR}_1 \times \mathtt{SHPAR}_2 \times \mathtt{SHPAR}_3 + (\pi/4)((\mathtt{SHPAR}_4)^2 \times \mathtt{SHPAR}_5)]$, although the exact number may differ because of the dipoles are required to be located on a rectangular lattice. The dipole spacing d in physical units is determined from the specified value of a_{eff} and the number N of dipoles in the target: $d = (4\pi/3N)^{1/3}a_{\mathrm{eff}}$. This option requires 7 shape parameters:

The pertinent line in `ddscat.par` should read

$\mathtt{SHPAR}_1$ $\mathtt{SHPAR}_2$ $\mathtt{SHPAR}_3$ $\mathtt{SHPAR}_4$ $\mathtt{SHPAR}_5$ $\mathtt{SHPAR}_6$ $\mathtt{SHPAR}_7$

where
$\mathtt{SHPAR}_1$ = [disk thickness (in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)]$/d$ [material 1]
$\mathtt{SHPAR}_2$ = (disk diameter)$/d$
$\mathtt{SHPAR}_3$ = (brick thickness in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)$/d$ [material 2]

SHPAR$_4$ = (brick length in $\hat{\mathbf{y}}_{TF}$ direction)/d
SHPAR$_5$ = (brick length in $\hat{\mathbf{z}}_{TF}$ direction)/d
SHPAR$_6$ = periodicity in $\hat{\mathbf{y}}_{TF}$ direction/d
SHPAR$_7$ = periodicity in $\hat{\mathbf{z}}_{TF}$ direction/d

The overall extent of the TUC (the "computational volume") is determined by parameters (SHPAR1+SHPAR4),
max(SHPAR$_2$,SHPAR$_4$, and max(SHPAR$_3$,SHPAR$_5$). The periodicity in the TF y and z directions is
determined by parameters SHPAR$_6$ and SHPAR$_7$.
The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the
file ddscat.par.

The target is a periodic structure, of infinite extent in the target y- and z- directions. The target axes
(in the TF) are set to $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{TF} = (1,0,0)_{TF}$ – i.e., normal to the "slab" – and $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{TF} = (0,1,0)_{TF}$.
The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual
orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident
normal to the slab.

Sample calculation: Subdirectory examples_exp/DSKRCTPBC contains ddscat.par for cal-
culating scattering by a 0.0500μm thick Si$_3$N$_4$ slab with a periodic array of Au disks, with period-
icity 0.0800μm, disk diameter 0.0500μm, and disk height 0.0400μm, for light with wavelength $\lambda = 0.5320\mu$m. The radiation is incident at an angle of $60°$ relative to the surface normal.

20.7 HEXGONPBC = Target consisting of homogeneous hexagonal prism re-peated in target y and/or z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of a periodic or biperiodic array of hexagonal
prisms. The individual prisms are assumed to be homogeneous and isotropic, just as for option RCTNGL
(see §19.18).
Let us refer to a single hexagonal prism as the Target Unit Cell (TUC). The TUC is then repeated in
the target y- and z-directions, with periodicities PYD$\times d$ and PZD$\times d$, where d is the lattice spacing. To
repeat in only one direction, set either PYD or PZD to zero.
This option requires 5 shape parameters: The pertinent line in ddscat.par should read

SHPAR$_1$ SHPAR$_2$ SHPAR3 SHPAR4 SHPAR$_5$

whereSHPAR$_1$, SHPAR$_2$, SHPAR$_3$, SHPAR$_4$, SHPAR$_5$ are numbers:
SHPAR$_1$ = prism length along prism axis (in units of d) in units of d
SHPAR$_2$ = 2×length of one hexagonal side/d
SHPAR$_3$ = 1,2,3,4,5 or 6 to specify prism orientation in the TF (see below)
SHPAR$_4$ = PYD = periodicity in TF y direction/d
SHPAR$_5$ = PZD = periodicity in TF z direction/d

The overall size of the TUC (in terms of numbers of dipoles) is determined by parameters SHPAR$_1$,
SHPAR$_2$, and SHPAR$_3$. The periodicity in the TF y and z directions is determined by parameters SHPAR$_4$
and SHPAR$_5$.
The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in
the file ddscat.par, with the usual correspondence $d = (4\pi/3N)^{1/3}a_{\text{eff}}$, where N is the number of
dipoles in the TUC.

With target option HEXGONPBC, the target becomes a periodic structure, of infinite extent in the
target y- and z- directions (assuming both NPY and NPZ are nonzero).

The target axes (in the TF) are set to $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{TF} = (1,0,0)_{TF}$ – i.e., normal to the "slab" – and
$\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{TF} = (0,1,0)_{TF}$.

The individual hexagons may have any of 6 different orientations relative to the slab: Let unit vectors
$\hat{\mathbf{h}}$ be $\parallel$ to the axis of the hexagonal prism, and let unit vector $\hat{\mathbf{f}}$ be normal to one of the rectangular faces
of the hexagonal prism. Then
SHPAR3=1 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{x}}_{TF}$, $\hat{\mathbf{f}} \parallel \hat{\mathbf{y}}_{TF}$

SHPAR3=2 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{x}}_{\mathrm{TF}}, \hat{\mathbf{f}} \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$
SHPAR3=3 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{y}}_{\mathrm{TF}}, \hat{\mathbf{f}} \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$
SHPAR3=4 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{y}}_{\mathrm{TF}}, \hat{\mathbf{f}} \parallel \hat{\mathbf{z}}_{\mathrm{TF}}$
SHPAR3=5 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{z}}_{\mathrm{TF}}, \hat{\mathbf{f}} \parallel \hat{\mathbf{x}}_{\mathrm{TF}}$
SHPAR3=6 for $\hat{\mathbf{h}} \parallel \hat{\mathbf{z}}_{\mathrm{TF}}, \hat{\mathbf{f}} \parallel \hat{\mathbf{y}}_{\mathrm{TF}}$

For example, one could construct a single infinite hexagonal column with the following line in ddscat.par:

2.0 100.0 3 2.0 0.

The TUC would be a thin hexagonal "slice" containing two layers of dipoles. The edges of the hexagon would be about $50d$ in extent, so the TUC would have approximately $(3\sqrt{3}/2) \times 50^2 \times 2 = 12990$ dipoles (13024 in the actual realization) within a $90 \times 2 \times 100$ "extended target volume". The TUC would be oriented with the hexagonal axis in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction, with $\hat{\mathbf{z}}_{\mathrm{TF}}$ normal to a rectangular faces of the prism (SHPAR3=3), and the structure would repeat in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction with a period of $2 \times d$ (SHPAR4=2.0). SHPAR5=0 means that there will be no repetition in the $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction.

Note that SHPAR$_1$, SHPAR$_2$, SHPAR$_4$, and SHPAR$_5$ need not be integers. However, SHPAR$_5$, determining the orientation of the prisms in the TF, can only take on the values 1,2,3,4,5,6.

Important Note: For technical reasons, PYD and PZD must not be smaller than the "extended" target extent in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ and $\hat{\mathbf{z}}_{\mathrm{TF}}$ directions. When the GPFAFT option is used for the 3-dimensional FFT calculations, the extended target volume always has dimensions/$d = 2^a 3^b 5^c$, where a, b, and c are nonnegative integers, with (dimension/d) ≥ 1).

The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the periodic structure.

20.8   LYRSLBPBC = Target consisting of layered slab, extended in target y and z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of an array of multilayer bricks, layered in the $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction. The size of each brick in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ and $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction is specified. Up to 4 layers are allowed.
The bricks are repeated in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ and $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction with a specified periodicity. If $L_y = P_y$ and $L_z = P_z$, then the target consists of a continuous multilayer slab. For this case, it is most economical to set $L_y/d = L_z/d = P_y/d = P_z/d = 1$.
If $P_y = 0$, then repetition in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction is suppressed – the target repeats only in the $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction.
If $P_z = 0$, then repetition in the $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction is suppressed – the target repeats only in the $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction.
The upper surface of the slab is asssume to be located at $x_{\mathrm{TF}} = 0$. The lower surface of the slab is at $x_{\mathrm{TF}} = -L_x = -$ SHPAR1$\times d$.
The multilayer slab geometry is specified with 9 parameters. The pertinent line in ddscat.par should read

SHPAR$_1$ SHPAR$_2$ SHPAR$_3$ SHPAR$_4$ SHPAR$_5$ SHPAR$_6$ SHPAR$_7$ SHPAR$_8$ SHPAR$_9$

where
SHPAR$_1$ = L_x/d = (brick thickness in $\hat{\mathbf{x}}_{\mathrm{TF}}$ direction)$/d$
SHPAR$_2$ = L_y/d = (brick extent in $\hat{\mathbf{y}}_{\mathrm{TF}}$ direction)$/d$
SHPAR$_3$ = L_z/d = (brick extent in $\hat{\mathbf{z}}_{\mathrm{TF}}$ direction)$/d$
SHPAR$_4$ = fraction of the slab with composition 1
SHPAR$_5$ = fraction of the slab with composition 2
SHPAR$_6$ = fraction of the slab with composition 3

SHPAR_7 = fraction of the slab with composition 4
$\text{SHPAR}_8 = P_y/d$ = (periodicity in $\hat{\mathbf{y}}_{\text{TF}}$ direction)/d (0 to suppress repetition in $\hat{\mathbf{y}}_{\text{TF}}$ direction)
$\text{SHPAR}_9 = P_z/d$ = (periodicity in $\hat{\mathbf{z}}_{\text{TF}}$ direction)/d (0 to suppress repetition in $\hat{\mathbf{z}}_{\text{TF}}$ direction)

For a slab with only one layer, set $\text{SHPAR}_5 = 0$, $\text{SHPAR}_6 = 0$, $\text{SHPAR}_7 = 0$.
For a slab with only two layers, set $\text{SHPAR}_6 = 0$ and $\text{SHPAR}_7 = 0$.
For a slab with only three layers, set $\text{SHPAR}_7 = 0$.
The user must set NCOMP equal to the number of nonzero thickness layers.
The number N of dipoles in one TUC is $N = \text{nint}(\text{SHPAR}_1) \times \text{nint}(\text{SHPAR}_2) \times \text{nint}(\text{SHPAR}_3)$.
    The fractions SHPAR_2, SHPAR_3, SHPAR_4, and SHPAR_5 *must* sum to 1. The number of dipoles in each of the layers will be integers that are close to $\text{nint}(\text{SHPAR}_1 * \text{SHPAR}_4)$, $\text{nint}(\text{SHPAR}_1 * \text{SHPAR}_5)$, $\text{nint}(\text{SHPAR}_1 * \text{SHPAR}_6)$, $\text{nint}(\text{SHPAR}_1 * \text{SHPAR}_7)$,
    The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file ddscat.par. Because of the way a_{eff} is defined ($4\pi a_{\text{eff}}^3/3 \equiv Nd^3$), it should be set to

$$a_{\text{eff}} = (3/4\pi)^{1/3} N^{1/3} d = (3/4\pi)^{1/3} (L_x L_y L_z)^{1/3}$$

.

    With target option LYRSLBPBC, the target becomes a periodic structure, of infinite extent in the target y- and z- directions. The target axes (in the TF) are set to $\hat{\mathbf{a}}_1 = (1,0,0)_{\text{TF}}$ – i.e., normal to the "slab" – and $\hat{\mathbf{a}}_2 = (0,1,0)_{\text{TF}}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the slab.
    For this option, there are only two allowed scattering directions, corresponding to transmission and specular reflection. **DDSCAT** will calculate both the transmission and reflection coefficients.
The last two lines in ddscat.par should appear as in the following example ddscat.par file. This example is for a slab with two layers: the slab is 26 dipole layers thick; the first layer comprises 76.92% of the thickness, the second layer 23.08% of the thickness. The wavelength is 0.532μm, the thickness is $L_x = (4\pi/3)^{1/3} N_x^{2/3} a_{\text{eff}} = (4\pi/3)^{1/3} (26)^{2/3} 0.009189 = 0.1300\mu$m.
The upper layer thickness is $0.2308 L_x = 0.0300\mu$m
ddscat.par is set up to calculate a single orientation: in the Lab Frame, the target is rotated through an angle $\Theta = 120°$, with $\Phi = 0$. In this orientation, the incident radiation is propagating in the $(-0.5, 0.866, 0)$ direction in the Target Frame, so that it is impinging on target layer 2 (Au).

```
' ========== Parameter file for v7.1.0 ==================='
'**** PRELIMINARIES ****'
'NOTORQ' = CMTORQ*6 (DOTORQ, NOTORQ) -- either do or skip torque calculations
'PBCGS2' = CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT' = CMETHD*6 (GPFAFT, FFTMKL)
'GKDLDR' = CALPHA*6 (GKDLDR, LATTDR)
'NOTBIN' = CBINFLAG (ALLBIN, ORIBIN, NOTBIN)
'**** Initial Memory Allocation ****'
26  1  1  = upper bounds on size of TUC
'**** Target Geometry and Composition ****'
'LYRSLBPBC' = CSHAPE*9 shape directive
26 1 1 0.7692 0.2308 0 0 1 1 = shape parameters SHPAR1 - SHPAR9
2        = NCOMP = number of dielectric materials
'/u/draine/work/DDA/diel/Eagle_2000' = refractive index 1
'/u/draine/work/DDA/diel/Au_evap'    = refractive index 2
'**** Error Tolerance ****'
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
5.00e-3 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
0.5 = ETASCA (number of angles is proportional to [(3+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
0.5320 0.5320 1 'INV' = wavelengths (first,last,how many,how=LIN,INV,LOG)
```

```
'**** Effective Radii (micron) **** '
0.009189 0.009189 1 'LIN' = eff. radii (first,last,how many,how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
'**** Specify which output files to write ****'
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA)
'**** Prescribe Target Rotations ****'
0.   0.   1  = BETAMI, BETAMX, NBETA (beta=rotation around a1)
120. 120. 1  = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
0.   0.   1  = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0  0   0    = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6 = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41 = indices ij of elements to print
'**** Specify Scattered Directions ****'
'TFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
1 = number of scattering orders
0.  0. = (M,N) for scattering
```

20.9   RCTGL_PBC = Target consisting of homogeneous rectangular brick, extended in target y and z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of a biperiodic array of rectangular bricks. The bricks are assumed to be homogeneous and isotropic, just as for option RCTNGL (see §19.18).

Let us refer to a single rectangular brick as the Target Unit Cell (TUC). The TUC is then repeated in the $y_{\rm TF}$- and $z_{\rm TF}$-directions, with periodicities PYAEFF$\times a_{\rm eff}$ and PZAEFF$\times a_{\rm eff}$, where $a_{\rm eff} \equiv (3V_{\rm TUC}/4\pi)^{1/3}$, where $V_{\rm TUC}$ is the total volume of solid material in one TUC. This option requires 5 shape parameters:

The pertinent line in ddscat.par should read

SHPAR$_1$ SHPAR$_2$ SHPAR$_3$ SHPAR$_4$ SHPAR$_5$

where
SHPAR$_1$ = (brick thickness)/d in the $x_{\rm TF}$ direction
SHPAR$_2$ = (brick thickness)/d in the $y_{\rm TF}$ direction
SHPAR$_3$ = (brick thickness)/d in the $z_{\rm TF}$ direction
SHPAR$_4$ = periodicity/d in the $y_{\rm TF}$ direction
SHPAR$_5$ = periodicity/d in the $z_{\rm TF}$ direction

The overall size of the TUC (in terms of numbers of dipoles) is determined by parameters SHPAR$_1$, SHPAR$_2$, and SHPAR$_3$. The periodicity in the $y_{\rm TF}$ and $z_{\rm TF}$ directions is determined by parameters SHPAR$_4$ and SHPAR$_5$.

The physical size of the TUC is specified by the value of $a_{\rm eff}$ (in physical units, e.g. cm), specified in the file ddscat.par.

With target option RCTGL_PBC, the target becomes a periodic structure, of infinite extent in the target y- and z- directions. The target axes (in the TF) are set to $\hat{\bf a}_1 = (1,0,0)_{\rm TF}$ – i.e., normal to the "slab" – and $\hat{\bf a}_2 = (0,1,0)_{\rm TF}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above); for example, $\Theta = 0$ would be for radiation incident normal to the slab.

Sample Calculation: Subdirectory examples_exp/RCTGL_PBC contains ddscat.par for scattering by an infinite slab, constituted from $16 \times 1 \times 1$ dipole TUCs.

20.10 RECRECPBC = Rectangular solid resting on top of another rectangular solid, repeated periodically in target y and z directions using periodic boundary conditions

The TUC consists of a single rectangular "brick", of material 1, resting on top of a second rectangular brick, of material 2. The centroids of the two bricks along a line in the $\hat{\mathbf{x}}_{\text{TF}}$ direction. The bricks are assumed to be homogeneous, and materials 1 and 2 are assumed to be isotropic. The TUC is then repeated in the y_{TF}- and z_{TF}-directions, with periodicities $\text{SHPAR}_4 \times d$ and $\text{SHPAR}_5 \times d$. is the total volume of solid material in one TUC. This option requires 5 shape parameters:
The pertinent line in `ddscat.par` should read

SHPAR_1 SHPAR_2 SHPAR3 SHPAR4 SHPAR_5

where
SHPAR_1 = (upper brick thickness)/d in the $\hat{\mathbf{x}}_{\text{TF}}$ direction
SHPAR_2 = (upper brick thickness)/d in the $\hat{\mathbf{y}}_{\text{TF}}$ direction
SHPAR_3 = (upper brick thickness)/d in the $\hat{\mathbf{z}}_{\text{TF}}$ direction
SHPAR_4 = (lower brick thickness)/d in the $\hat{\mathbf{x}}_{\text{TF}}$ direction
SHPAR_5 = (lower brick thickness)/d in the $\hat{\mathbf{y}}_{\text{TF}}$ direction
SHPAR_6 = (lower brick thickness)/d in the $\hat{\mathbf{z}}_{\text{TF}}$ direction
SHPAR_7 = periodicity/d in the $\hat{\mathbf{y}}_{\text{TF}}$ direction
SHPAR_8 = periodicity/d in the $\hat{\mathbf{z}}_{\text{TF}}$ direction

The actual numbers of dipoles N_{1x}, N_{1y}, N_{1z}, along each dimension of the upper brick, and N_{2x}, N_{2y}, N_{2z} along each dimension of the lower brick, just be integers. Usually, $N_{1x} = \text{nint}(\text{SHPAR}_1)$, $N_{1y} = \text{nint}(\text{SHPAR}_2)$, $N_{1z} = \text{nint}(\text{SHPAR}_3)$, $N_{2x} = \text{nint}(\text{SHPAR}_4)$, $N_{2y} = \text{nint}(\text{SHPAR}_5)$, $N_{2z} = \text{nint}(\text{SHPAR}_6)$, where $\text{nint}(x)$ is the integer nearest to x, but under some circumstances N_{1x}, N_{1y}, N_{1z}, N_{2x}, N_{2y}, N_{2z} might be larger or smaller by 1 unit.

The overall size of the TUC (in terms of numbers of dipoles) is determined by parameters SHPAR_1 − SHPAR_6:

$$N = (N_{1x} \times N_{1y} \times N_{1z}) + (N_{2x} \times N_{2y} \times N_{2z}) \tag{34}$$

The periodicity in the $\hat{\mathbf{y}}_{\text{TF}}$ and $\hat{\mathbf{z}}_{\text{TF}}$ directions is determined by parameters SHPAR_7 and SHPAR_8.
The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file `ddscat.par`:

$$d = (4\pi/3N)^{1/3} a_{\text{eff}} \tag{35}$$

The target is a periodic structure, of infinite extent in the $\hat{\mathbf{y}}_{\text{TF}}$ and $\hat{\mathbf{z}}_{\text{TF}}$ directions. The target axes are set to $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{\text{TF}}$ – i.e., normal to the "slab" – and $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{\text{TF}}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above) specifying the orientation of the target axes $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ relative to the direction of incidence; for example, $\Theta = 0$ would be for radiation incident normal to the slab.

The scattering directions are specified by specifying the diffraction order (M, N); for each diffraction order one transmitted wave direction and one reflected wave direction will be calculated, with the dimensionless 4×4 scattering matrix $S^{(2d)}$ calculated for each scattering direction. At large distances from the infinite slab, the scattered Stokes vector in the (M,N) diffraction order is

$$I_{sca,i}(M, N) = \sum_{j=1}^{4} S_{ij}^{(2d)} I_{in,j} \tag{36}$$

where $I_{in,j}$ is the incident Stokes vector. See Draine & Flatau (2008) for interpretation of the S_{ij} as transmission and reflection efficiencies.

20.11   SLBHOLPBC = Target consisting of a periodic array of rectangular blocks, each containing a cylindrical hole

Individual blocks have extent (a, b, c) in the $(\hat{\mathbf{x}}_{TF}, \hat{\mathbf{y}}_{TF}, \hat{\mathbf{z}}_{TF})$ directions, and the cylindrical hole has radius r. The period in the $\hat{\mathbf{y}}_{TF}$-direction is P_y, and the period in the $\hat{\mathbf{z}}_{TF}$-direction is P_z.

The pertinent line in `ddscat.par` should consist of

SHPAR$_1$ SHPAR$_2$ SHPAR$_3$ SHPAR$_4$ SHPAR$_5$ SHPAR$_6$

where SHPAR$_1 = a/d$ (d is the interdipole spacing)

SHPAR$_2 = b/a$

SHPAR$_3 = c/a$

SHPAR$_4 = r/a$

SHPAR$_5 = P_y/d$

SHPAR$_6 = P_z/d$.

Ideally, a/d =SHPAR$_1$, b/d =SHPAR$_2 \times$ SHPAR$_1$, and c/d =SHPAR$_3 \times$ SHPAR$_1$ will be integers (so that the cubic lattice can accurately approximate the desired target). If $P_y = 0$ and $P_z > 0$ the target is periodic in the $\hat{\mathbf{z}}_{TF}$-direction only.

If $P_y > 0$ and $P_z = 0$ the target is periodic in the $\hat{\mathbf{y}}_{TF}$-direction only.

If $P_y > 0$ it is required that $P_y \geq b$, and if $P_z > 0$ it is required that $P_z \geq c$, so that the blocks do not overlap.

With $P_y = b$ and $P_z = c$, the blocks are juxtaposed to form a periodic array of cylindrical holes in a solid slab.

Example: `ddscat_SLBHOLPBC.par` is a sample `ddscat.par` for a periodic array of cylindrical holes in a slab of thickness a, with holes of radius r, and period P_y and P_d

20.12   SPHRN_PBC = Target consisting of group of N spheres, extended in target y and z directions using periodic boundary conditions

This option causes **DDSCAT** to create a target consisting of a periodic array of $N-$sphere structures, where one $N-$sphere structure consists of N spheres, just as for target option NANSPH (see §19.23). Each sphere can be of arbitary composition, and can be anisotropic if desired. Information for the description of one N-sphere structure is supplied via an external file, just as for target option NANSPH – see §19.23).

Let us refer to a single N-sphere structure as the Target Unit Cell (TUC). The TUC is then repeated in the y_{TF}- and z_{TF}-directions, with periodicities PYAEFF$\times a_{eff}$ and PZAEFF$\times a_{eff}$, where $a_{eff} \equiv (3V_{TUC}/4\pi)^{1/3}$, where V_{TUC} is the total volume of solid material in one TUC. This option requires 3 shape parameters:

DIAMX = maximum extent of target in the target frame x direction/d

PYAEFF = periodicity in target y direction/a_{eff}

PZAEFF = periodicity in target z direction/a_{eff}.

   The pertinent line in `ddscat.par` should read

SHPAR$_1$ SHPAR$_2$ SHPAR$_3$ *'filename'* (quotes must be used)

where

SHPAR$_1$ = target diameter in x direction (in Target Frame) in units of d

SHPAR$_2$= PYAEFF

SHPAR$_3$= PZAEFF.

filename is the name of the file specifying the locations and relative sizes of the spheres.

The overall size of the TUC (in terms of numbers of dipoles) is determined by parameter SHPAR$_1$, which is the extent of the multisphere target in the x-direction, in units of the lattice spacing d. The physical size of the TUC is specified by the value of a_{eff} (in physical units, e.g. cm), specified in the file `ddscat.par`.

The location of the spheres in the TUC, and their composition, is specified in file *'filename'*. Please consult §19.23 above for detailed information concerning the information in this file, and its arrangement.

Note that while the spheres can be anisotropic and of differing composition, they can of course also be isotropic and of a single composition, in which case the relevant lines in the file *'filename'* should read

$x_1\ y_1\ z_1\ r_1$ 1 1 1 0 0 0
$x_2\ y_2\ z_2\ r_2$ 1 1 1 0 0 0
$x_3\ y_3\ z_3\ r_3$ 1 1 1 0 0 0
...

i.e., every sphere has isotropic composition ICOMP=1 and the three dielectric function orientation angles are set to zero.

When the user uses target option SPHRN_PBC, the target now becomes a periodic structure, of infinite extent in the target y- and z- directions. The target axis $\hat{\mathbf{a}}_1 = \hat{\mathbf{x}}_{LF} = (1, 0, 0)_{TF}$ – i.e., normal to the "slab" – and target axis $\hat{\mathbf{a}}_2 = \hat{\mathbf{y}}_{LF} = (0, 1, 0)_{TF}$. The orientation of the incident radiation relative to the target is, as for all other targets, set by the usual orientation angles β, Θ, and Φ (see §17 above). The scattering directions are, just as for other targets, determined by the scattering angles θ_s, ϕ_s (see §21 below).

The scattering problem for this infinite structure, assumed to be illuminated by an incident monochromatic plane wave, is essentially solved "exactly", in the sense that the electric polarization of each of the constituent dipoles is due to the electric field produced by the incident plane wave plus *all* of the other dipoles in the infinite target.

However, the assumed target will, of course, act as a perfect diffraction grating if the scattered radiation is calculated as the coherent sum of all the oscillating dipoles in this periodic structure: the far-field scattered intensity would be zero in all directions except those where the Bragg scattering condition is satisfied, and in those directions the far-field scattering intensity would be infinite.

To suppress this singular behavior, we calculate the far-field scattered intensity as though the separate TUCs scatter incoherently. The scattering efficiency Q_{sca} and the absorption efficiency Q_{abs} are defined to be the scattering and absorption cross section per TUC, divided by πa_{eff}^2, where $a_{eff} \equiv (3V_{TUC}/4\pi)^{1/3}$, where V_{TUC} is the volume of solid material per TUC.

Note: the user is allowed to set the target periodicity in the target y_{TF} (or z_{TF}) direction to values that could be smaller than the total extent of one TUC in the target y_{TF} (or z_{TF}) direction. This is physically allowable, *provided that the spheres from one TUC do not overlap with the spheres from neighboring TUCs*. Note that **DDSCAT** does *not* check for such overlap.

20.13   TRILYRPBC = Three stacked rectangular blocks, repeated periodically

The target unit cell (TUC) consists of a stack of 3 rectangular blocks with centers on the $\hat{\mathbf{x}}_{TF}$ axis. The TUC is repeated in either the $\hat{\mathbf{y}}_{TF}$ direction, the $\hat{\mathbf{z}}_{TF}$ direction, or both. A total of 11 shape parameters must be specified:

SHPAR$_1$ = x-thickness of upper layer/d [material 1]
SHPAR$_2$ = y-width/d of upper layer
SHPAR$_3$ = z-width/d of upper layer
SHPAR$_4$ = x-thickness/d of middle layer [material 2]
SHPAR$_5$ = y-width/d of middle layer
SHPAR$_6$ = z-width/d of middle layer
SHPAR$_7$ = x-width/d of lower layer
SHPAR$_8$ = y-width/d of lower layer
SHPAR$_9$ = z-width/d of lower layer
SHPAR$_{10}$ = period/d in y direction
SHPAR$_{11}$= period/d in z direction

21 Scattering Directions

21.1 Isolated Finite Targets

DDSCAT calculates scattering in selected directions, and elements of the scattering matrix are reported in the output files w*xxx*r*yyy*k*zzz*.sca . The scattering direction is specified through angles θ_s and ϕ_s (not to be confused with the angles Θ and Φ which specify the orientation of the target relative to the incident radiation!).

For isolated finite targets (*i.e.,* PBC *not* employed) there are two options for specifying the scattering direction, with the option determined by the value of the string CMDFRM read from the input file ddscat.par.

1. If the user specifies CMDFRM='LFRAME', then the angles θ, ϕ input from ddscat.par are understood to specify the scattering directions relative to the Lab Frame (the frame where the incident beam is in the $x-$direction).

   When CMDFRM='LFRAME', the angle θ is simply the scattering angle θ_s: the angle between the incident beam (in direction $\hat{\mathbf{x}}_{\mathrm{LF}}$) and the scattered beam ($\theta_s = 0$ for forward scattering, $\theta_s = 180°$ for backscattering).

   The angle ϕ specifies the orientation of the "scattering plane" relative to the $\hat{\mathbf{x}}_{\mathrm{LF}} - \hat{\mathbf{y}}_{\mathrm{LF}}$ plane. When $\phi = 0$ the scattering plane is assumed to coincide with the $\hat{\mathbf{x}}_{\mathrm{LF}} - \hat{\mathbf{y}}_{\mathrm{LF}}$ plane. When $\phi = 90°$ the scattering plane is assumed to coincide with the $\hat{\mathbf{x}}_{\mathrm{LF}} - \hat{\mathbf{z}}_{\mathrm{LF}}$ plane. Within the scattering plane the scattering directions are specified by $0 \leq \theta \leq 180°$. Thus:

$$\hat{\mathbf{n}}_s = \hat{\mathbf{x}}_{\mathrm{LF}} \cos\theta + \hat{\mathbf{y}}_{\mathrm{LF}} \sin\theta \cos\phi + \hat{\mathbf{z}}_{\mathrm{LF}} \sin\theta \sin\phi \quad , \tag{37}$$

2. If the user specifies CMDFRM='TFRAME', then the angles θ, ϕ input from ddscat.par are understood to specify the scattering directions $\hat{\mathbf{n}}_{\mathbf{s}}$ relative to the Target Frame (the frame defined by target axes $\hat{\mathbf{x}}_{\mathrm{TF}}$, $\hat{\mathbf{y}}_{\mathrm{TF}}$, $\hat{\mathbf{z}}_{\mathrm{TF}}$). θ is the angle between $\hat{\mathbf{n}}_s$ and $\hat{\mathbf{x}}_{\mathrm{TF}}$, and ϕ is the angle between the $\hat{\mathbf{n}}_s - \hat{\mathbf{x}}_{\mathrm{TF}}$ plane and the $\hat{\mathbf{x}}_{\mathrm{TF}} - \hat{\mathbf{y}}_{\mathrm{TF}}$ plane. Thus:

$$\hat{\mathbf{n}}_s = \hat{\mathbf{x}}_{\mathrm{TF}} \cos\theta + \hat{\mathbf{y}}_{\mathrm{TF}} \sin\theta \cos\phi + \hat{\mathbf{z}}_{\mathrm{TF}} \sin\theta \sin\phi \quad . \tag{38}$$

Scattering directions for which the scattering properties are to be calculated are set in the parameter file ddscat.par by specifying one or more scattering planes (determined by the value of ϕ_s) and for each scattering plane, the number and range of θ_s values. The only limitation is that the number of scattering directions not exceed the parameter MXSCA in DDSCAT.f (in the code as distributed it is set to MXSCA=1000).

21.2 Scattering Directions for Targets that are Periodic in 1 Dimension

For targets that are periodic, scattering is only allowed in certain directions (see Draine & Flatau 2008). If the user has chosen a PBC target (e.g, CYLNDRPBC, HEXGONPBC, or RCTGL_PBC), SPHRN_PBC but has set one of the periodicities to zero, then the target is periodic in only one dimension – e.g., CYLNDRPBC could be used to construct a single infinite cylinder.

In this case, the scattering directions are specified by giving an integral diffraction order $M = 0, \pm1, \pm2, ...$ and one angle, the azimuthal angle ζ around the target repetition axis. The diffraction order M determines the projection of $\mathbf{k}_s$ onto the repetition direction. For a given order M, the scattering angles with $\zeta = 0 \rightarrow 2\pi$ form a cone around the repetition direction.

For example, if PYD > 0 (target repeating in the y_{TF} direction), then M determines the value of $k_{sy} = \mathbf{k}_s \cdot \hat{\mathbf{y}}_{\mathrm{TF}}$, where $\hat{\mathbf{y}}_{\mathrm{TF}}$ is the unit vector in the Target Frame $y-$direction:

$$k_{sy} = k_{0y} + 2\pi M/L_y \tag{39}$$

where $k_{0y} \equiv \mathbf{k}_0 \cdot \hat{\mathbf{y}}_{\mathrm{TF}}$, where $\mathbf{k}_0$ is the incident k vector. Note that the diffraction order M *must* satisfy the condition

$$(k_{0y} - k_0)(L_y/2\pi) < M < (k_0 - k_{0y})(L_y/2\pi) \tag{40}$$

where $L_y = \text{PYD} \times d$ is the periodicity along the y axis in the Target Frame. $M = 0$ is always an allowed diffraction order.

The azimuthal angle ζ defines a right-handed rotation of the scattering direction around the target repetition axis. Thus for a target repetition axis $\hat{\mathbf{y}}_{\text{TF}}$,

$$k_{sx} = k_\perp \cos\zeta \quad , \tag{41}$$
$$k_{sz} = k_\perp \sin\zeta \quad , \tag{42}$$

where $k_\perp = (k_0^2 - k_{sy}^2)^{1/2}$, with $k_{sy} = k_{0y} + 2\pi M/L_y$. For a target with repetition axis z_{TF},

$$k_{sx} = k_\perp \cos\zeta \quad , \tag{43}$$
$$k_{sy} = k_\perp \sin\zeta \quad , \tag{44}$$

where $k_\perp = (k_0^2 - k_{sz}^2)^{1/2}$, $k_{sz} = k_{0z} + 2\pi M/L_z$.

The user selects a diffraction order M and the azimuthal angles ζ to be used for that M via one line in ddscat.par. An example would be to use CYLNDRPBC to construct an infinite cylinder with the cylinder direction in the $\hat{\mathbf{y}}_{\text{TF}}$ direction:

```
' ============== Parameter file for v7.1.0 ===================='
'**** PRELIMINARIES ****'
'NOTORQ' = CMTORQ*6 (DOTORQ, NOTORQ) -- either do or skip torque calculations
'PBCGS2' = CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT' = CMETHD*6 (GPFAFT, FFTMKL)
'GKDLDR' = CALPHA*6 (GKDLDR, LATTDR)
'NOTBIN' = CBINFLAG (NOTBIN, ORIBIN, ALLBIN)
'**** Initial Memory Allocation ****'
50 50 50 = size allowance for target generation
'**** Target Geometry and Composition ****'
'CYLNDRPBC' = CSHAPE*9 shape directive
2.0 20. 2 2.0 0. = shape parameters SHPAR1, SHPAR2, SHPAR3, SHPAR4, SHPAR5,
1         = NCOMP = number of dielectric materials
'/u/draine/work/DDA/diel/m1.33_0.01' = name of file containing dielectric function
'**** Error Tolerance ****'
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
5.00e-3 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
0.5 = ETASCA (number of angles is proportional to [(3+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
6.283185 6.283185 1 'INV' = wavelengths (first,last,how many,how=LIN,INV,LOG)
'**** Effective Radii (micron) **** '
2 2 1 'LIN' = eff. radii (first, last, how many, how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.)
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA))
'**** Prescribe Target Rotations ****'
0.   0.   1  = BETAMI, BETAMX, NBETA (beta=rotation around a1)
60. 60.   1  = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
0.   0.   1  = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0   0   0   = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6 = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41 = indices ij of elements to print
'**** Specify Scattered Directions ****'
'TFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
1 = number of scattering cones
0.  0. 360. 30 = M, zeta_min, zeta_max, dzeta (in degrees)
```

In this example, a single diffraction order $M = 0$ is selected, and ζ is to run from $\zeta_{\min} = 0$ to $\zeta_{\max} = 360°$ in increments of $\delta\zeta = 30°$.

There may be additional lines, one per diffraction order. Remember, however, that every diffraction order must satisfy eq. (40).

21.3 Scattering Directions for Targets for Doubly-Periodic Targets

If the user has specified nonzero periodicity in both the y and z directions, then the scattering directions are specified by two integers – the diffraction orders M, N for the $\hat{\mathbf{y}}, \hat{\mathbf{z}}$ directions. The scattering directions are

$$\mathbf{k}_s = \pm \frac{k_n}{k_0}\left(\mathbf{k}_0 \cdot \hat{\mathbf{x}}_{\mathrm{TF}}\right)\hat{\mathbf{x}}_{\mathrm{TF}} + \left(\mathbf{k}_0 \cdot \hat{\mathbf{y}}_{\mathrm{TF}} + \frac{2\pi M}{L_y}\right)\hat{\mathbf{y}}_{\mathrm{TF}} + \left(\mathbf{k}_0 \cdot \hat{\mathbf{z}}_{\mathrm{TF}} + \frac{2\pi N}{L_z}\right)\hat{\mathbf{z}}_{\mathrm{TF}} \qquad (45)$$

$$k_n \equiv \left[k_0^2 - \left(\mathbf{k}_0 \cdot \hat{\mathbf{y}}_{\mathrm{TF}} + \frac{2\pi M}{L_y}\right)^2 + \left(\mathbf{k}_0 \cdot \hat{\mathbf{z}}_{\mathrm{TF}} + \frac{2\pi N}{L_z}\right)^2\right]^{1/2} \qquad (46)$$

where the $+$ sign gives transmission, and the $-$ sign gives reflection. The integers M and N *must* together satisfy the inequality

$$(k_{0y} + 2\pi M/L_y)^2 + (k_{0z} + 2\pi N/L_z)^2 < k_0^2 \qquad (47)$$

which, for small values of L_y and L_z, may limit the scattering to only $(M, N) = (0, 0)$. [Of course, $(0, 0)$ is *always* allowed]. For each (M, N) specified in ddscat.par, **DDSCAT 7.1** will calculate the generalized Mueller matrix $S_{ij}^{(2d)}(M, N)$ – see §At large distances from the infinite slab, the scattered Stokes vector in the (M, N) diffraction order is

$$I_{sca,i}(M, N) = \sum_{j=1}^{4} S_{ij}^{(2d)}(M, N)I_{in,j} \qquad (48)$$

where $I_{in,j}$ is the incident Stokes vector, and $S_{ij}^{(2d)}(M, N)$ is the generalization of the 4×4 Müller scattering matrix to targets that are periodic in 2-directions (Draine & Flatau 2008). There are distinct $S_{ij}^{(2d)}(M, N)$ for transmission and for reflection, corresponding to the $\pm$ in eq. (45).

Draine & Flatau (2008, eq. 69-71) show how the $S_{ij}^{(2d)}(M, N)$ are easily related to familiar "transmission coefficients" and "reflection coefficients".

Here is a sample ddscat.par file as an example:

```
' ============== Parameter file for v7.1.0 ==================='
'**** PRELIMINARIES ****'
'NOTORQ' = CMTORQ*6 (DOTORQ, NOTORQ) -- either do or skip torque calculations
'PBCGS2' = CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT' = CMETHD*6 (GPFAFT, FFTMKL)
'GKDLDR' = CALPHA*6 (GKDLDR, LATTDR)
'NOTBIN' = CBINFLAG (NOTBIN, ORIBIN, ALLBIN)
'**** Initial Memory Allocation ****'
50 50 50 = dimensioning allowance for target generation
'**** Target Geometry and Composition ****'
'RCTGL_PBC' = CSHAPE*9 shape dirctive
20.0 1.0 1.0 1.0 1.0 = shape parameters PAR1, PAR2, PAR3,...
1         = NCOMP = number of dielectric materials
'/u/draine/work/DDA/diel/m1.33_0.01' = name of file containing dielectric function
'**** CONJUGATE GRADIENT DEFINITIONS ****'
0         = INIT (TO BEGIN WITH |X0> = 0)
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
5.00e-3 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
0.5 = ETASCA (number of angles is proportional to [(3+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
6.283185 6.283185 1 'INV' = wavelengths (first,last,how many,how=LIN,INV,LOG)
'**** Effective Radii (micron) **** '
2 2 1 'LIN' = eff. radii (first, last, how many, how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.)
```

```
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA))
'**** Prescribe Target Rotations ****'
0.   0.   1  = BETAMI, BETAMX, NBETA (beta=rotation around a1)
60. 60.   1  = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
0.   0.   1  = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0   0   0  = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6 = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41 = indices ij of elements to print
'**** Specify Scattered Directions ****'
'TFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
1 = number of scattering orders
0   0 = M, N (diffraction orders)
```

22 Incident Polarization State

Recall that the "Lab Frame" is defined such that the incident radiation is propagating along the $\hat{\mathbf{x}}_{\mathrm{LF}}$ axis. **DDSCAT** allows the user to specify a general elliptical polarization for the incident radiation, by specifying the (complex) polarization vector $\hat{\mathbf{e}}_{01}$. The orthonormal polarization state $\hat{\mathbf{e}}_{02} = \hat{\mathbf{x}}_{\mathrm{LF}} \times \hat{\mathbf{e}}_{01}^*$ is generated automatically if ddscat.par specifies IORTH=2.

For incident linear polarization, one can simply set $\hat{\mathbf{e}}_{01} = \hat{\mathbf{y}}$ by specifying

(0,0) (1,0) (0,0)

in ddscat.par; then $\hat{\mathbf{e}}_{02} = \hat{\mathbf{z}}$. For polarization mode $\hat{\mathbf{e}}_{01}$ to correspond to right-handed circular polarization, set $\hat{\mathbf{e}}_{01} = (\hat{\mathbf{y}} + i\hat{\mathbf{z}})/\sqrt{2}$ by specifying (0,0) (1,0) (0,1) in ddscat.par (**DDSCAT** automatically takes care of the normalization of $\hat{\mathbf{e}}_{01}$); then $\hat{\mathbf{e}}_{02} = (i\hat{\mathbf{y}} + \hat{\mathbf{z}})/\sqrt{2}$, corresponding to left-handed circular polarization.

23 Averaging over Scattering Directions: $g(1) = \langle\cos\theta_s\rangle$, etc.

23.1 Angular Averaging

An example of scattering by a nonspherical target is shown in Fig. 8, showing the scattering for a tilted cube. Results are shown for four different scattering planes.

DDSCAT automatically carries out numerical integration of various scattering properties, including

- $\langle\cos\theta_s\rangle$;
- $\langle\cos^2\theta_s\rangle$;
- $\mathbf{g} = \langle\cos\theta_s\rangle\hat{\mathbf{x}}_{\mathrm{LF}} + \langle\sin\theta_s\cos\phi_s\rangle\hat{\mathbf{y}} + \langle\sin\theta_s\sin\phi_s\rangle\hat{\mathbf{z}}$ (see §15);
- $\mathbf{Q}_\Gamma$, provided option DOTORQ is specified (see §15).

The angular averages are accomplished by evaluating the scattered intensity for selected scattering directions (θ_s, ϕ_s), and taking the appropriately weighted sum. Suppose that we have N_θ different values of θ_s,

$$\theta = \theta_j, \quad j = 1, ..., N_\theta \quad , \tag{49}$$

and for each value of θ_j, $N_\phi(j)$ different values of ϕ_s:

$$\phi_s = \phi_{j,k}, \quad k = 1, ..., N_\phi(j) \quad . \tag{50}$$

For a given j, the values of $\phi_{j,k}$ are assumed to be uniformly spaced: $\phi_{j,k+1} - \phi_{j,k} = 2\pi/N_\phi(j)$. The angular average of a quantity $f(\theta_s, \phi_s)$ is approximated by

$$\langle f\rangle \equiv \frac{1}{4\pi}\int_0^\pi \sin\theta_s d\theta_s \int_0^{2\pi} d\phi_s f(\theta_s, \phi_s) \approx \frac{1}{4\pi}\sum_{j=1}^{N_\theta}\sum_{k=1}^{N_\phi(j)} f(\theta_j, \phi_{j,k})\Omega_{j,k} \tag{51}$$

$$\Omega_{j,k} = \frac{\pi}{N_\phi(j)}\left[\cos(\theta_{j-1}) - \cos(\theta_{j+1})\right] \quad , \quad j = 2, ..., N_\theta - 1 \quad . \tag{52}$$
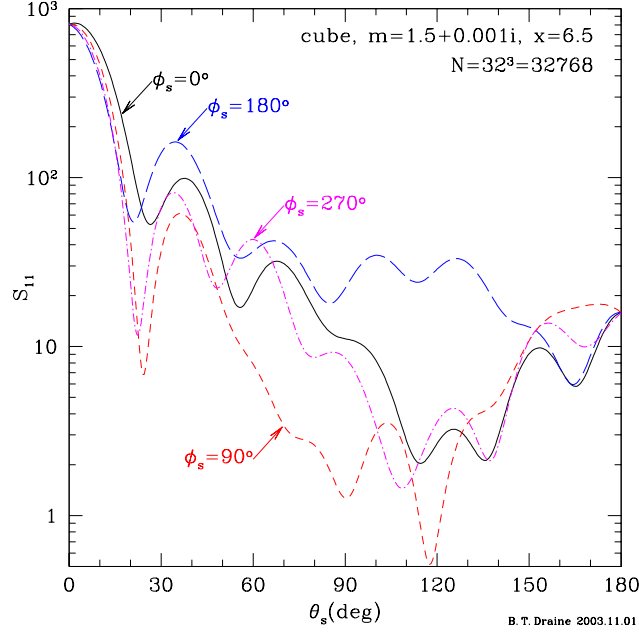
Figure 8: Scattered intensity for incident unpolarized light for a cube with $m = 1.5 + 0.001i$ and $x = 2\pi a_{\rm eff}/\lambda = 6.5$ (i.e., $d/\lambda = 1.6676$, where d is the length of a side). The cube is tilted with respect to the incident radiation, with $\Theta = 30°$, and rotated by $\beta = 15°$ around its axis to break reflection symmetry. The Mueller matrix element S_{11} is shown for 4 different scattering planes. The strong forward scattering lobe is evident. It is also seen that the scattered intensity is a strong function of scattering angle ϕ_s as well as θ_s – at a given value of θ_s (e.g., $\theta_s = 120°$), the scattered intensity can vary by orders of magnitude as ϕ_s changes by $90°$.

$$\Omega_{1,k} = \frac{2\pi}{N_\phi(1)}\left[1 - \frac{\cos(\theta_1) + \cos(\theta_2)}{2}\right] \quad, \tag{53}$$

$$\Omega_{N_\theta,k} = \frac{2\pi}{N_\phi(N_\theta)}\left[\frac{\cos(\theta_{N_\theta - 1}) + \cos(\theta_{N_\theta})}{2} + 1\right] \quad. \tag{54}$$

For a sufficiently large number of scattering directions

$$N_{\rm sca} \equiv \sum_{j=1}^{N_\theta} N_\phi(j) \tag{55}$$

the sum (51) approaches the desired integral, but the calculations can be a significant cpu-time burden, so efficiency is an important consideration.

23.2   Selection of Scattering Angles θ_s, ϕ_s

Beginning with **DDSCAT 6.1**, an improved approach is taken to evaluation of the angular average. Since targets with large values of $x = 2\pi a_{\rm eff}/\lambda$ in general have strong forward scattering, it is important to obtain good sampling of the forward scattering direction. To implement a preferential sampling of the forward scattering directions, the scattering directions (θ, ϕ) are chosen so that θ values correspond to equal intervals in a monotonically increasing function $s(\theta)$. The function $s(\theta)$ is chosen to have a negative second derivative $d^2 s/d\theta^2 < 0$ so that the density of scattering directions will be higher for small values of θ. **DDSCAT** takes

$$s(\theta) = \theta + \frac{\theta}{\theta + \theta_0} \quad. \tag{56}$$

This provides increased resolution (i.e., increased $ds/d\theta$) for $\theta < \theta_0$. We want this for the forward scattering lobe, so we take

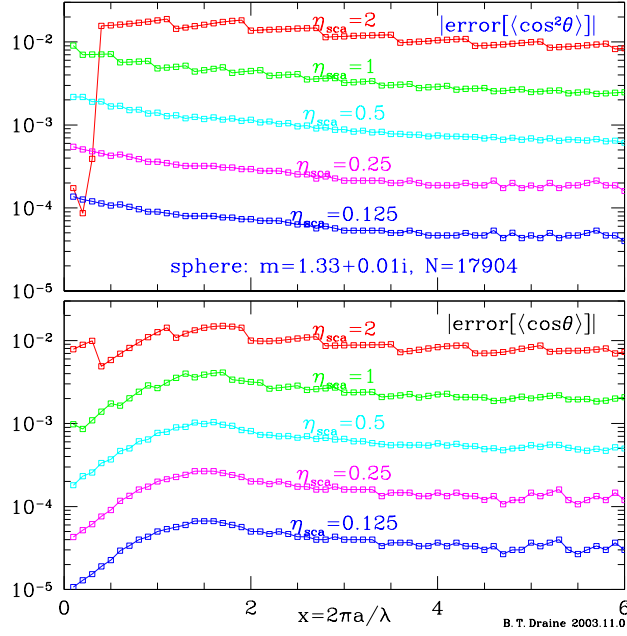$$\theta_0 = \frac{2\pi}{1 + x} \quad. \tag{57}$$

Figure 9: Errors in $\langle \cos \theta \rangle$ and $\langle \cos^2 \theta \rangle$ calculated for a $N = 17904$ dipole pseudosphere with $m = 1.33 + 0.01i$, as functions of $x = 2\pi a/\lambda$. Results are shown for different values of the parameter η.

The θ values run from $\theta = 0$ to $\theta = \pi$, corresponding to uniform increments

$$\Delta s = \frac{1}{N_\theta - 1}\left(\pi + \frac{\pi}{\pi + \theta_0}\right) \quad . \tag{58}$$

If we now require that

$$\max[\Delta\theta] \approx \frac{\Delta s}{(ds/d\theta)_{\theta=\pi}} = \eta \frac{\pi/2}{3 + x} \quad , \tag{59}$$

we determine the number of values of θ:

$$N_\theta = 1 + \frac{2(3 + x)}{\eta} \frac{[1 + 1/(\pi + \theta_0)]}{[1 + \theta_0/(\pi + \theta_0)^2]} \quad . \tag{60}$$

Thus for small values of x, $\max[\Delta\theta] = 30°\eta$, and for $x \gg 1$, $\max[\Delta\theta] \to 90°\eta/x$. For a sphere, minima in the scattering pattern are separated by $\sim 180°/x$, so $\eta = 1$ would be expected to marginally resolve structure in the scattering function. Smaller values of η will obviously lead to improved sampling of the scattering function, and more accurate angular averages.

The scattering angles θ_j used for the angular averaging are then given by

$$\theta_j = \frac{(s_j - 1 - \theta_0) + \left[(1 + \theta_0 - s_j)^2 + 4\theta_0 s_j\right]^{1/2}}{2} \quad , \tag{61}$$

where

$$s_j = \frac{(j - 1)\pi}{N_\theta - 1}\left[1 + \frac{1}{\pi + \theta_0}\right] \quad j = 1, ..., N_\theta \quad . \tag{62}$$

For each θ_j, we must choose values of ϕ. For $\theta_1 = 0$ and $\theta_{N_\theta} = \pi$ only a single value of ϕ is needed (the scattering is independent of ϕ in these two directions). For $0 < \theta_j < \pi$ we use

$$N_\phi = \max\{3, \text{nint}\left[4\pi \sin(\theta_j)/(\theta_{j+1} - \theta_{j-1})\right]\} \quad , \tag{63}$$

where $\text{nint} = $ nearest integer. This provides sampling in ϕ consistent with the sampling in θ.
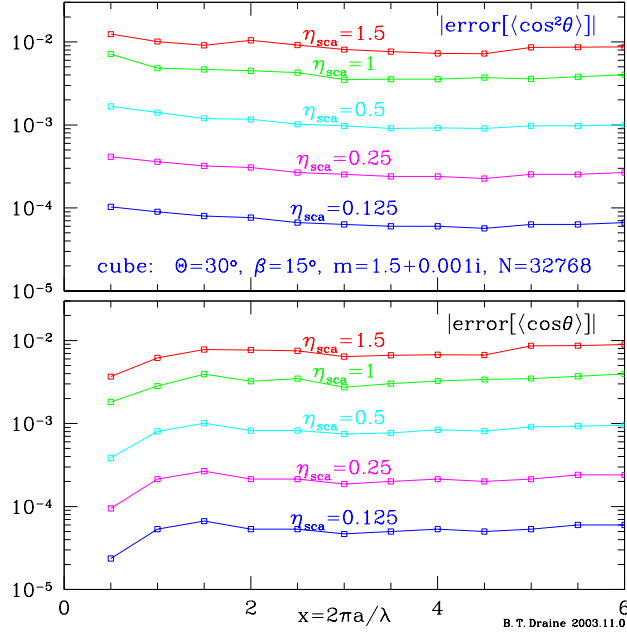
Figure 10: Same as Fig. 9, but for a $N = 32768$ dipole cube with $m = 1.5 + 0.001i$.

23.3   Accuracy of Angular Averaging as a Function of η

Figure 9 shows the absolute errors in $\langle \cos \theta \rangle$ and $\langle \cos^2 \theta \rangle$ calculated for a sphere with refractive index $m = 1.33 + 0.01i$ using the above prescription for choosing scattering angles. The error is shown as a function of scattering parameter x. We see that accuracies of order 0.01 are attained with $\eta = 1$, and that the above prescription provides an accuracy which is approximately independent of x. We recommend using values of $\eta \leq 1$ unless accuracy in the angular averages is not important.

24   Scattering by Finite Targets: The Mueller Matrix

24.1   Two Orthogonal Incident Polarizations (`IORTH=2`)

Throughout the following discussion, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ are unit vector defining the Lab Frame (thus $\hat{\mathbf{k}}_0 = \hat{\mathbf{x}}$).

DDSCAT internally computes the scattering properties of the dipole array in terms of a complex scattering matrix $f_{ml}(\theta_s, \phi_s)$ (Draine 1988), where index $l = 1, 2$ denotes the incident polarization state, $m = 1, 2$ denotes the scattered polarization state, and θ_s, ϕ_s specify the scattering direction. Normally **DDSCAT** is used with `IORTH=2` in `ddscat.par`, so that the scattering problem will be solved for both incident polarization states ($l = 1$ and 2); in this subsection it will be assumed that this is the case.

Incident polarization states $l = 1, 2$ correspond to polarization states $\hat{\mathbf{e}}_{01}$, $\hat{\mathbf{e}}_{02}$; recall that polarization state $\hat{\mathbf{e}}_{01}$ is user-specified, and $\hat{\mathbf{e}}_{02} = \hat{\mathbf{x}} \times \hat{\mathbf{e}}_{01}^*$.[10][11] Scattered polarization state $m = 1$ corresponds to linear polarization of the scattered wave parallel to the scattering plane ($\hat{\mathbf{e}}_1 = \hat{\mathbf{e}}_{\|s} = \hat{\theta}_s$) and $m = 2$ corresponds to linear polarization perpendicular to the scattering plane (in the $+\hat{\phi}_s$ direction). The scattering matrix f_{ml} was defined (Draine 1988) so that the scattered electric field $\mathbf{E}_s$ is related to the incident electric field $\mathbf{E}_i(0)$ at the origin (where the target is assumed to be located) by

$$\begin{pmatrix} \mathbf{E}_s \cdot \hat{\theta}_s \\ \mathbf{E}_s \cdot \hat{\phi}_s \end{pmatrix} = \frac{\exp(i\mathbf{k}_s \cdot \mathbf{r})}{kr} \begin{pmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{01}^* \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{02}^* \end{pmatrix} \quad . \tag{64}$$

---

[10] Draine (1988) adopted the convention $\hat{\mathbf{e}}_{02} = \hat{\mathbf{x}} \times \hat{\mathbf{e}}_{01}^*$. The customary definition of $\hat{\mathbf{e}}_{i\perp}$ is $\hat{\mathbf{e}}_{i\perp} \equiv \hat{\mathbf{e}}_{i\|} \times \hat{\mathbf{k}}$. Thus, if $\hat{\mathbf{e}}_{01} = \hat{\mathbf{e}}_{i\|}$, then $\hat{\mathbf{e}}_{02} = -\hat{\mathbf{e}}_{i\perp}$.

[11] A frequent choice is $\hat{\mathbf{e}}_{01} = \hat{\mathbf{y}}_{\mathrm{LF}}$, with $\hat{\mathbf{e}}_{02} = \hat{\mathbf{x}}_{\mathrm{LF}} \times \hat{\mathbf{y}}_{\mathrm{LF}} = \hat{\mathbf{z}}_{\mathrm{LF}}$.

The 2×2 complex *scattering amplitude matrix* (with elements S_1, S_2, S_3, and S_4) is defined so that (see Bohren & Huffman 1983)

$$\begin{pmatrix} \mathbf{E}_s \cdot \hat{\theta}_s \\ -\mathbf{E}_s \cdot \hat{\phi}_s \end{pmatrix} = \frac{\exp(i\mathbf{k}_s \cdot \mathbf{r})}{-ikr} \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\parallel} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\perp} \end{pmatrix} \quad , \tag{65}$$

where $\hat{\mathbf{e}}_{i\parallel}$, $\hat{\mathbf{e}}_{i\perp}$ are (real) unit vectors for incident polarization parallel and perpendicular to the scattering plane (with the customary definition of $\hat{\mathbf{e}}_{i\perp} = \hat{\mathbf{e}}_{i\parallel} \times \hat{\mathbf{x}}_{\mathrm{LF}}$).

From (64,65) we may write

$$\begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\parallel} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\perp} \end{pmatrix} = -i \begin{pmatrix} f_{11} & f_{12} \\ -f_{21} & -f_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{01}^* \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{02}^* \end{pmatrix} \quad . \tag{66}$$

Let

$$\begin{aligned} a &\equiv \hat{\mathbf{e}}_{01}^* \cdot \hat{\mathbf{y}}_{\mathrm{LF}} \quad , & (67) \\ b &\equiv \hat{\mathbf{e}}_{01}^* \cdot \hat{\mathbf{z}}_{\mathrm{LF}} \quad , & (68) \\ c &\equiv \hat{\mathbf{e}}_{02}^* \cdot \hat{\mathbf{y}}_{\mathrm{LF}} \quad , & (69) \\ d &\equiv \hat{\mathbf{e}}_{02}^* \cdot \hat{\mathbf{z}}_{\mathrm{LF}} \quad . & (70) \end{aligned}$$

Note that since $\hat{\mathbf{e}}_{01}, \hat{\mathbf{e}}_{02}$ could be complex (i.e., elliptical polarization), the quantities a, b, c, d are complex. Then

$$\begin{pmatrix} \hat{\mathbf{e}}_{01}^* \\ \hat{\mathbf{e}}_{02}^* \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \hat{\mathbf{y}}_{\mathrm{LF}} \\ \hat{\mathbf{z}}_{\mathrm{LF}} \end{pmatrix} \tag{71}$$

and eq. (66) can be written

$$\begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\parallel} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\perp} \end{pmatrix} = i \begin{pmatrix} -f_{11} & -f_{12} \\ f_{21} & f_{22} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{y}}_{\mathrm{LF}} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{z}}_{\mathrm{LF}} \end{pmatrix} \quad . \tag{72}$$

The incident polarization states $\hat{\mathbf{e}}_{i\parallel}$ and $\hat{\mathbf{e}}_{i\perp}$ are related to $\hat{\mathbf{x}}_{\mathrm{LF}}, \hat{\mathbf{y}}_{\mathrm{LF}}, \hat{\mathbf{z}}_{\mathrm{LF}}$ by

$$\begin{pmatrix} \hat{\mathbf{y}}_{\mathrm{LF}} \\ \hat{\mathbf{z}}_{\mathrm{LF}} \end{pmatrix} = \begin{pmatrix} \cos\phi_s & \sin\phi_s \\ \sin\phi_s & -\cos\phi_s \end{pmatrix} \begin{pmatrix} \hat{\mathbf{e}}_{i\parallel} \\ \hat{\mathbf{e}}_{i\perp} \end{pmatrix} ; \tag{73}$$

substituting (73) into (72) we obtain

$$\begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\parallel} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\perp} \end{pmatrix} = i \begin{pmatrix} -f_{11} & -f_{12} \\ f_{21} & f_{22} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \cos\phi_s & \sin\phi_s \\ \sin\phi_s & -\cos\phi_s \end{pmatrix} \begin{pmatrix} \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\parallel} \\ \mathbf{E}_i(0) \cdot \hat{\mathbf{e}}_{i\perp} \end{pmatrix} \tag{74}$$

Eq. (74) must be true for all $\mathbf{E}_i(0)$, so we obtain an expression for the complex scattering amplitude matrix in terms of the f_{ml}:

$$\begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} = i \begin{pmatrix} -f_{11} & -f_{12} \\ f_{21} & f_{22} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \cos\phi_s & \sin\phi_s \\ \sin\phi_s & -\cos\phi_s \end{pmatrix} \quad . \tag{75}$$

This provides the 4 equations used in subroutine `GETMUELLER` to compute the scattering amplitude matrix elements:

$$\begin{aligned} S_1 &= -i\left[f_{21}(b\cos\phi_s - a\sin\phi_s) + f_{22}(d\cos\phi_s - c\sin\phi_s)\right] \quad , & (76) \\ S_2 &= -i\left[f_{11}(a\cos\phi_s + b\sin\phi_s) + f_{12}(c\cos\phi_s + d\sin\phi_s)\right] \quad , & (77) \\ S_3 &= i\left[f_{11}(b\cos\phi_s - a\sin\phi_s) + f_{12}(d\cos\phi_s - c\sin\phi_s)\right] \quad , & (78) \\ S_4 &= i\left[f_{21}(a\cos\phi_s + b\sin\phi_s) + f_{22}(c\cos\phi_s + d\sin\phi_s)\right] \quad . & (79) \end{aligned}$$

24.2   Stokes Parameters

It is both convenient and customary to characterize both incident and scattered radiation by 4 "Stokes parameters" – the elements of the "Stokes vector". There are different conventions in the literature; we adhere to the definitions of the Stokes vector (I,Q,U,V) adopted in the excellent treatise by Bohren & Huffman (1983), to which the reader is referred for further detail. Here are some examples of Stokes vectors $(I, Q, U, V) = (1, Q/I, U/I, V/I)I$:

- $(1, 0, 0, 0)I$: unpolarized light (with intensity I);
- $(1, 1, 0, 0)I$: 100% linearly polarized with **E** parallel to the scattering plane;
- $(1, -1, 0, 0)I$: 100% linearly polarized with **E** perpendicular to the scattering plane;
- $(1, 0, 1, 0)I$: 100% linearly polarized with **E** at $+45°$ relative to the scattering plane;
- $(1, 0, -1, 0)I$: 100% linearly polarized with **E** at $-45°$ relative to the scattering plane;
- $(1, 0, 0, 1)I$: 100% right circular polarization (*i.e.,* negative helicity);
- $(1, 0, 0, -1)I$: 100% left circular polarization (*i.e.,* positive helicity).

24.3   Relation Between Stokes Parameters of Incident and Scattered Radiation: The Mueller Matrix

It is convenient to describe the scattering properties of a finite target in terms of the 4×4 Mueller matrix S_{ij} relating the Stokes parameters (I_i, Q_i, U_i, V_i) and (I_s, Q_s, U_s, V_s) of the incident and scattered radiation:

$$
\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix} . \tag{80}
$$

Once the amplitude scattering matrix elements are obtained, the Mueller matrix elements can be computed (Bohren & Huffman 1983):

$$
\begin{aligned}
S_{11} &= \left(|S_1|^2 + |S_2|^2 + |S_3|^2 + |S_4|^2 \right)/2 \ , \\
S_{12} &= \left(|S_2|^2 - |S_1|^2 + |S_4|^2 - |S_3|^2 \right)/2 \ , \\
S_{13} &= \mathrm{Re}\left(S_2 S_3^* + S_1 S_4^* \right) \ , \\
S_{14} &= \mathrm{Im}\left(S_2 S_3^* - S_1 S_4^* \right) \ , \\
S_{21} &= \left(|S_2|^2 - |S_1|^2 + |S_3|^2 - |S_4|^2 \right)/2 \ , \\
S_{22} &= \left(|S_1|^2 + |S_2|^2 - |S_3|^2 - |S_4|^2 \right)/2 \ , \\
S_{23} &= \mathrm{Re}\left(S_2 S_3^* - S_1 S_4^* \right) \ , \\
S_{24} &= \mathrm{Im}\left(S_2 S_3^* + S_1 S_4^* \right) \ , \\
S_{31} &= \mathrm{Re}\left(S_2 S_4^* + S_1 S_3^* \right) \ , \\
S_{32} &= \mathrm{Re}\left(S_2 S_4^* - S_1 S_3^* \right) \ , \\
S_{33} &= \mathrm{Re}\left(S_1 S_2^* + S_3 S_4^* \right) \ , \\
S_{34} &= \mathrm{Im}\left(S_2 S_1^* + S_4 S_3^* \right) \ , \\
S_{41} &= \mathrm{Im}\left(S_4 S_2^* + S_1 S_3^* \right) \ , \\
S_{42} &= \mathrm{Im}\left(S_4 S_2^* - S_1 S_3^* \right) \ , \\
S_{43} &= \mathrm{Im}\left(S_1 S_2^* - S_3 S_4^* \right) \ , \\
S_{44} &= \mathrm{Re}\left(S_1 S_2^* - S_3 S_4^* \right) \ . \tag{81}
\end{aligned}
$$

These matrix elements are computed in `DDSCAT` and passed to subroutine `WRITESCA` which handles output of scattering properties. Although the Muller matrix has 16 elements, only 9 are independent.

The user can select up to 9 distinct Muller matrix elements to be printed out in the output files w*xxx*r*yyy*k*zzz*.sca and w*xxx*r*yyy*ori.avg; this choice is made by providing a list of indices in ddscat.par (see Appendix A).

If the user does not provide a list of elements, WRITESCA will provide a "default" set of 6 selected elements: S_{11}, S_{21}, S_{31}, S_{41} (these 4 elements describe the intensity and polarization state for scattering of unpolarized incident radiation), S_{12}, and S_{13}.

In addition, WRITESCA writes out the linear polarization P of the scattered light for incident unpolarized light (see Bohren & Huffman 1983):

$$P = \frac{(S_{21}^2 + S_{31}^2)^{1/2}}{S_{11}} \quad . \tag{82}$$

24.4 Polarization Properties of the Scattered Radiation

The scattered radiation is fully characterized by its Stokes vector (I_s, Q_s, U_s, V_s). As discussed in Bohren & Huffman (eq. 2.87), one can determine the linear polarization of the Stokes vector by operating on it by the Mueller matrix of an ideal linear polarizer:

$$\mathbf{S}_{\mathrm{pol}} = \frac{1}{2} \begin{pmatrix} 1 & \cos 2\xi & \sin 2\xi & 0 \\ \cos 2\xi & \cos^2 2\xi & \cos 2\xi \sin 2\xi & 0 \\ \sin 2\xi & \sin 2\xi \cos 2\xi & \sin^2 2\xi & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{83}$$

where ξ is the angle between the unit vector $\hat{\theta}_s$ parallel to the scattering plane ("SP") and the "transmission" axis of the linear polarizer. Therefore the intensity of light polarized parallel to the scattering plane is obtained by taking $\xi = 0$ and operating on (I_s, Q_s, U_s, V_s) to obtain

$$I(\mathbf{E}_s \parallel \mathrm{SP}) = \frac{1}{2}(I_s + Q_s) \tag{84}$$

$$= \frac{1}{2k^2 r^2} \left[(S_{11} + S_{21})I_i + (S_{12} + S_{22})Q_i + (S_{13} + S_{23})U_i + (S_{14} + S_{24})V_i \right] . \tag{85}$$

Similarly, the intensity of light polarized perpendicular to the scattering plane is obtained by taking $\xi = \pi/2$:

$$I(\mathbf{E}_s \perp \mathrm{SP}) = \frac{1}{2}(I_s - Q_s) \tag{86}$$

$$= \frac{1}{2k^2 r^2} \left[(S_{11} - S_{21})I_i + (S_{12} - S_{22})Q_i + (S_{13} - S_{23})U_i + (S_{14} - S_{24})V_i \right] . \tag{87}$$

24.5 Relation Between Mueller Matrix and Scattering Cross Sections

Differential scattering cross sections can be obtained directly from the Mueller matrix elements by noting that

$$I_s = \frac{1}{r^2} \left(\frac{dC_{\mathrm{sca}}}{d\Omega} \right)_{s,i} I_i \quad . \tag{88}$$

Let SP be the "scattering plane": the plane containing the incident and scattered directions of propagation. Here we consider some special cases:

- Incident light unpolarized: Stokes vector $s_i = I(1, 0, 0, 0)$:
    - cross section for scattering with polarization $\mathbf{E}_s \parallel$ SP:

$$\frac{dC_{\mathrm{sca}}}{d\Omega} = \frac{1}{2k^2} \left(|S_2|^2 + |S_3|^2 \right) = \frac{1}{2k^2} (S_{11} + S_{21}) \tag{89}$$

    - cross section for scattering with polarization $\mathbf{E}_s \perp$ SP:

$$\frac{dC_{\mathrm{sca}}}{d\Omega} = \frac{1}{2k^2} \left(|S_1|^2 + |S_4|^2 \right) = \frac{1}{2k^2} (S_{11} - S_{21}) \tag{90}$$

– total intensity of scattered light:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{2k^2} \left(|S_1|^2 + |S_2|^2 + |S_3|^2 + |S_4|^2 \right) = \frac{1}{k^2} S_{11} \tag{91}$$

- Incident light polarized with $\mathbf{E}_i \parallel$ SP: Stokes vector $s_i = I(1, 1, 0, 0)$:
  – cross section for scattering with polarization $\mathbf{E}_s \parallel$ to SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} |S_2|^2 = \frac{1}{2k^2} \left(S_{11} + S_{12} + S_{21} + S_{22} \right) \tag{92}$$

  – cross section for scattering with polarization $\mathbf{E}_s \perp$ to SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} |S_4|^2 = \frac{1}{2k^2} \left(S_{11} + S_{12} - S_{21} - S_{22} \right) \tag{93}$$

  – total scattering cross section:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} \left(|S_2|^2 + |S_4|^2 \right) = \frac{1}{k^2} \left(S_{11} + S_{12} \right) \tag{94}$$

- Incident light polarized with $\mathbf{E}_i \perp$ SP: Stokes vector $s_i = I(1, -1, 0, 0)$:
  – cross section for scattering with polarization $\mathbf{E}_s \parallel$ to SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} |S_3|^2 = \frac{1}{2k^2} \left(S_{11} - S_{12} + S_{21} - S_{22} \right) \tag{95}$$

  – cross section for scattering with polarization $\mathbf{E}_s \perp$ SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} |S_1|^2 = \frac{1}{2k^2} \left(S_{11} - S_{12} - S_{21} + S_{22} \right) \tag{96}$$

  – total scattering cross section:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} \left(|S_1|^2 + |S_3|^2 \right) = \frac{1}{k^2} \left(S_{11} - S_{12} \right) \tag{97}$$

- Incident light linearly polarized at angle γ to SP: Stokes vector $s_i = I(1, \cos 2\gamma, \sin 2\gamma, 0)$:
  – cross section for scattering with polarization $\mathbf{E}_s \parallel$ to SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{2k^2} \left[(S_{11} + S_{21}) + (S_{12} + S_{22}) \cos 2\gamma + (S_{13} + S_{23}) \sin 2\gamma \right] \tag{98}$$

  – cross section for scattering with polarization $\mathbf{E}_s \perp$ SP:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{2k^2} \left[(S_{11} - S_{21}) + (S_{12} - S_{22}) \cos 2\gamma + (S_{13} - S_{23}) \sin 2\gamma \right] \tag{99}$$

  – total scattering cross section:

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k^2} \left[S_{11} + S_{12} \cos 2\gamma + S_{13} \sin 2\gamma \right] \tag{100}$$

24.6 One Incident Polarization State Only (`IORTH=1`)

In some cases it may be desirable to limit the calculations to a single incident polarization state – for example, when each solution is very time-consuming, and the target is known to have some symmetry so that solving for a single incident polarization state may be sufficient for the required purpose. In this case, set IORTH=1 in ddscat.par.

When IORTH=1, only f_{11} and f_{21} are available; hence, **DDSCAT** cannot automatically generate the Mueller matrix elements. In this case, the output routine WRITESCA writes out the quantities $|f_{11}|^2$, $|f_{21}|^2$, $\text{Re}(f_{11} f_{21}^*)$, and $\text{Im}(f_{11} f_{21}^*)$ for each of the scattering directions.

The differential scattering cross section for scattering with polarization $\mathbf{E}_s \parallel$ and $\perp$ to the scattering plane are

$$\left(\frac{dC_{\rm sca}}{d\Omega}\right)_{s,\parallel} = \frac{1}{k^2}|f_{11}|^2 \tag{101}$$

$$\left(\frac{dC_{\rm sca}}{d\Omega}\right)_{s,\perp} = \frac{1}{k^2}|f_{21}|^2 \tag{102}$$

Note, however, that if `IPHI` is greater than 1, **DDSCAT** will automatically set `IORTH=2` even if `ddscat.par` specified `IORTH=1`: this is because when more than one value of the target orientation angle Φ is required, there is no additional "cost" to solve the scattering problem for the second incident polarization state, since when solutions are available for two orthogonal states for some particular target orientation, the solution may be obtained for another target orientation differing only in the value of Φ by appropriate linear combinations of these solutions. Hence we may as well solve the "complete" scattering problem so that we can compute the complete Mueller matrix.

25   Scattering by Periodic Targets: Generalized Mueller Matrix

The Mueller scattering matrix $S_{ij}(\theta)$ described above was originally defined (see, e.g., Bohren & Huffman 1983) to describe scattering of incident plane waves by finite targets, such as aerosol particles or dust grains.

Draine & Flatau (2008) have extended the Mueller scattering matrix formalism to also apply to targets that are periodic and infinite in one or two dimensions (e.g., an infinite chain of particles, or a two-dimensional array of particles).

25.1   Mueller Matrix $S_{ij}^{(1d)}$ for Targets Periodic in One Direction

The dimensionless 4×4 matrix $S_{ij}^{(1d)}(M, \zeta)$ describes the scattering properties of targets that are periodic in one dimension. In the radiation zone, for incident Stokes vector $I_{\rm in}$, the scattered Stokes vector in direction (M, ζ) (see §21.2) is (see Draine & Flatau 2008, eq. 63)

$$I_{{\rm sca},i}(M, \zeta) = \frac{1}{k_0 R} \sum_{j=1}^{4} S_{ij}^{(1d)}(M, \zeta)\, I_{{\rm in},j} \quad, \tag{103}$$

where R is the distance from the target repetition axis.

DDSCAT 7.1 reports the scattering matrix elements $S_{ij}^{(nd)}$ in the output files w*aaa*r*bbb*k*ccc*`.sca`.

25.2   Mueller Matrix $S_{ij}^{(2d)}(M, N)$ for Targets Periodic in Two Directions

For targets that are periodic in two directions, the scattering intensities are described by the dimensionless 4×4 matrix $S_{ij}^{(2d)}(M, N)$. In the radiation zone, for incident Stokes vector $I_{\rm in}$, the scattered Stokes vector in scattering order (M, N) is (see Draine & Flatau 2008, eq. 64)

$$I_{{\rm sca},i}(M, N) = \sum_{j=1}^{4} S_{ij}^{(2d)}(M, N)\, I_{{\rm in},j} \quad, \tag{104}$$

where integers (M, N) define the scattering order (see §21.3). For given (M, N) there are actually two possible scattering directions – corresponding to transmission and reflection (see §21.3), and for each there is a value of $S_{ij}^{(2d)}(M, N)$.

For targets with 2-d periodicity, the scattering matrix elements $S_{ij}^{(2d)}(M, N)$ are directly related to the usual transmission coefficient and reflection coefficient (see Draine & Flatau 2008, eq. 69-71).

26   Composite Targets with Anisotropic Constituents

Section 19 includes targets composed of anisotropic materials (ANIELLIPS, ANIRCTNGL, ANI_ELL_2, ANI_ELL_3). However, in each of these cases it is assumed that the dielectric tensor of the target material is diagonal in the "Target Frame". For targets consisting of a single material (in a single domain), it is obviously possible to choose the "Target Frame" to coincide with a frame in which the dielectric tensor is diagonal.

However, for inhomogeneous targets containing anisotropic materials as, e.g., inclusions, the optical axes of the constituent material may be oriented differently in different parts of the target. In this case, it is obviously not possible to choose a single reference frame such that the dielectric tensor is diagonalized for all of the target material.

To extend DDSCAT to cover this case, we must allow for off-diagonal elements of the dielectric tensor, and therefore of the dipole polarizabilities. It will be assumed that the dielectric tensor ϵ is symmetric (this excludes magnetooptical materials – check this).

Let the material at a given location in the grain have a dielectric tensor with complex eigenvalues $\epsilon^{(j)}$, $j = 1 - 3$. These are the diagonal elements of the dielectric tensor in a frame where it is diagonalized (i.e., the frame coinciding with the principal axes of the dielectric tensor). Let this frame in which the dielectric tensor is diagonalized have unit vectors $\hat{\mathbf{e}}_j$ corresponding to the principal axes of the dielectric tensor. We need to describe the orientation of the "Dielectric Frame" (DF) – defined by the "dielectric axes" $\hat{\mathbf{e}}_j$ – relative to the Target Frame. It is convenient to do so with rotation angles analogous to the rotation angles Θ, Φ, and β used to describe the orientation of the Target Frame in the Lab Frame: Suppose that we start with unit vectors $\hat{\mathbf{e}}_j$ aligned with the target frame $\hat{\mathbf{x}}_j$.

1. Rotate the DF through an angle θ_{DF} around axis $\hat{\mathbf{y}}_{TF}$, so that θ_{DF} is now the angle between $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{x}}_{TF}$.

2. Now rotate the DF through an angle ϕ_{DF} around axis $\hat{\mathbf{x}}_{TF}$, in such a way that $\hat{\mathbf{e}}_2$ remains in the $\hat{\mathbf{x}}_{TF} - \hat{\mathbf{e}}_1$ plane.

3. Finally, rotate the DF through an angle β_{DF} around axis $\hat{\mathbf{e}}_1$.

The unit vectors $\hat{\mathbf{e}}_i$ are related to the TF basis vectors $\hat{\mathbf{x}}_{TF}$, $\hat{\mathbf{y}}_{TF}$, $\hat{\mathbf{z}}_{TF}$ by:

$$\hat{\mathbf{e}}_1 = \hat{\mathbf{x}}_{TF} \cos\theta_{DF} + \hat{\mathbf{y}}_{TF} \sin\theta_{DF} \cos\phi_{DF} + \hat{\mathbf{z}}_{TF} \sin\theta_{DF} \sin\phi_{DF} \tag{105}$$

$$\hat{\mathbf{e}}_2 = -\hat{\mathbf{x}}_{TF} \sin\theta_{DF} \cos\beta_{DF} + \hat{\mathbf{y}}_{TF}[\cos\theta_{DF} \cos\beta_{DF} \cos\phi_{DF} - \sin\beta_{DF} \sin\phi_{DF}]$$
$$+\hat{\mathbf{z}}_{TF}[\cos\theta_{DF} \cos\beta_{DF} \sin\phi_{DF} + \sin\beta_{DF} \cos\phi_{DF}] \tag{106}$$

$$\hat{\mathbf{e}}_3 = \hat{\mathbf{x}}_{TF} \sin\theta_{DF} \sin\beta_{DF} - \hat{\mathbf{y}}_{TF}[\cos\theta_{DF} \sin\beta_{DF} \cos\phi_{DF} + \cos\beta_{DF} \sin\phi_{DF}]$$
$$-\hat{\mathbf{z}}_{TF}[\cos\theta_{DF} \sin\beta_{DF} \sin\phi_{DF} - \cos\beta_{DF} \cos\phi_{DF}] \tag{107}$$

or, equivalently:

$$\hat{\mathbf{x}}_{TF} = \hat{\mathbf{e}}_1 \cos\theta_{DF} - \hat{\mathbf{e}}_2 \sin\theta_{DF} \cos\beta_{DF} + \hat{\mathbf{e}}_3 \sin\theta_{DF} \sin\beta_{DF} \tag{108}$$

$$\hat{\mathbf{y}}_{TF} = \hat{\mathbf{e}}_1 \sin\theta_{DF} \cos\phi_{DF} + \hat{\mathbf{e}}_2[\cos\theta_{DF} \cos\beta_{DF} \cos\phi_{DF} - \sin\beta_{DF} \sin\phi_{DF}]$$
$$-\hat{\mathbf{e}}_3[\cos\theta_{DF} \sin\beta_{DF} \cos\phi_{DF} + \cos\beta_{DF} \sin\phi_{DF}] \tag{109}$$

$$\hat{\mathbf{z}}_{TF} = \hat{\mathbf{e}}_1 \sin\theta_{DF} \sin\phi_{DF} + \hat{\mathbf{e}}_2[\cos\theta_{DF} \cos\beta_{DF} \sin\phi_{DF} + \sin\beta_{DF} \cos\phi_{DF}]$$
$$-\hat{\mathbf{e}}_3[\cos\theta_{DF} \sin\beta_{DF} \sin\phi_{DF} - \cos\beta_{DF} \cos\phi_{DF}] \tag{110}$$

Define the rotation matrix $R_{ij} \equiv \hat{\mathbf{x}}_i \cdot \hat{\mathbf{e}}_j$:

$$R_{ij} = \tag{111}$$

$$\begin{pmatrix} \cos\theta_{DF} & \sin\theta_{DF} \cos\phi_{DF} & \sin\theta_{DF} \sin\phi_{DF} \\ -\sin\theta_{DF} \cos\beta_{DF} & \cos\theta_{DF} \cos\beta_{DF} \cos\phi_{DF} - \sin\beta_{DF} \sin\phi_{DF} & \cos\theta_{DF} \cos\beta_{DF} \sin\phi_{DF} + \sin\beta_{DF} \cos\phi_{DF} \\ \sin\theta_{DF} \sin\beta_{DF} & -\cos\theta_{DF} \sin\beta_{DF} \cos\phi_{DF} - \cos\beta_{DF} \sin\phi_{DF} & -\cos\theta_{DF} \sin\beta_{DF} \sin\phi_{DF} + \cos\beta_{DF} \cos\phi_{DF} \end{pmatrix}$$
$$\tag{112}$$

and its inverse

$$(R^{-1})_{ij} = \tag{113}$$

$$
\begin{pmatrix}
\cos\theta_{\mathrm{DF}} & -\sin\theta_{\mathrm{DF}}\cos\beta_{\mathrm{DF}} & \sin\theta_{\mathrm{DF}}\sin\beta_{\mathrm{DF}} \\
\sin\theta_{\mathrm{DF}}\cos\phi_{\mathrm{DF}} & \cos\theta_{\mathrm{DF}}\cos\beta_{\mathrm{DF}}\cos\phi_{\mathrm{DF}}-\sin\beta_{\mathrm{DF}}\sin\phi_{\mathrm{DF}} & -\cos\theta_{\mathrm{DF}}\sin\beta_{\mathrm{DF}}\cos\phi_{\mathrm{DF}}-\cos\beta_{\mathrm{DF}}\sin\phi_{\mathrm{DF}} \\
\sin\theta_{\mathrm{DF}}\sin\phi_{\mathrm{DF}} & \cos\theta_{\mathrm{DF}}\cos\beta_{\mathrm{DF}}\sin\phi_{\mathrm{DF}}+\sin\beta_{\mathrm{DF}}\cos\phi_{\mathrm{DF}} & -\cos\theta_{\mathrm{DF}}\sin\beta_{\mathrm{DF}}\sin\phi_{\mathrm{DF}}+\cos\beta_{\mathrm{DF}}\cos\phi_{\mathrm{DF}}
\end{pmatrix}
\tag{114}
$$

The dielectric tensor is diagonal in the DF. If we calculate the dipole polarizabilility tensor in the DF it will also be diagonal, with elements

$$
\alpha^{\mathrm{DF}} = \begin{pmatrix}
\alpha_{11}^{\mathrm{DF}} & 0 & 0 \\
0 & \alpha_{22}^{\mathrm{DF}} & 0 \\
0 & 0 & \alpha_{33}^{\mathrm{DF}}
\end{pmatrix}
\tag{115}
$$

The polarizability tensor in the TF is given by

$$
(\alpha^{\mathrm{TF}})_{im} = R_{ij}(\alpha^{\mathrm{DF}})_{jk}(R^{-1})_{km}
\tag{116}
$$

Thus, we can describe a general anisotropic material if we provide, for each lattice site, the three diagonal elements $\epsilon_{jj}^{\mathrm{DF}}$ of the dielectric tensor in the DF, and the three rotation angles θ_{DF}, β_{DF}, and ϕ_{DF}. We first use the LDR prescription and the elements to obtain the three diagonal elements $\alpha_{jj}^{\mathrm{DF}}$ of the polarizability tensor in the DF. We then calculate the polarizability tensor α^{TF} using eq. (116).

27   Postprocessing: Calculating E and B In or Near the Target

For some scientific applications (e.g., surface-enhanced Raman scattering) one wishes to calculate the electric field just outside the target boundary. It may also be of interest to calculate the electromagnetic field at positions within the target volume. **DDSCAT** includes tools to carry out such calculations.

When **DDSCAT** is run with option `IWRPOL=1`, it creates files w*xxx*r*yyy*k*zzz*.pol*n* for *n*=1 and (if `IORTH=2`) *n*=2. These files store the solution for the dipole polarizations, allowing postprocessing. Of particular interest is calculation of the electromagnetic field at locations in or near the target.

To facilitate this, we provide a Fortran subroutine `READPOL` (in the file `readpol.f90`) that reads in data from the w*xxx*r*yyy*k*zzz*.pol*n* file.

In addition, we provide a Fortran program `DDfield.f90` that calls subroutine `READPOL`, and uses the data read in by `READPOL` to calculate the electric and magnetic field at locations specified by the user. The **E** and **B** contributions from the oscillating dipoles are calculated [including retardation effects – see, e.g., equations (7) and (10) from Draine & Weingartner (1996)] giving the "exact" electromagnetic field contributed by the oscillating dipoles. The incident plane wave field is added to the field generated by the oscillating dipoles to obtain the total **E** and **B** at the specified location.

The user is interested in the continuous and finite field in a real target, as opposed to the field generated by an array of oscillating point dipoles, which diverges as one approaches any one of the dipoles. To suppress the divergences, the contributions of dipoles within a distance d of the selected point is obtained by multiplying the "exact" contribution from the point dipole by a factor $\phi(r)$ that goes to zero more rapidly than r^3, thus ensuring that the electric field contribution from an individual dipole goes to zero as we approach the dipole location. This is desired, because the discrete dipole approximation is based on the assumption that a given dipole is polarized by the electric field from the incident wave plus the electric field contributed by all *other* dipoles. When dealing with periodic (i.e., infinite) targets, the function $\phi(r)$ smoothly suppresses the contributions from distant dipoles, allowing the summations to be truncated. Please refer to Draine & Flatau (2008) for further discussion of $\phi(r)$ and examples of results calculated by `DDfield`.

To calculate the electric and magnetic field at user-selected locations:

- Run `ddscat` with `WRPOL=1` to create a file with the stored polarization (for example, `w000r000k000.pol1`)

- Compile and link the `DDfield` code, by entering the `src` directory and typing
  `make ddfield`
  This will create an executable named `DDfield`

- Use an editor to create a file `ddfield.in` providing the name of the file (*in quotes!, where "quote" should be the "apostrophe" character*) containing the stored target polarization,
  followed by the value of the *interaction cutoff parameter* γ (see Draine & Flatau 2008, eq. 79) to be used,
  followed by the information defining a "track" along which **E** and **B** will be sampled. The track is specified by the beginning and end points (x_1, y_1, z_1) and (x_N, y_N, z_N) in the TF, in units of dipole spacing d, followed by an integer specifying the number N of points in the track. Thus, for example:
  '*filename*'
  γ
  $x_1/d \quad y_1/d \quad z_1/d \quad x_N/d \quad y_N/d \quad z_N/d \quad N \quad$ *for track 1*
  $x_1/d \quad y_1/d \quad z_1/d \quad x_N/d \quad y_N/d \quad z_N/d \quad N \quad$ *for track 2*
  ...
  $x_1/d \quad y_1/d \quad z_1/d \quad x_N/d \quad y_N/d \quad z_N/d \quad N \quad$ *for last track*

  Here $x_j/d \quad y_j/d \quad z_j/d$ are integer or decimal numbers giving the coordinates (in the "Target Frame", in units of the lattice spacing d) of the positions at which the electromagnetic field is to be evaluated.

- Type
      ddfield
  to run the executable.

- The output will be written to two files, `DDfield.E` and `DDBfield.B`, containing the electric and magnetic fields (given as complex vectors) at each chosen location. The fields are evaluated at a time when the factor $e^{-i\omega t}$ is 1 (e.g., $t = 0, 2\pi/\omega, ...$).

27.1 Sample Calculation

Here is an example of an input file `ddfield.in`:

```
'w000r000k000.pol1'      = name of file with stored polarization
5.00e-3 = gamma (interaction cutoff parameter)
-64.   0.  0. 32.  0.  0. 481    (xa,ya,za , xb,yb,zb , NAB)
```

The above example will sample the EM field at 481 points uniformly spaced along a track running from $(x/d, y/d, z/d) = (-64, 0, 0)$ to $(32, 0, 0)$ at intervals of $\delta x = 0.2d$.

Here's a second example of an input file `ddfield.in`:

```
'w000r000k000.pol1'      = name of file with stored polarization
5.00e-3 = gamma (interaction cutoff parameter)
-64. 32.64 32.64 32 32.64 32.64 481  (xa,ya,za , xb,yb,zb , NAB)
```

Note that x, y, z are specified in the **Target Frame**, and in units of d. To properly locate these you will need to know the location of the TF origin $(0, 0, 0)$ – see the target descriptions in §§19,20.

We have run `DDfield` on the output created by the "test problem" of a rectangular gold block with dimensions 0.5μm $\times 1\mu$m $\times 1\mu$m illuminated by a plane wave with wavelength $\lambda = 0.5\mu$m incident normal to the 1μm $\times 1\mu$m surface. The Au target has refractive index $m = 0.9656 + 1.8628i$ (dielectric function $\epsilon = -2.5374 + 3.5975i$). (see §8).

For the $(x, 0, 0)$ track running through the center of the slab, the output `DDfield.E` file will look like

```
    131072 = number of dipoles in Target
Extent of occupied lattice sites
      1        32 = JXMIN,JXMAX
      1        64 = JYMIN,JYMAX
      1        64 = JZMIN,JZMAX
 -32.000000     0.000000 = (x_TF/d)min,(x_TF/d)max
 -32.000000    32.000000 = (y_TF/d)min,(y_TF/d)max
 -32.000000    32.000000 = (z_TF/d)min,(z_TF/d)max
  -0.499997     0.000000 = xmin(TF),xmax(TF) (phys. units)
  -0.499997     0.499997 = ymin(TF),ymax(TF) (phys. units)
  -0.499997     0.499997 = zmin(TF),zmax(TF) (phys. units)
   0.015625 = d (phys units)
```
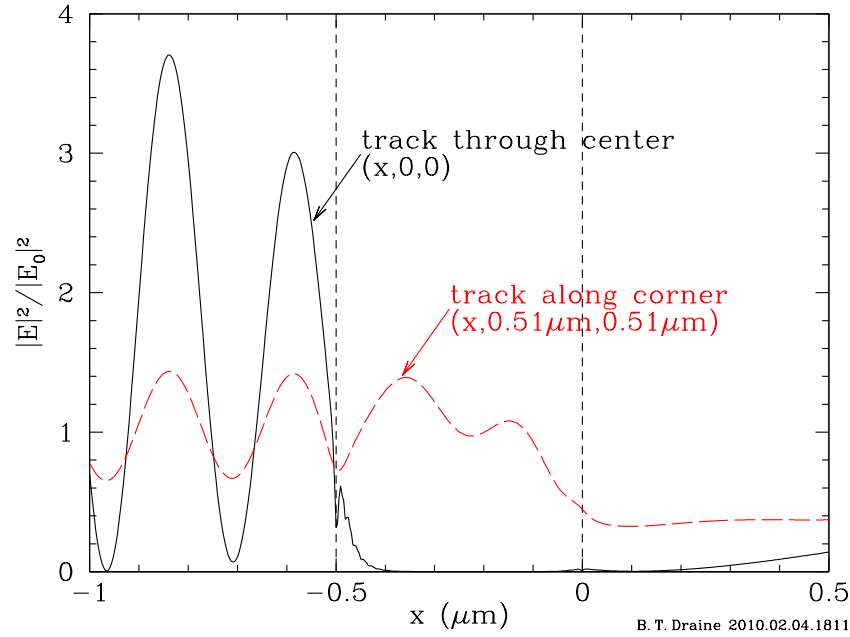
Figure 11: Solid line: $|E|^2$ on track passing through center of Au block for the sample problem calculated using target option `RCTGLPRSM`. Dotted lines show where the Au block surface is located. Note how weak the **E** field is inside the Au. Dashed line: $|E|^2$ on track passing near the corner of the slab. Incident radiation is propagating in the $+x$ direction.

```
  0.000000     0.000000 = PYD,PZD = period_y/dy, period_z/dz
  0.000000     0.000000 = period_y, period_z (phys. units)
  0.500000 = wavelength in ambient medium (phys units)
  0.196349 = k_x*d for incident wave
  0.000000 = k_y*d for incident wave
  0.000000 = k_z*d for incident wave
5.000E-03 = gamma (parameter for summation cutoff)
 0.000000  0.000000 = (Re,Im)E_inc,x(0,0,0)
 1.000000  0.000000 = (Re,Im)E_inc,y(0,0,0)
 0.000000  0.000000 = (Re,Im)E_inc,z(0,0,0)
   x/d       y/d      z/d       ----- E_x -----     ----- E_y ------    ----- E_z -----
 -64.0000  0.0000   0.0000   0.00000  0.00000   0.26693 -0.79540   0.00000  0.00000
 -63.8000  0.0000   0.0000   0.00000  0.00000   0.23994 -0.72895   0.00000  0.00000
 -63.6000  0.0000   0.0000   0.00000  0.00000   0.21246 -0.66168   0.00000  0.00000
 -63.4000  0.0000   0.0000   0.00000  0.00000   0.18452 -0.59368   0.00000  0.00000
 -63.2000  0.0000   0.0000   0.00000  0.00000   0.15614 -0.52505   0.00000  0.00000
 -63.0000  0.0000   0.0000   0.00000  0.00000   0.12738 -0.45588   0.00000  0.00000
 -62.8000  0.0000   0.0000   0.00000  0.00000   0.09826 -0.38630   0.00000  0.00000
 -62.6000  0.0000   0.0000   0.00000  0.00000   0.06882 -0.31641   0.00000  0.00000
 -62.4000  0.0000   0.0000   0.00000  0.00000   0.03910 -0.24629   0.00000  0.00000
 -62.2000  0.0000   0.0000   0.00000  0.00000   0.00915 -0.17606   0.00000  0.00000
 -62.0000  0.0000   0.0000   0.00000  0.00000  -0.02102 -0.10582   0.00000  0.00000
 -61.8000  0.0000   0.0000   0.00000  0.00000  -0.05135 -0.03568   0.00000  0.00000
 -61.6000  0.0000   0.0000   0.00000  0.00000  -0.08178  0.03426   0.00000  0.00000
 -61.4000  0.0000   0.0000   0.00000  0.00000  -0.11230  0.10390   0.00000  0.00000
 -61.2000  0.0000   0.0000   0.00000  0.00000  -0.14287  0.17314   0.00000  0.00000
 -61.0000  0.0000   0.0000   0.00000  0.00000  -0.17343  0.24187   0.00000  0.00000
...
  30.0000  0.0000   0.0000   0.00000  0.00000  -0.34868 -0.04369   0.00000  0.00000
  30.2000  0.0000   0.0000   0.00000  0.00000  -0.34974 -0.05307   0.00000  0.00000
  30.4000  0.0000   0.0000   0.00000  0.00000  -0.35052 -0.06257   0.00000  0.00000
  30.6000  0.0000   0.0000   0.00000  0.00000  -0.35103 -0.07216   0.00000  0.00000
  30.8000  0.0000   0.0000   0.00000  0.00000  -0.35124 -0.08185   0.00000  0.00000
  31.0000  0.0000   0.0000   0.00000  0.00000  -0.35119 -0.09163   0.00000  0.00000
  31.2000  0.0000   0.0000   0.00000  0.00000  -0.35082 -0.10148   0.00000  0.00000
  31.4000  0.0000   0.0000   0.00000  0.00000  -0.35020 -0.11141   0.00000  0.00000
  31.6000  0.0000   0.0000   0.00000  0.00000  -0.34926 -0.12140   0.00000  0.00000
  31.8000  0.0000   0.0000   0.00000  0.00000  -0.34804 -0.13144   0.00000  0.00000
  32.0000  0.0000   0.0000   0.00000  0.00000  -0.34645 -0.14151   0.00000  0.00000
```

In the example given, the incident wave is propagating in the $+x$ direction. The first layer of dipoles in the rectangular target is at $x/d = -31.5$, and the last layer is at $x/d = -0.5$. The "surface" of the target is at $x/d = -32$ ($x = -0.50\mu$m) and $x/d = 0$ ($x = 0$).

Figure 11 shows how $|E|^2$ varies along the tracks specified by the above two sample `ddfield.in` files. As expected, the wave is strongly suppressed in the interior of the Au block.

28 Finale

This User Guide is somewhat inelegant, but we hope that it will prove useful. The structure of the ddscat.par file is intended to be simple and suggestive so that, after reading the above notes once, the user may not have to refer to them again.

Known bugs in **DDSCAT** will be posted at the **DDSCAT** web site,

http://www.astro.princeton.edu/~draine/DDSCAT.html

and the latest version of **DDSCAT** will always be available at this site. The source code is also available at

http://code.google.com/p/ddscat/

There is also a wiki:

http://ddscat.wikidot.com/start

Users are encouraged to provide B. T. Draine (draine@astro.princeton.edu) with their email address; email notification of bug fixes, and any new releases of **DDSCAT**, will be made known to those who do!

P. J. Flatau maintains the WWW page "SCATTERLIB - Light Scattering Codes Library" with URL http://atol.ucsd.edu/~pflatau. The SCATTERLIB Internet site is a library of light scattering codes. Emphasis is on providing source codes (mostly FORTRAN). However, other information related to scattering on spherical and non-spherical particles is collected: an extensive list of references to light scattering methods, refractive index, etc. This URL page contains section on the discrete dipole approximation.

Concrete suggestions for improving **DDSCAT** (and this User Guide) are welcomed.

Users of **DDSCAT** may wish to cite papers describing DDA theory and its implementation, such as Draine (1988), Draine & Flatau (2004), and Draine & Flatau (2008). The latter reference describes extension of the DDA to periodic structures, and generalization of the Mueller scattering matrix to describe scattering by 1-d and 2-d periodic structures.

To cite this User Guide, we suggest the following citation:

Draine, B.T., & Flatau, P.J. 2010, "User Guide for the Discrete Dipole Approximation Code DDSCAT (Version 7.1)", http://arxiv.org/abs/1002.1505

Finally, the authors have one special request: We would appreciate preprints and (especially!) reprints of any papers which make use of **DDSCAT**!

29 Acknowledgments

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A Understanding and Modifying `ddscat.par`

In order to use DDSCAT to perform the specific calculations of interest to you, it will be necessary to modify the `ddscat.par` file. Here we list the sample `ddscat.par` file, followed by a discussion of how to modify this file as needed. Note that all numerical input data in DDSCAT is read with free-format `READ(IDEV,*)...` statements. Therefore you do not need to worry about the precise format in which integer or floating point numbers are entered on a line. The crucial thing is that lines in `ddscat.par` containing numerical data have the correct number of data entries, with any informational comments appearing *after* the numerical data on a given line.

```
' ========= Parameter file for v7.1.0 ==================='
'**** Preliminaries ****'
'NOTORQ' = CMTORQ*6 (NOTORQ, DOTORQ) -- either do or skip torque calculations
'PBCGS2' = CMDSOL*6 (PBCGS2, PBCGST, PETRKP) -- select solution method
'GPFAFT' = CMDFFT*6 (GPFAFT, FFTMKL)
'GKDLDR' = CALPHA*6 (GKDLDR, LATTDR
'NOTBIN' = CBINFLAG (NOTBIN, ORIBIN, ALLBIN)
'**** Initial Memory Allocation ****'
100 100 100 = dimensioning allowance for target generation
'**** Target Geometry and Composition ****'
'RCTGLPRSM' = CSHAPE*9 shape directive
32 64 64  = shape parameters 1 - 3
1         = NCOMP = number of dielectric materials
'../diel/Au_evap' = file with refractive index 1
'**** Error Tolerance ****'
1.00e-5 = TOL = MAX ALLOWED (NORM OF |G>=AC|E>-ACA|X>)/(NORM OF AC|E>)
'**** Interaction cutoff parameter for PBC calculations ****'
1.00e-2 = GAMMA (1e-2 is normal, 3e-3 for greater accuracy)
'**** Angular resolution for calculation of <cos>, etc. ****'
0.5 = ETASCA (number of angles is proportional to [(3+x)/ETASCA]^2 )
'**** Wavelengths (micron) ****'
0.5000 0.5000 1 'LIN' = wavelengths (first,last,how many,how=LIN,INV,LOG)
'**** Effective Radii (micron) **** '
0.49237 0.49237 1 'LIN' = aeff (first,last,how many,how=LIN,INV,LOG)
'**** Define Incident Polarizations ****'
(0,0) (1.,0.) (0.,0.) = Polarization state e01 (k along x axis)
2 = IORTH  (=1 to do only pol. state e01; =2 to also do orth. pol. state)
'**** Specify which output files to write ****'
1 = IWRKSC (=0 to suppress, =1 to write ".sca" file for each target orient.
1 = IWRPOL (=0 to suppress, =1 to write ".pol" file for each (BETA,THETA)
'**** Prescribe Target Rotations ****'
0.   0.   1  = BETAMI, BETAMX, NBETA  (beta=rotation around a1)
0.   0.   1  = THETMI, THETMX, NTHETA (theta=angle between a1 and k)
0.   0.   1  = PHIMIN, PHIMAX, NPHI (phi=rotation angle of a1 around k)
'**** Specify first IWAV, IRAD, IORI (normally 0 0 0) ****'
0   0   0    = first IWAV, first IRAD, first IORI (0 0 0 to begin fresh)
'**** Select Elements of S_ij Matrix to Print ****'
6 = NSMELTS = number of elements of S_ij to print (not more than 9)
11 12 21 22 31 41 = indices ij of elements to print
'**** Specify Scattered Directions ****'
'LFRAME' = CMDFRM (LFRAME, TFRAME for Lab Frame or Target Frame)
2 = number of scattering planes
0.  0. 180. 5 = phi, thetan_min, thetan_max, dtheta (in deg) for plane 1
90. 0. 180. 5 = phi, thetan_min, thetan_max, dtheta (in deg) for plane 2
```

Lines	Comments
1-2	comment lines
3	`NOTORQ` if torque calculation is not required;
	`DOTORQ` if torque calculation is required.
4	`PBCGS2` is recommended; other options are `PBCGST` and `PETRKP` (see §11).
5	`GPFAFT` is supplied as default, but `FFTMKL` is recommended if `DDSCAT` has been compiled with the Intel® Math Kernal Library (see §§6.5, 12).
6	`GKDLDR` is recommended as the prescription for polarizabilities (see §13)
7	`NOTBIN` for no unformatted binary output.
	`ORIBIN` for unformatted binary dump of orientational averages only;
	`ALLBIN` for full unformatted binary dump (§10.2);
8	comment line
9	initial memory allocation NX,NY,NZ. These must be large enough to accomodate the target that will be generated.
10	comment line
11	specify choice of target shape (see §19 for description of options `RCTGLPRSM`, `ELLIPSOID`, `TETRAHDRN`, ...)
12	shape parameters SHPAR1, SHPAR2, SHPAR3, ... (see §19).
13	number of different dielectric constant tables (§14).
14	name(s) of dielectric constant table(s) (one per line).
15	comment line
16	`TOL` = error tolerance h: maximum allowed value of $|A^\dagger E - A^\dagger AP|/|A^\dagger E|$ [see eq.(18)].
17	comment line
18	`GAMMA`= interaction cutoff parameter γ (see Draine & Flatau 2009)
	the value of γ does not affect calculations for isolated targets
19	comment line
20	`ETASCA` – parameter η controlling angular averages (§23).
21	comment line
22	λ – first, last, how many, how chosen.
23	comment line
24	a_{eff} – first, last, how many, how chosen.
25	comment line
26	specify x,y,z components of (complex) incident polarization $\hat{\mathbf{e}}_{01}$ (§22)
27	`IORTH` = 2 to do both polarization states (normal);
	`IORTH` = 1 to do only one incident polarization.
28	comment line
29	`IWRKSC` = 0 to suppress writing of ".sca" files;
	`IWRKSC` = 1 to enable writing of ".sca" files.
30	`IWRPOL` = 0 to suppress writing of ".pol" files.
	`IWRPOL` = 1 to write ".pol" files.
31	comment line
32	β (see §17) – first, last, how many .
33	Θ (see §17) – first, last, how many.
34	Φ (see §17) – first, last, how many.
35	comment line
36	`IWAV0 IRAD0 IORI0` – starting values of integers IWAV IRAD IORI (normally `0 0 0`).
37	comment line
38	N_S = number of scattering matrix elements (must be ≤ 9)
39	indices ij of N_S elements of the scattering matrix S_{ij}
40	comment line
41	specify whether scattered directions are to be specified by CMDFRM=`'LFRAME'` or `'TFRAME'`.
42	= number of scattering planes to follow
43	ϕ_s for first scattering plane, $\theta_{s,min}$, $\theta_{s,max}$, how many θ_s values;
44,...	ϕ_s for 2nd,... scattering plane, ...

B   w*xxx*r*yyy*.avg **Files**

The file w000r000ori.avg contains the results for the first wavelength (w000) and first target radius
(r000) averaged over orientations (.avg). The w000r000ori.avg file generated by the sample
calculation should look like the following:

```
 DDSCAT --- DDSCAT 7.1.0 [10.02.04]
 TARGET --- Rectangular prism; NX,NY,NZ=  32  64  64
 GPFAFT --- method of solution
 GKDLDR --- prescription for polarizabilies
 RCTGLPRSM --- shape
  131072     = NAT0 = number of dipoles
  0.03173411 = d/aeff for this target [d=dipole spacing]
    0.015625 = d (physical units)
  AEFF=      0.492370 = effective radius (physical units)
  WAVE=      0.500000 = wavelength (physical units)
K*AEFF=      6.187304 = 2*pi*aeff/lambda
n= ( 0.9656 ,  1.8628), eps.= ( -2.5374 ,  3.5975)  |m|kd=  0.4120 for subs. 1
   TOL= 1.000E-05 = error tolerance for CCG method
( 1.00000  0.00000  0.00000) = target axis A1 in Target Frame
( 0.00000  1.00000  0.00000) = target axis A2 in Target Frame
  NAVG=  2292 = (theta,phi) values used in comp. of Qsca,g
( 0.19635  0.00000  0.00000) = k vector (latt. units) in Lab Frame
( 0.00000, 0.00000)( 1.00000, 0.00000)( 0.00000, 0.00000)=inc.pol.vec. 1 in LF
( 0.00000, 0.00000)( 0.00000, 0.00000)( 1.00000, 0.00000)=inc.pol.vec. 2 in LF
    0.000    0.000 = beta_min, beta_max ;  NBETA = 1
    0.000    0.000 = theta_min, theta_max; NTHETA= 1
    0.000    0.000 = phi_min, phi_max   ;  NPHI = 1

  0.5000 = ETASCA = param. controlling # of scatt. dirs used to calculate <cos> etc.
 Results averaged over    1 target orientations
                 and    2 incident polarizations
         Qext      Qabs      Qsca      g(1)=<cos>  <cos^2>    Qbk       Qpha
JO=1:  3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
JO=2:  3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
mean:  3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
Qpol= -4.5300E-06                                         dQpha= -1.0133E-06
        Qsca*g(1)   Qsca*g(2)   Qsca*g(3)   iter  mxiter  Nsca
JO=1:  1.1179E+00 -9.4339E-08  3.3191E-07    27    117   2292
JO=2:  1.1179E+00  1.9882E-07 -2.6904E-08    29    117   2292
mean:  1.1179E+00  5.2242E-08  1.5250E-07
         Mueller matrix elements for selected scattering directions in Lab Frame
  theta   phi    Pol.    S_11       S_12       S_21       S_22       S_31       S_41
   0.00   0.00  0.00000  1.2306E+03 -1.4038E-03 -1.404E-03  1.231E+03 -5.918E-05 -2.785E-05
   5.00   0.00  0.01832  1.0648E+03 -1.9511E+01 -1.951E+01  1.065E+03 -9.344E-05  8.054E-07
  10.00   0.00  0.08034  6.7623E+02 -5.4325E+01 -5.433E+01  6.762E+02 -9.059E-05  1.788E-05
  15.00   0.00  0.21696  2.9300E+02 -6.3568E+01 -6.357E+01  2.930E+02 -4.868E-05  7.888E-05
  20.00   0.00  0.52316  7.4600E+01 -3.9028E+01 -3.903E+01  7.460E+01  1.372E-05  4.646E-05
  25.00   0.00  0.47166  2.1356E+01 -1.0073E+01 -1.007E+01  2.136E+01  3.462E-05 -1.389E-05
  30.00   0.00  0.09869  3.8576E+01 -3.8070E+00 -3.807E+00  3.858E+01  1.067E-05 -8.347E-05
  35.00   0.00  0.33427  4.8965E+01 -1.6368E+01 -1.637E+01  4.897E+01 -2.223E-05 -1.148E-04
  40.00   0.00  0.69023  3.7585E+01 -2.5942E+01 -2.594E+01  3.759E+01 -5.071E-05 -9.225E-05
  45.00   0.00  0.93616  2.2608E+01 -2.1165E+01 -2.116E+01  2.261E+01 -4.507E-05 -2.219E-07
  50.00   0.00  0.55260  1.6124E+01 -8.9100E+00 -8.910E+00  1.612E+01 -2.009E-05  5.881E-05
  55.00   0.00  0.04414  1.5380E+01 -6.7895E-01 -6.789E-01  1.538E+01  3.102E-05  1.028E-04
  60.00   0.00  0.00152  1.4134E+01  2.1518E-02  2.152E-02  1.413E+01  4.444E-05  9.157E-05
  65.00   0.00  0.25433  1.0795E+01 -2.7454E+00 -2.745E+00  1.079E+01  5.736E-05  6.703E-05
  70.00   0.00  0.61640  7.1817E+00 -4.4268E+00 -4.427E+00  7.182E+00  4.303E-05  3.109E-05
  75.00   0.00  0.84301  4.7205E+00 -3.9795E+00 -3.979E+00  4.721E+00  2.952E-05  5.581E-06
  80.00   0.00  0.83319  3.3467E+00 -2.7884E+00 -2.788E+00  3.347E+00  1.446E-05 -5.168E-06
  85.00   0.00  0.83162  2.5365E+00 -2.1094E+00 -2.109E+00  2.536E+00  1.247E-05 -1.128E-05
  90.00   0.00  0.95712  2.1245E+00 -2.0334E+00 -2.033E+00  2.124E+00  1.498E-05 -9.050E-06
  95.00   0.00  0.97305  2.1420E+00 -2.0843E+00 -2.084E+00  2.142E+00  2.119E-05 -6.176E-06
 100.00   0.00  0.86407  2.4048E+00 -2.0779E+00 -2.078E+00  2.405E+00  2.250E-05 -4.506E-07
 105.00   0.00  0.86090  2.6074E+00 -2.2447E+00 -2.245E+00  2.607E+00  1.945E-05  6.889E-07
 110.00   0.00  0.95634  2.8343E+00 -2.7105E+00 -2.711E+00  2.834E+00  1.241E-05 -5.764E-06
 115.00   0.00  0.84227  3.7313E+00 -3.1428E+00 -3.143E+00  3.731E+00  7.830E-06 -2.114E-05
 120.00   0.00  0.53216  5.8481E+00 -3.1121E+00 -3.112E+00  5.848E+00  4.552E-06 -4.294E-05
 125.00   0.00  0.31008  8.7198E+00 -2.7039E+00 -2.704E+00  8.720E+00  1.571E-05 -5.892E-05
```

```
130.00    0.00   0.21846   1.0852E+01  -2.3708E+00  -2.371E+00   1.085E+01   3.464E-05  -6.386E-05
135.00    0.00   0.19080   1.0801E+01  -2.0610E+00  -2.061E+00   1.080E+01   4.566E-05  -4.999E-05
140.00    0.00   0.14140   8.1464E+00  -1.1519E+00  -1.152E+00   8.146E+00   4.584E-05  -2.501E-05
145.00    0.00   0.01267   3.8742E+00   4.9092E-02   4.909E-02   3.874E+00   3.123E-05  -1.770E-06
150.00    0.00   0.35726   1.7618E+00  -6.2942E-01  -6.294E-01   1.762E+00   5.787E-06   1.075E-05
155.00    0.00   0.45976   1.1004E+01  -5.0593E+00  -5.059E+00   1.100E+01  -2.023E-05   6.036E-06
160.00    0.00   0.25129   4.5243E+01  -1.1369E+01  -1.137E+01   4.524E+01  -3.670E-05  -1.867E-05
165.00    0.00   0.12705   1.1280E+02  -1.4331E+01  -1.433E+01   1.128E+02  -2.745E-05  -4.470E-05
170.00    0.00   0.05271   2.0294E+02  -1.0697E+01  -1.070E+01   2.029E+02  -8.684E-06  -9.197E-05
175.00    0.00   0.01266   2.8300E+02  -3.5830E+00  -3.583E+00   2.830E+02   6.964E-06  -1.170E-04
180.00    0.00   0.00000   3.1528E+02   1.0529E-03   1.053E-03   3.153E+02   3.305E-05  -1.139E-04
  0.00   90.00   0.00000   1.2306E+03   1.4038E-03   1.404E-03   1.231E+03   6.016E-05  -2.801E-05
  5.00   90.00   0.01833   1.0648E+03  -1.9514E+01  -1.951E+01   1.065E+03   2.780E-05  -3.678E-05
 10.00   90.00   0.08033   6.7623E+02  -5.4322E+01  -5.432E+01   6.762E+02   1.102E-05  -3.231E-05
 15.00   90.00   0.21697   2.9299E+02  -6.3570E+01  -6.357E+01   2.930E+02   1.738E-05  -2.438E-05
 20.00   90.00   0.52318   7.4600E+01  -3.9029E+01  -3.903E+01   7.460E+01   2.034E-05  -1.601E-05
 25.00   90.00   0.47167   2.1356E+01  -1.0073E+01  -1.007E+01   2.136E+01  -1.107E-06  -1.376E-05
 30.00   90.00   0.09869   3.8576E+01  -3.8071E+00  -3.807E+00   3.858E+01  -2.730E-05  -1.969E-05
 35.00   90.00   0.33427   4.8965E+01  -1.6367E+01  -1.637E+01   4.896E+01  -4.634E-05  -2.751E-05
 40.00   90.00   0.69023   3.7585E+01  -2.5943E+01  -2.594E+01   3.759E+01  -3.474E-05  -2.855E-05
 45.00   90.00   0.93616   2.2608E+01  -2.1165E+01  -2.116E+01   2.261E+01  -2.394E-06  -2.566E-05
 50.00   90.00   0.55260   1.6124E+01  -8.9099E+00  -8.910E+00   1.612E+01   3.199E-05  -2.475E-05
 55.00   90.00   0.04413   1.5380E+01  -6.7869E-01  -6.787E-01   1.538E+01   5.216E-05  -3.188E-05
 60.00   90.00   0.00154   1.4133E+01   2.1708E-02   2.171E-02   1.413E+01   4.590E-05  -3.833E-05
 65.00   90.00   0.25432   1.0795E+01  -2.7453E+00  -2.745E+00   1.079E+01   2.070E-05  -3.406E-05
 70.00   90.00   0.61638   7.1818E+00  -4.4267E+00  -4.427E+00   7.182E+00  -6.848E-06  -1.910E-05
 75.00   90.00   0.84300   4.7205E+00  -3.9794E+00  -3.979E+00   4.721E+00  -2.576E-05   9.569E-07
 80.00   90.00   0.83319   3.3466E+00  -2.7883E+00  -2.788E+00   3.347E+00  -2.862E-05   1.663E-05
 85.00   90.00   0.83162   2.5364E+00  -2.1093E+00  -2.109E+00   2.536E+00  -1.826E-05   2.157E-05
 90.00   90.00   0.95713   2.1244E+00  -2.0333E+00  -2.033E+00   2.124E+00  -7.100E-08   1.742E-05
 95.00   90.00   0.97305   2.1420E+00  -2.0842E+00  -2.084E+00   2.142E+00   1.977E-05   1.030E-05
100.00   90.00   0.86407   2.4047E+00  -2.0778E+00  -2.078E+00   2.405E+00   3.345E-05   7.257E-06
105.00   90.00   0.86090   2.6073E+00  -2.2446E+00  -2.245E+00   2.607E+00   3.586E-05   1.214E-05
110.00   90.00   0.95634   2.8342E+00  -2.7104E+00  -2.710E+00   2.834E+00   2.374E-05   2.154E-05
115.00   90.00   0.84225   3.7312E+00  -3.1426E+00  -3.143E+00   3.731E+00   6.297E-07   2.754E-05
120.00   90.00   0.53214   5.8481E+00  -3.1120E+00  -3.112E+00   5.848E+00  -2.385E-05   2.262E-05
125.00   90.00   0.31007   8.7197E+00  -2.7037E+00  -2.704E+00   8.720E+00  -3.821E-05   6.028E-06
130.00   90.00   0.21846   1.0852E+01  -2.3708E+00  -2.371E+00   1.085E+01  -3.448E-05  -1.354E-05
135.00   90.00   0.19080   1.0801E+01  -2.0610E+00  -2.061E+00   1.080E+01  -1.698E-05  -2.486E-05
140.00   90.00   0.14140   8.1462E+00  -1.1519E+00  -1.152E+00   8.146E+00   1.131E-06  -2.232E-05
145.00   90.00   0.01267   3.8740E+00   4.9075E-02   4.908E-02   3.874E+00   6.794E-06  -9.904E-06
150.00   90.00   0.35722   1.7617E+00  -6.2933E-01  -6.293E-01   1.762E+00  -1.560E-07   1.926E-06
155.00   90.00   0.45974   1.1005E+01  -5.0592E+00  -5.059E+00   1.100E+01  -8.574E-06   1.684E-06
160.00   90.00   0.25128   4.5243E+01  -1.1369E+01  -1.137E+01   4.524E+01  -7.389E-06  -1.695E-05
165.00   90.00   0.12704   1.1280E+02  -1.4331E+01  -1.433E+01   1.128E+02   1.518E-06  -5.206E-05
170.00   90.00   0.05271   2.0294E+02  -1.0698E+01  -1.070E+01   2.029E+02   8.093E-06  -9.152E-05
175.00   90.00   0.01267   2.8300E+02  -3.5861E+00  -3.586E+00   2.830E+02  -2.762E-06  -1.182E-04
180.00   90.00   0.00000   3.1528E+02  -1.0834E-03  -1.083E-03   3.153E+02  -3.244E-05  -1.142E-04
```

C   w*xxx*r*yyy*k*zzz*.sca **Files**

The w000r000k000.sca file contains the results for the first wavelength (w000), first target radius
(r000), and first orientation (k000). The w000r000k000.sca file created by the sample calculation
should look like the following:

```
 DDSCAT --- DDSCAT 7.1.0 [10.02.04]
 TARGET --- Rectangular prism; NX,NY,NZ=  32  64  64
 GPFAFT --- method of solution
 GKDLDR --- prescription for polarizabilities
 RCTGLPRSM --- shape
  131072     = NAT0 = number of dipoles
  0.03173411 = d/aeff for this target [d=dipole spacing]
    0.015625 = d (physical units)
----- physical extent of target volume in Target Frame ------
     -0.499997       0.000000 = xmin,xmax (physical units)
     -0.499997       0.499997 = ymin,ymax (physical units)
     -0.499997       0.499997 = zmin,zmax (physical units)
   AEFF=      0.492370 = effective radius (physical units)
   WAVE=      0.500000 = wavelength (physical units)
K*AEFF=      6.187304 = 2*pi*aeff/lambda
n= ( 0.9656 ,  1.8628), eps.= ( -2.5374 ,  3.5975)  |m|kd=  0.4120 for subs. 1
   TOL= 1.000E-05 = error tolerance for CCG method
( 1.00000  0.00000  0.00000) = target axis A1 in Target Frame
( 0.00000  1.00000  0.00000) = target axis A2 in Target Frame
   NAVG=  2292 = (theta,phi) values used in comp. of Qsca,g
( 0.19635  0.00000  0.00000) = k vector (latt. units) in TF
( 0.00000, 0.00000)( 1.00000, 0.00000)( 0.00000, 0.00000)=inc.pol.vec. 1 in TF
( 0.00000, 0.00000)( 0.00000, 0.00000)( 1.00000, 0.00000)=inc.pol.vec. 2 in TF
( 1.00000  0.00000  0.00000) = target axis A1 in Lab Frame
( 0.00000  1.00000  0.00000) = target axis A2 in Lab Frame
( 0.19635  0.00000  0.00000) = k vector (latt. units) in Lab Frame
( 0.00000, 0.00000)( 1.00000, 0.00000)( 0.00000, 0.00000)=inc.pol.vec. 1 in LF
( 0.00000, 0.00000)( 0.00000, 0.00000)( 1.00000, 0.00000)=inc.pol.vec. 2 in LF
 BETA =  0.000 = rotation of target around A1
 THETA=  0.000 = angle between A1 and k
  PHI =  0.000 = rotation of A1 around k
 0.5000 = ETASCA = param. controlling # of scatt. dirs used to calculate <cos> etc.
         Qext       Qabs       Qsca      g(1)=<cos>  <cos^2>     Qbk       Qpha
JO=1: 3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
JO=2: 3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
mean: 3.6494E+00 1.2208E+00 2.4287E+00  4.6029E-01 8.7798E-01 2.6214E+00 -1.7030E-01
Qpol= -4.5300E-06                                            dQpha= -1.0133E-06
         Qsca*g(1)   Qsca*g(2)   Qsca*g(3)    iter   mxiter  Nsca
JO=1: 1.1179E+00 -9.4339E-08  3.3191E-07      27    117    2292
JO=2: 1.1179E+00  1.9882E-07 -2.6904E-08      29    117    2292
mean: 1.1179E+00  5.2242E-08  1.5250E-07
          Mueller matrix elements for selected scattering directions in Lab Frame
   theta   phi   Pol.    S_11      S_12        S_21       S_22        S_31        S_41
   0.00   0.00  0.00000  1.2306E+03 -1.4038E-03 -1.404E-03  1.231E+03 -5.918E-05 -2.785E-05
   5.00   0.00  0.01832  1.0648E+03 -1.9511E+01 -1.951E+01  1.065E+03 -9.344E-05  8.054E-07
  10.00   0.00  0.08034  6.7623E+02 -5.4325E+01 -5.433E+01  6.762E+02 -9.059E-05  1.788E-05
  15.00   0.00  0.21696  2.9300E+02 -6.3568E+01 -6.357E+01  2.930E+02 -4.868E-05  7.888E-05
  20.00   0.00  0.52316  7.4600E+01 -3.9028E+01 -3.903E+01  7.460E+01  1.372E-05  4.646E-05
  25.00   0.00  0.47166  2.1356E+01 -1.0073E+01 -1.007E+01  2.136E+01  3.462E-05 -1.389E-05
  30.00   0.00  0.09869  3.8576E+01 -3.8070E+00 -3.807E+00  3.858E+01  1.067E-05 -8.347E-05
  35.00   0.00  0.33427  4.8965E+01 -1.6368E+01 -1.637E+01  4.897E+01 -2.223E-05 -1.148E-04
  40.00   0.00  0.69023  3.7585E+01 -2.5942E+01 -2.594E+01  3.759E+01 -5.071E-05 -9.225E-05
  45.00   0.00  0.93616  2.2608E+01 -2.1165E+01 -2.116E+01  2.261E+01 -4.507E-05 -2.219E-07
  50.00   0.00  0.55260  1.6124E+01 -8.9100E+00 -8.910E+00  1.612E+01 -2.009E-05  5.881E-05
  55.00   0.00  0.04414  1.5380E+01 -6.7895E-01 -6.789E-01  1.538E+01  3.102E-05  1.028E-04
  60.00   0.00  0.00152  1.4134E+01  2.1518E-02  2.152E-02  1.413E+01  4.444E-05  9.157E-05
  65.00   0.00  0.25433  1.0795E+01 -2.7454E+00 -2.745E+00  1.079E+01  5.736E-05  6.703E-05
  70.00   0.00  0.61640  7.1817E+00 -4.4268E+00 -4.427E+00  7.182E+00  4.303E-05  3.109E-05
  75.00   0.00  0.84301  4.7205E+00 -3.9795E+00 -3.979E+00  4.721E+00  2.952E-05  5.581E-06
  80.00   0.00  0.83319  3.3467E+00 -2.7884E+00 -2.788E+00  3.347E+00  1.446E-05 -5.168E-06
  85.00   0.00  0.83162  2.5365E+00 -2.1094E+00 -2.109E+00  2.536E+00  1.247E-05 -1.128E-05
  90.00   0.00  0.95712  2.1245E+00 -2.0334E+00 -2.033E+00  2.124E+00  1.498E-05 -9.050E-06
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 95.00    0.00   0.97305   2.1420E+00  -2.0843E+00  -2.084E+00   2.142E+00   2.119E-05  -6.176E-06
100.00    0.00   0.86407   2.4048E+00  -2.0779E+00  -2.078E+00   2.405E+00   2.250E-05  -4.506E-07
105.00    0.00   0.86090   2.6074E+00  -2.2447E+00  -2.245E+00   2.607E+00   1.945E-05   6.889E-07
110.00    0.00   0.95634   2.8343E+00  -2.7105E+00  -2.711E+00   2.834E+00   1.241E-05  -5.764E-06
115.00    0.00   0.84227   3.7313E+00  -3.1428E+00  -3.143E+00   3.731E+00   7.830E-06  -2.114E-05
120.00    0.00   0.53216   5.8481E+00  -3.1121E+00  -3.112E+00   5.848E+00   4.552E-06  -4.294E-05
125.00    0.00   0.31008   8.7198E+00  -2.7039E+00  -2.704E+00   8.720E+00   1.571E-05  -5.892E-05
130.00    0.00   0.21846   1.0852E+01  -2.3708E+00  -2.371E+00   1.085E+01   3.464E-05  -6.386E-05
135.00    0.00   0.19080   1.0801E+01  -2.0610E+00  -2.061E+00   1.080E+01   4.566E-05  -4.999E-05
140.00    0.00   0.14140   8.1464E+00  -1.1519E+00  -1.152E+00   8.146E+00   4.584E-05  -2.501E-05
145.00    0.00   0.01267   3.8742E+00   4.9092E-02   4.909E-02   3.874E+00   3.123E-05  -1.770E-06
150.00    0.00   0.35726   1.7618E+00  -6.2942E-01  -6.294E-01   1.762E+00   5.787E-06   1.075E-05
155.00    0.00   0.45976   1.1004E+01  -5.0593E+00  -5.059E+00   1.100E+01  -2.023E-05   6.036E-06
160.00    0.00   0.25129   4.5243E+01  -1.1369E+01  -1.137E+01   4.524E+01  -3.670E-05  -1.867E-05
165.00    0.00   0.12705   1.1280E+02  -1.4331E+01  -1.433E+01   1.128E+02  -2.745E-05  -4.470E-05
170.00    0.00   0.05271   2.0294E+02  -1.0697E+01  -1.070E+01   2.029E+02  -8.684E-06  -9.197E-05
175.00    0.00   0.01266   2.8300E+02  -3.5830E+00  -3.583E+00   2.830E+02   6.964E-06  -1.170E-04
180.00    0.00   0.00000   3.1528E+02   1.0529E-03   1.053E-03   3.153E+02   3.305E-05  -1.139E-04
  0.00   90.00   0.00000   1.2306E+03   1.4038E-03   1.404E-03   1.231E+03   6.016E-05  -2.801E-05
  5.00   90.00   0.01833   1.0648E+03  -1.9514E+01  -1.951E+01   1.065E+03   2.780E-05  -3.678E-05
 10.00   90.00   0.08033   6.7623E+02  -5.4322E+01  -5.432E+01   6.762E+02   1.102E-05  -3.231E-05
 15.00   90.00   0.21697   2.9299E+02  -6.3570E+01  -6.357E+01   2.930E+02   1.738E-05  -2.438E-05
 20.00   90.00   0.52318   7.4600E+01  -3.9029E+01  -3.903E+01   7.460E+01   2.034E-05  -1.601E-05
 25.00   90.00   0.47167   2.1356E+01  -1.0073E+01  -1.007E+01   2.136E+01  -1.107E-06  -1.376E-05
 30.00   90.00   0.09869   3.8576E+01  -3.8071E+00  -3.807E+00   3.858E+01  -2.730E-05  -1.969E-05
 35.00   90.00   0.33427   4.8965E+01  -1.6367E+01  -1.637E+01   4.896E+01  -4.634E-05  -2.751E-05
 40.00   90.00   0.69023   3.7585E+01  -2.5943E+01  -2.594E+01   3.759E+01  -3.474E-05  -2.855E-05
 45.00   90.00   0.93616   2.2608E+01  -2.1165E+01  -2.116E+01   2.261E+01  -2.394E-06  -2.566E-05
 50.00   90.00   0.55260   1.6124E+01  -8.9099E+00  -8.910E+00   1.612E+01   3.199E-05  -2.475E-05
 55.00   90.00   0.04413   1.5380E+01  -6.7869E-01  -6.787E-01   1.538E+01   5.216E-05  -3.188E-05
 60.00   90.00   0.00154   1.4133E+01   2.1708E-02   2.171E-02   1.413E+01   4.590E-05  -3.833E-05
 65.00   90.00   0.25432   1.0795E+01  -2.7453E+00  -2.745E+00   1.079E+01   2.070E-05  -3.406E-05
 70.00   90.00   0.61638   7.1818E+00  -4.4267E+00  -4.427E+00   7.182E+00  -6.848E-06  -1.910E-05
 75.00   90.00   0.84300   4.7205E+00  -3.9794E+00  -3.979E+00   4.721E+00  -2.576E-05   9.569E-07
 80.00   90.00   0.83319   3.3466E+00  -2.7883E+00  -2.788E+00   3.347E+00  -2.862E-05   1.663E-05
 85.00   90.00   0.83162   2.5364E+00  -2.1093E+00  -2.109E+00   2.536E+00  -1.826E-05   2.157E-05
 90.00   90.00   0.95713   2.1244E+00  -2.0333E+00  -2.033E+00   2.124E+00  -7.100E-08   1.742E-05
 95.00   90.00   0.97305   2.1420E+00  -2.0842E+00  -2.084E+00   2.142E+00   1.977E-05   1.030E-05
100.00   90.00   0.86407   2.4047E+00  -2.0778E+00  -2.078E+00   2.405E+00   3.345E-05   7.257E-06
105.00   90.00   0.86090   2.6073E+00  -2.2446E+00  -2.245E+00   2.607E+00   3.586E-05   1.214E-05
110.00   90.00   0.95634   2.8342E+00  -2.7104E+00  -2.710E+00   2.834E+00   2.374E-05   2.154E-05
115.00   90.00   0.84225   3.7312E+00  -3.1426E+00  -3.143E+00   3.731E+00   6.297E-07   2.754E-05
120.00   90.00   0.53214   5.8481E+00  -3.1120E+00  -3.112E+00   5.848E+00  -2.385E-05   2.262E-05
125.00   90.00   0.31007   8.7197E+00  -2.7037E+00  -2.704E+00   8.720E+00  -3.821E-05   6.028E-06
130.00   90.00   0.21846   1.0852E+01  -2.3708E+00  -2.371E+00   1.085E+01  -3.448E-05  -1.354E-05
135.00   90.00   0.19080   1.0801E+01  -2.0610E+00  -2.061E+00   1.080E+01  -1.698E-05  -2.486E-05
140.00   90.00   0.14140   8.1462E+00  -1.1519E+00  -1.152E+00   8.146E+00   1.131E-06  -2.232E-05
145.00   90.00   0.01267   3.8740E+00   4.9075E-02   4.908E-02   3.874E+00   6.794E-06  -9.904E-06
150.00   90.00   0.35722   1.7617E+00  -6.2933E-01  -6.293E-01   1.762E+00  -1.560E-07   1.926E-06
155.00   90.00   0.45974   1.1005E+01  -5.0592E+00  -5.059E+00   1.100E+01  -8.574E-06   1.684E-06
160.00   90.00   0.25128   4.5243E+01  -1.1369E+01  -1.137E+01   4.524E+01  -7.389E-06  -1.695E-05
165.00   90.00   0.12704   1.1280E+02  -1.4331E+01  -1.433E+01   1.128E+02   1.518E-06  -5.206E-05
170.00   90.00   0.05271   2.0294E+02  -1.0698E+01  -1.070E+01   2.029E+02   8.093E-06  -9.152E-05
175.00   90.00   0.01267   2.8300E+02  -3.5861E+00  -3.586E+00   2.830E+02  -2.762E-06  -1.182E-04
180.00   90.00   0.00000   3.1528E+02  -1.0834E-03  -1.083E-03   3.153E+02  -3.244E-05  -1.142E-04
```

D   w*xxx*r*yyy*k*zzz*.pol*n* **Files**

The w000r000k000.pol1 file contains the polarization solution for the first wavelength (w000), first target radius (r000), first orientation (k000), and first incident polarization (pol1). In order to limit the size of this file, it has been written as an *unformatted* file. This preserves full machine precision for the data, is quite compact, and can be read efficiently, but unfortunately the file is **not** fully portable because different computer architectures (e.g., Linux vs. MS Windows) have adopted different standards for storage of "unformatted" data. However, anticipating that many users will be computing within a single architecture, the distribution version of **DDSCAT** uses this format.

Additional warning: even on a single architecture, users should be alert to the possibility that different compilers may follow different conventions for reading/writing unformatted files.

The file contains the following information:

- The location of each dipole in the target frame.

- $(k_x, k_y, k_z)d$, where **k** is the incident k vector.

- (E_{0x}, E_{0y}, E_{0z}), the complex polarization vector of the incident wave.

- $\alpha^{-1}d^3$, the inverse of the symmmetric complex polarizability tensor for each of the dipoles in the target.

- (P_x, P_y, P_z), the complex polarization vector for each of the dipoles.

The interested user should consult the routine writepol.f, or the to see how this information has been organized in the unformatted file. The user can, of course, simply use the routine readpol.f to read this file and load the information into memory.

Note that a subroutine readpol.f90 is already provided that reads the stored file, and the program DDfield.f90 (which uses readpol.f90) is provided to calculate **E** and **B** at user-selected postions – see §27.

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