# OpTool User Guide

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## 1. Introduction

This tool produces complex dust particle opacities right from the command line. It is derived from Michiel Min's DHS OpacityTool and also implements Ryo Tazaki's MMF theory for highly porous aggregates.

## 1.1. Capabilities

- stand-alone tool, fully command line driven, no input files need to be edited
- full scattering matrix output in several formats, including for RADMC-3D
- combining materials through mixing into a complex grain with porosity
- a useful collection of built-in materials for standard applications in astronomy
- an easy way to use external refractive index data for more specialized applications
- two computational methods: (i) **DHS** (**Distribution of Hollow Spheres**) for *irregular grains* and *low-porosity* aggregates. Standard **Mie theory** for *perfect spheres* is included as a limiting case. (ii) **MMF** (**Modified Mean Field**) theory for *high-porosity/fractal aggregates*.
- Python interface module for easy postprocessing and cross-tool use.

### 1.2. Terms of use

optool is distributed under the MIT license and can be used, changed and redistributed freely. The relevant references for this tool are listed below. Depending on which parts of optool you are using, please reference the corresponding papers.

- optool: https://github.com/cdominik/optool.git
- DHS model for irregular grains: Min et al. 2005, A&A, 432, 909
- MMF model for aggregates: Tazaki & Tanaka 2018, ApJ 860, 79
- DIANA standard Opacities: Woitke, Min et al. 2016, A&A 586, 103
- Third party software: Toon et al. 1981, Applied Optics 20, 3657
- References to refractive index data used in your particular application.

## 2. Examples

A simple grain made only of the default pyroxene, for the default grain size distribution  $(a^{-3.5}$  powerlaw from 0.05 to  $3000\mu\text{m}$ ), on the default wavelength grid  $(0.05\mu\text{m}$  to 1cm).

```
optool pyr
```

Include the scattering matrix in the produced output

```
optool pyr -s
```

Reproduce the DIANA standard dust model, using a specific pyroxene (70% Mg) and carbon, in a mass ratio 0.87/0.13, and with a porosity of 25%.

```
optool pyr-mg70 0.87 c 0.13 -p 0.25
```

List the built-in materials

```
optool -c
```

Add an ice mantle (built-in data from Warren+08) that is 20% of the core mass

```
optool pyr-mg70 0.87 c 0.13 -m ice-w 0.2 -p 0.25
```

Like the previous example, but use ice refractive index data from a separate file.

```
optool pyr-mg70 0.87 c 0.13 -p 0.25 -m data/ice_hudgins.dat 0.2
```

Pure ice grains in a narrow size distribution from 1 to 3 microns, with 15 sample sizes following an  $f(a) \propto a^{-2.5}$  powerlaw size distribution. Also, restrict the wavelength range to  $10\text{-}100\mu\text{m}$ , and turn off DHS to get perfect spheres.

```
optool ice -a 1 3 2.5 15 -l 10 100 -fmax 0
```

For silicon carbide, compute the opacity of a single grains size  $(2.5\mu \text{m})$  at  $\lambda=8.9\mu\text{m}$ .

```
optool -a 2.5 -1 8.9 sic
```

Represent the default dust model (DIANA, you also get this when you do not give any materials at all) in 42 grain sizes, and produce input files for RADMC-3D, one for each grain size, with full scattering matrix, chopping 3 degrees from the scattering peak.

```
optool -na 42 -d -s -radmc -chop 3
```

Use MMF to compute the opacities of dust aggregates made of pyroxene monomers. Use a monomer radius of 2.5 microns to construct aggregates with radii of gyration in the range between 1 and 3 cm, and a filling factor of 5% (i.e. a porosity of 0.95)

```
optool pyr -a 1e4 3e4 -mmf 2.5 -p 0.95
```

## 3. Compiling optool

On most systems, you can download and compile optool with these simple steps, using the freely available GNU FORTRAN compiler gfortran.

```
git clone https://github.com/cdominik/optool.git
cd optool
make multi=true
```

The executable is called optool, and you should put it on your execution path. To use the Intel fortran compiler, to use multiple cores for speed (highly recommended if your system supports it), or to be able to write FITS files<sup>1</sup>, use one or more of the following parameters during compilation:

You can also find binaries for Mac and Linux at my homepage.

## 4. Command line arguments

-h Show a compact help message about command line options.

## 4.1. Grain composition

-c List available built-in materials (the keys for the -c and -m options).

### [-c] KEY-or-FILE [MFRAC]

Specify a material to include in the grain. KEYorFILE can be the key for a builtin material, or the path to the correct lnk file. MFRAC is the *mass* fraction (default 1.0) of the material. You can give up to 10 materials to build up the grain. Mass fractions do not have to add up to one, they will be renormalized. All materials will be mixed together using the *Bruggeman* rule, and vacuum can be added through the porosity. A -c switch before each KEY-or-FILE is optional.

### -m KEY-or-FILE [MFRAC]

Like -c, but place this material into the grain mantle. Multiple mantle materials will be mixed using the Bruggeman rule, and than that mix will be added to the core using the *Maxwell-Garnett* rule. The -m is *not* optional, it must be present.

## 4.2. Grain geometry and computational method

See Appendix A for a brief discussion of the merits of the different methods.

<sup>&</sup>lt;sup>1</sup>This requires the cfitsio library to be installed on your system.

### -p POROSITY [P\_MANTLE]

Porosity, the *volume* fraction of vacuum, a number smaller than 1. The default is 0. A single value will apply to both core and mantle, but a second value will be specific for the mantle (and may be 0).

### -dhs [FMAX]

Use the *Distribution of Hollow Spheres* (DHS, Min 2005) approach to model deviations from prefect sphericity and low-porosity aggregates. **This is the default method**. Spheres with inner holes with volume fractions between 0 and  $f_{max}$  (default 0.8) are averaged to mimic irregularities.  $f_{max}$ =0 means to use solid spheres (Mie theory), i.e. perfectly regular grains. **-fmax** can be used instead of **-dhs** for backward compatibility.

#### -mie

Do a standard Mie calculation. This is short for **-dhs 0** (or **-fmax 0**).

### -mmf [AMONO]

Use Modified Mean Field theory (MMF, Tazaki 2018) to compute the opacities of highly porous or fractal aggregates. Particles will then be aggregates with the characteristic radius given by the -a switch. The volume filling factor f = 1 - p is specified through the porosity (-p), and a fractal dimension will be chosen appropriately.  $a_{\text{mono}}$  is the monomer radius, with default  $0.1\mu\text{m}$ . Monomers will have the composition given by the -c and -m switches.

### 4.3. Grain size distribution

### -a AMIN [AMAX [APOW [NA]]]

Specify (minimum) grain radius, and optionally maximum grain radius, the size distribution powerlaw and the number of size bins. You may also use options to set individual values with **-amin**, **-amax**, **-apow**, **-na**. The defaults are 0.05  $\mu$ m, 3000  $\mu$ m, 3.5, and 10 per size decade with a fixed minimum of 5, respectively. If only a single size is specified with **-a**, then  $a_{max}=a_{min}$  and  $n_a=1$  are implied.

### 4.4. Wavelength grid

### -1 LMIN [LMAX [NLAM]]

Specifiy the (minimum) wavelength, and optionally the maximum wavelength and the number of wavelengths points for the construction of the wavelength grid. The default values are 0.05  $\mu$ m, 10000  $\mu$ m, and 300, respectively. You may also use the options -lmin, -lmax, and -nlam (or -nl) to set individual values. If only one wavelength is specified with -l, then  $\lambda_{\text{max}} = \lambda_{\text{min}}$  and  $n_{\lambda} = 1$  are implied.

#### -1 FILE

Read the wavelength grid from FILE. The file may start with comment lines, and the first non-comment line needs to contain the number of wavelength values in the data block below it. In the data block, the first column is expected to hold the wavelength values, in  $\mu$ m. For example, an lnk file could be used here.

### 4.5. Controlling the output

The standard output is the file dustkappa.dat, with the opacities and the asymmetry parameter g. The following options control and extend the output.

#### -o [DIR]

Put the output files in directory DIR instead of the current working directory. ./output will be used if DIR is not specified.

### -s [NANG]

Include the full scattering matrix in the output. NANG can optionally specify the number of equally-spaced angular grid points to cover the range of angles between 0 and 180 degrees. The default for NANG is 180 and should normally not be changed.

### -chop [NDEG]

Cut out the first NDEG (2 if unspecified) degrees of the forward scattering peak and compensate by a reduction in the scattering cross section.

#### -d [NSUB]

Divide the computation up into NA parts to produce a file for each grain size. Each size will actually be an average over a small range of NSUB grains around the real size, to smear out resonances. The default for NSUB is 5.

#### -fits

Write dustkappa.fits with the absorption cross sections and scattering matrix elements, instead of ASCII output. With the -d switch, NA files will be written.

#### -radmc [LABEL]

RADMC-3D uses a different angular grid and normalization for the scattering matrix, so the output has to be adapted for it. The extension of the files will be changed to .inp, and if you specify LABEL, it will be used in the file name(s).

## 5. Material properties

optool needs refractive index data to work. For your convenience, a useful list of materials is compiled into optool, but you can also find and use other data. No matter where the data is from, you should *always* cite the original laboratory papers.

### 5.1. Built-in materials

To access one of the built-in materials, specify the corresponding key string like pyr-mg70 instead of the path to an lnk file. In each material class I have selected a useful default, accessible with an even simpler generic key.

-c Key	-c Key	Material	State	$\rho$	$\lambda_{min}$	$\lambda_{\sf max}$	Reference
generic	full key			g/cm <sup>3</sup>	$\mu$ m	$\mu$ m	
	pyr-mg100	$MgSiO_3$	amorph	2.71	0.2	500	Dorschner+95
	pyr-mg95	$Mg_{0.95}Fe_{0.05}SiO_3$	amorph	2.74	0.2	500	Dorschner+95
	pyr-mg80	$Mg_{0.8}Fe_{0.2}SiO_3$	amorph	2.9	0.2	500	Dorschner+95
pyr	pyr-mg70	$Mg_{0.7}Fe_{0.3}SiO_3$	amorph	3.01	0.2	500	Dorschner+95
	pyr-mg60	$Mg_{0.6}Fe_{0.4}SiO_3$	amorph	3.1	0.2	500	Dorschner+95
	pyr-mg50	$Mg_{0.5}Fe_{0.5}SiO_3$	amorph	3.2	0.2	500	Dorschner+95
	pyr-mg40	$Mg_{0.4}Fe_{0.6}SiO_3$	amorph	3.3	0.2	500	Dorschner+95
ens	pyr-c-mg96	$Mg_{0.96}Fe_{0.04}SiO3$	cryst	2.8	2.0	99	Jäger+98
ol	ol-mg50	MgFeSiO <sub>4</sub>	amorph	3.71	0.2	500	Dorschner+95
	ol-mg40	Mg <sub>0.8</sub> Fe <sub>1.2</sub> SiO <sub>4</sub>	amorph	3.71	0.2	500	Dorschner+95
for	ol-c-mg100	Mg <sub>2</sub> SiO <sub>4</sub>	cryst	3.33	3.0	250	Steyer+74
	astrosil	MgFeSiO4	mixed	3.3	6e-5	1e5	Draine+03
С	C-Z	С	amorph?	1.8	0.05	1e4	Zubko+96
	c-p	C	amorph	1.8	0.11	800	Preibisch+93
gra	c-gra	C graphite	cryst	2.16?	0.001	1000	Draine+03
org	c-org	CHON organics	amorph	1.4	0.1	1e5	Henning+96
	c-nano	C nano-diamond	cryst	2.3	0.02	110	Mutschke+04
ice	ice-w	Water ice	cryst	0.92	0.04	2e6	Warren+08
iron	fe-c	Fe	metal	7.87	0.1	1e5	Henning+96
	fes	FeS	metal	4.83	0.1	1e5	Henning+96
	sic	SiC	cryst	3.22	0.001	1000	Laor93
cor	cor-c	$Al_2O_3$	cryst	4.0	0.5	40	Koike+95

## 5.2. External refractory index files (lnk files)

optool can use external refractive index data in files with the following format:

- The file may start with several comment lines (lines starting with !, #, or \*).
- The next line contains two numbers, the number of wavelengths  $n_{\lambda}$  and the specific weight  $\rho$  of the material in g/cm<sup>3</sup>
- Then follow three columns of data:  $\lambda[\mu m]$ , and the real and imaginary parts of the refractive index, n and k.

You can find refractive index data in the Jena database, and associated with original papers in the literature. Don't forget to add the line with  $n_{\lambda}$  and  $\rho$ ! If for some reason it is not convenient to add that line to the file, optool will count the lines and you can specify the density after the mass fraction, like this: optool -c path/to/file.lnk 0.7 3.42. The appendix contains information on how to compile frequently-used external materials into the program.

## Output files

#### dustkappa.dat

This is an ASCII file containing the basic opacity results. It starts with a comment section describing the dust model, followed by the format number (3, currently),

followed by the number of wavelengths in the grid, both on lines by themselves. Then follows a block with these columns:

- 1. wavelength  $\lambda$  [micron]
- 2. mass absorption cross section  $\kappa_{\rm abs} \, [{\rm cm}^2/{\rm g}]$
- 3. mass scattering cross section  $\kappa_{\rm sca}$  [cm<sup>2</sup>/g]
- 4. asymmetry parameter g

### dustkapscatmat.dat

ASCII file with cross sections and full scattering matrix. The comment section at the start of the file explains the structure. See the appendix for information about the normalization of the scattering matrix. And see the <code>-radmc</code> switch which will modify the output to make sure it can be used as an input file for RADMC-3D.

### dustkappa.fits

The FITS-file (ending in '.fits') is written instead of the ASCII output when using the -fits switch. It has two HDU blocks. The first block contains the cross sections per unit mass. This is an  $n_{\lambda} \times 4$  matrix with these columns:

- 1. wavelengths in  $[\mu m]$
- 2. mass extinction cross section  $\kappa_{\rm ext}$  in [cm<sup>2</sup>/g]
- 3. mass absorption cross section  $\kappa_{\rm abs}$  in [cm<sup>2</sup>/g]
- 4. mass scattering cross section  $\kappa_{\rm sca}$  in [cm<sup>2</sup>/g]

The second HDU block contains the scattering matrix elements. It is a  $n_{\lambda} \times 6 \times n_{\rm ang}$  matrix, containing the 6 elements of the scattering matrix for  $n_{\rm ang}$  equidistant scattering angles from forward scattering (element 0) to backward scattering (element  $n_{\rm ang}$ -1), for each wavelength value. The stored matrix elements are  $F_{11}$ ,  $F_{12}$ ,  $F_{22}$ ,  $F_{33}$ ,  $F_{34}$ , and  $F_{44}$ .

## 7. Python interface

optool comes with a python module optool.py that runs optool in the background<sup>2</sup> and puts all computed quantities as numpy arrays into a python object. This makes it straight forward to inspect and further process the output, for example to produce custom opacity files for use in an radiative transfer tool. Here is how to use the module:

```
>>> import optool
>>> p = optool.particle('~/bin/optool pyr 0.8 -m ice 0.2 -na 24 -d')
```

The argument to optool.particle() must be a valid shell command<sup>3</sup> to run optool, if necessary with the full path to the optool binary. Depending on the presence of the

<sup>&</sup>lt;sup>2</sup>The module runs the command as a subprocess, with output to a temporary subdirectory in the current working directory. It then reads the output files and cleans up the temporary directory unless is called with the keep keyword argument: optool.particle('optool',keep=True).

<sup>&</sup>lt;sup>3</sup>The command may be given as string than can be split on whitespace, or, for example if the path to the binary contains whitespace, in list form ['/path/to my/command','arg1','arg2',...].

optool's -d switch, the command will produce opacities either for  $n_p = 1$  particle, or for  $n_p = n_a$  particles. Most of the attributes (with the exception of the global wavelength and angular grids) will therefore be arrays with the first dimension equal to  $n_p$ , even if  $n_p = 1$ . The object returned will have the following attributes:

Attribute	$\mathbf{Type}/\mathbf{Shape}$	Quantity	
cmd	string	The full command given in the particle() call	
radmc	boolean	Output follows RADMC conventions	
scat	boolean	Scattering matrix is available	
nlam	int	Number of wavelength points	
lam	float[nlam]	The wavelength grid	
nang	int	Number of scattering angles	
scatang	float[nang]	The angular grid	
materials	[ [] ]	Lists with location, $m_{frac}$ , $\rho$ , $material$	
np	int	Number of particles, either 1 or (with -d) n <sub>a</sub>	
fmax	float[np]	Maximum volume fraction of vacuum for DHS	
pcore, pmantle	float[np]	Porosity of the core/mantle material	
amin, amax	float[np]	min/max grain size used for each particle	
nsub	int[np]	Number of sizes averaged for each particle.	
apow	float[np]	Negative size distribution power law (e.g. 3.5)	
a1, a2, a3	fload[np]	Mean $\langle a \rangle$ , $\langle a^2 \rangle$ , and $\langle a^3 \rangle$ of the particle	
kabs,ksca,kext	float[np,nlam]	Absorption, scattering/extinction cross section	
gsca	float[np,nlam]	Asymmetry parameter	
f11,, f44	<pre>float[np,nlam,nang]</pre>	Scattering matrix element $F_{11}, \ldots, F_{44}$	
chop	float[np]	Degrees chopped off forward scattering	
plot()	method	Plot the cross sections and matrix elements	

The optool.plot() method will produce the following plots:

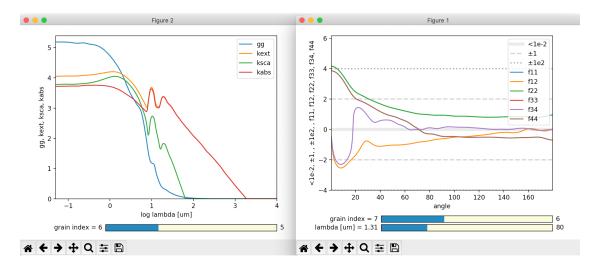


Figure 1: Screenshot of the plots created by running p.plot() on an optool particle.

- a plot showing the opacities  $\kappa_{\text{abs}}$ ,  $\kappa_{\text{sca}}$ , and  $\kappa_{\text{ext}}$  as a function of wavelength, along with the asymmetry parameter g (on a linear y-scale). Note that the blue g curve does not have its own axis, imagine the full g axis going from 0 to 1 for g.
- a plot showing the scattering matrix elements as a function of scattering angle, with sliders to go through grain sizes and wavelengths. When interpreting the y axis, note that we plot the positive/negative  $\log_{10}$  of positive/negative matrix elements, compressing the range from  $10^{-2}$  to  $10^2$  into a line (use the grey lines as a guide, ignore the y-axis labels).

## 8. Acknowledgments

- Charléne Lefévre for SIGMA, which triggered me to add a grain mantle using the Maxwell Garnett rule.
- Kees Dullemond for his python plotting routine viewarr (available on github).
- Jeroen Bouwman for some pointers to refractive index data.

## A. Computational methods in optool

FIXME: This needs to be improved.

The details and intricacies light scattering by small particles fill books and feed a vast literature. optool implements robust approximate methods that are fast, easy to use, and that can be used for a wide variety of applications. Here is a brief instruction on when to use which optool method:

- 1. Use standard Mie theory only if you have a good reason why you particles should actually be perfect spheres.
- 2. DHS takes into account geometric irregularities, so it makes the shape of solid state fetures more realistic (REF) and also produces realistic opacity enhancement conneced to irregularities, in particular enhancements in the Raghleigh limit (wavelength larger than particle size). It further provides a decent approximation for low porosity aggregates (Min+??), that are compact enough so that the properties of the monomers do not play a critical role. DHS is stable, fast, and delivers fully consistent scattering matrix elements.
- 3. In high-porosity aggregates, the properties of the monomers become critical for the correct determination of cross sections outside the Rayleigh limit, i. e. at wavelengths smaller than the overall size of the aggregate. Since DHS is unaware of the monomer properties, it is no longer reliable. This is an area that is covered well by MMF, which delivers accurate absorption and scattering cross sections for high porosity aggregates, as well as asymmetry parameters. The scattering matrix of MMF is reliable if the phase shift is....

## B. Units

Due to conventions in our field, the input and output of optool uses the following units

- microns for grain sizes and wavelengths
- g/cm<sup>3</sup> for mass densities of materials
- cm<sup>2</sup> g<sup>-1</sup> for opacities  $\kappa_{abs}$ ,  $\kappa_{sca}$ , and  $\kappa_{ext}$
- sr<sup>-1</sup> or cm<sup>2</sup> g<sup>-1</sup> sr<sup>-1</sup> for the scattering matrix elements, see below.

## C. Scattering Matrix: The fine print

### C.1. Phase function normalization

A number of different normalizations for the scattering matrix are being used in the literature and in computational tools. The differences are significant, and it is important to be aware of the choice. For optool we are using a convention (Hovenier (2004)) in which the average over all directions of the 1-1 element of the scattering matrix equals unity, i.e.

$$\oint_{(4\pi)} F_{11}(\lambda, \Theta) d\Omega = 4\pi \quad . \tag{1}$$

optool can also produce output for RADMC-3D which uses instead

$$\oint_{(4\pi)} Z_{11}(\lambda, \Theta) d\Omega = \kappa_{\rm sca}(\lambda) \quad . \tag{2}$$

The books by Bohren & Huffman and by Mishchenko use different normalizations again. As described in RADMC-3D's manual, these conventions can be matched by scaling all matrix elements with simple factors involving dust mass and wavenumber  $k = 2\pi/\lambda$ .

### C.2. Forward-scattering peak

Particles that are much larger than the wavelength of the considered radiation can show extreme forward scattering, were much of the *scattered* radiation is sent into just a few degrees around the forward direction. This can be difficult to handle for radiative transfer codes which have limited angular resolution or limited sampling. MCMax3D has the nspike keyword to deal with this issue. Other tools (e.g. RADMC-3D) require this to be taken care of by the process that creates the opacity files. The -chop switch specifies a number of degrees around the forward scattering direction. Inside that cone, the scattering matrix gets limited to the value at the edge of the cone. To compensate and ensure energy conservation, the scattering cross section will be reduced accordingly. As a result, the radiation that would be *scattered* into this narrow range of angles will be treated as if it did have *no interaction at all* with the grain.

### C.3. Angular grid

optool uses an angular grid in one degree steps from 0 to 180 degrees. The full degrees are the cell *interfaces* of that grid. optool computes the scattering matrix at the cell *midpoints*, i.e. at 0.5°, 1.5° etc to 179.5°, for a total of 180 values. The scattering matrix is normalized in this way, so that a numerical integral gives the correct result.

RADMC-3D requires the values of the scattering matrix on the cell *boundaries*, so at 0°, 1° etc to 180°, for a total of 181 values. For the input files for RADMC-3D, we interpolate and extend the computed values to the cell boundaries.

## D. How to ingest refractive index data for another material

Using external refractive index data means that you have to keep track of where those files are. It can be convenient to compile your favorite materials into optool, so that accessing them will be as simple as using the built-in materials. Here is how to do that:

- Give your lnk file a name exactly like pyr-mg70-Dorschner1995.lnk, where the start of the name (pyr-mg70) is the key to access the material and Dorschner1995 (the text after the final -) is the reference.
- 2. Put this file into the lnk\_data directory.
- 3. Optionally edit lnk\_data/lnk-help.txt, so that optool -c will list the new material. Note that, in order to define generic keys, optool looks for pairs that look like genkey -> fullkey in this file.
- 4. Run make ingest to update ref\_ind.f90, now including your new material.
- 5. Recompile and install the code.

### E. Internals

This appendix describes some key aspects of the internal workings of the code.

### Refractive Index Data

Measured refractive index data is obtained from data compiled into the code, or read-in from a file. That data is then interpolated and extrapolated onto the wavelengths grid requested for the computation. Extrapolation toward short wavelengths is done keeping the refractive indices constant. Extrapolation toward long wavelength assumes that the last two measured data points define a powerlaw. Interpolation in the measured grid is done using double-logarithmic interpolation.

#### Mixing

Once the refractive index for all involved materials is available, the core and the mantle mixtures are created independantly, using the Bruggeman rule. Mass fractions are converted into volume fractions, and porosity is implemented using vacuum as an additional material. The subroutine doing the mixing uses an iterative procedure that is very stable, also for a large number of components.

If there is a mantle, the Maxwell Garnett rule is applied with the core being treated an inclusion inside a mantle matrix.

#### DHS

In order to simulate irregularities in grains (irregular shapes, or the properties of low-porosity aggregates, optool averages the opacities of grains with an inner empty region, over a range of volume fractions of this inner region between 0 and  $f_{\rm max}$ . The subroutine used to compute the opacities and scattering matrix elements for these structures is DMiLay (Toon & Ackerman 1981). However, when the size parameter  $x=2\pi a/\lambda$  exceeds a value of  $10^4$ , then no DHS averaging is used. A standard Mie calculation is performed , using the routine MeerhoffMie (reference missing), for a fixed size parameter of 5000, with proper scaling to the actual size of the particle.

### **MMF**

FIXME: Document here the details of MMF

### **Computational Structure**

The computation of opacities and matrix elements follows this structure. Additional information can be obtained by reading the code.

```
,- Loop over all wavelengths lambda
| ,- Loop over all particle sizes a
| | ,- Loop over all DHS volume ratios f
| | | - Call DMiLay or (for large x) MeerhoffMie
| | '- Sum the weighted contributions of each DHS volume
| | OR
| | [ Apply MMF ]
| '- Sum weighted contributions of all particle sizes
'- Store the results for the current wavelength
```

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