Mie Scattering by Ensembles of Particles with Very Large Size Parameters

S. Wolf ^{a,b}, N. V. Voshchinnikov ^c

- ^a California Institute of Technology, 1201 East California Blvd, Mail Code 105-24, Pasadena CA 91125, USA
- ^bMax Planck Institute for Astronomy, Königstuhl 17, 69117 Heidelberg, Germany, swolf@mpia.de
- ^cSobolev Astronomical Institute, St. Petersburg University, Universitetskii prosp. 28, 198504 Stary Peterhof-St. Petersburg, Russia, nvv@astro.spbu.ru

Abstract

We present a computer program for the simulation of Mie scattering in case of arbitrarily large size parameters. The elements of the scattering matrix, efficiency factors as well as the corresponding cross sections, the albedo and the scattering asymmetry parameter are calculated. Single particles as well as particle ensembles consisting of several components and particle size distributions can be considered.

PACS: 94.10.Gb Absorption and scattering of radiation

Key words: Mie scattering, scattering matrix, efficiency factors, cross sections, radiative transfer – astrophysics, optics, geophysics, biophysics

1 Program summary

Title of program: **miex**

Catalogue identifier:

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Computer for which the program is designed and others on which it has been tested:

Computers: Any machine running standard FORTRAN 90; **miex** has been tested on an Intel Celeron processor (Redhat Linux 9.0, Intel Fortran Compiler 7.1), an Intel XEON processor (SuSE Linux 9.0, Intel Fortran Compiler 8.0), and a Sun-Blade-1000 (OS 8.5, Sun Workshop Compiler Fortran 90 2.0).

Installations: standard

Operating systems or monitors under which the program has been tested: Redhat Linux 9.0, SuSE Linux 9.0, Sun OS 8.5

Programming language used: Fortran 90

Memory required to execute with typical data: 1 MByte - several 100 MByte (see Sect. A for examples)

No. of bits in a word: 8

No. of processors used: 1

Has the code been vectorized or parallelized?: NO

No. of bytes in distributed program, including test data, etc.:

Distributed format: ASCII

Keywords: Mie scattering, size parameter, particle ensemble, scattering matrix, Stokes vector, efficiency factor, cross section, asymmetry parameter, albedo

Nature of the physical problem: Among a variety of applications, Mie scattering is of essential importance for the continuum radiative transfer in cosmic dust configurations. In this particular case, Mie theory describes the interaction of electromagnetic radiation with spherical dust grains on the basis of their complex refractive index and size parameter. Both, broad grain size distributions (radii a: nanometers – millimeters) and a very wide wavelength

range ($\lambda \approx 10^{-10} - 10^{-2} \,\mathrm{m}$) of the interacting radiation are considered. Previous numerical solutions to the Mie scattering problem are not appropriate to consider size parameters $x = 2\pi a/\lambda > 10^4 - 10^5$. In contrast to this, the presented code allows to consider arbitrary size parameters. It will be useful not only for applications in astrophysics but also in other fields of science (atmospheric and ocean optics, biophysics, etc.) and industry (particle sizing, ecology control measurements, etc.).

Method of solution: Calculations of Mie scattering coefficients and efficiency factors as outlined by Voshchinnikov (2004), combined with standard solutions of the scattering amplitude functions. Single scattering by particle ensembles is calculated by proper averaging of the respective parameters.

Restrictions on the complexity of the problem: Single Scattering

Typical running time: Seconds to minutes.

Unusual features of the program: None

References:

Bohren C.F., Huffman D.R., Absorption and scattering of light by small particles. John Wiley & Sons, New York (1983)

Voshchinnikov N.V.: "Optics of Cosmic Dust. I", Astrophysics and Space Physics Reviews 12, 1 (2004)

2 Introduction

The motivation for the development of the presented Mie scattering routine was given by the goal to model the continuum radiative transfer in the circumstellar environment of young stellar objects and X-ray halos where dust scattering and thermal dust reemission dominate the continuum radiation field. In the most approaches, dust grains are assumed to be homogeneous spheres. Their optical properties are defined through Mie theory with following input parameters: (a) the complex refractive index m = n + ik of a material relative to the surrounding medium and (b) the dimensionless size parameter

$$x = \frac{2\pi a}{\lambda},\tag{1}$$

connecting the particle radius a and the wavelength of the incident electromagnetic radiation λ . New findings suggest that the radii of the largest grains in circumstellar disks around young stellar objects may reach several millimeters to centimeters in radius (see, e.g., Calvet et al. 2002). Since the embedded stars emit a considerable amount of energy even in the ultraviolet wavelength range (effective temperature of a typical T Tauri star: $T_{\rm eff}$ =4000 K – Gullbring et al. 1998), the resulting size parameter x amounts up to 10^5-10^6 . In more evolved circumstellar disks, so-called "debris disks", the size parameter x may even exceed this value by several orders of magnitude. Furthermore, interstellar dust grains located near the line of sight toward distant X-ray sources will scatter some of its radiation and thus produce a diffuse halo around a point-like source. Observations are performed at energies $E \sim 10 \, {\rm keV}$ (or more see, e.g., Woo et al., 1994) that correspond to wavelengths $\lambda \sim 1.24 \, {\rm \AA}$. In this domain, the size parameter is equal to $x = 5067(a/\mu{\rm m})(E/{\rm keV})$ and exceeds 5×10^6 if $a > 100 \, \mu{\rm m}$.

For the solution of the described radiative transfer problems, the efficiency factors and scattering matrix are required. Under the assumption of spherical, homogeneous particles, these quantities are calculated from the Mie series solution. The most widely applied numerical Mie code is that from Bohren & Huffman (1983). It is based on the improved algorithm of Mie scattering of Wiscombe (1980, 1996) and is restricted to size parameters $\leq 2 \times 10^4$. Therefore, this numerical solution is not appropriate for the applications described above (see also Shah 1977, 1992 for Mie calculations in the size parameter regime $x \leq 10^5$).

The computer program presented in this article is based on the calculation of the Mie coefficients and efficiency factors for single particles as described by Voshchinnikov (2004). The calculations of the angular functions are based on the standard approach (see Wiscombe 1980, Bohren & Huffman 1983). We

successfully tested the direct implementation of Legendre functions (Zhang & Jin 1996) for the determination of the scattering amplitude functions as well, but only the fastest, i.e., the first approach is realized in the published version of the code. To account for particle size distributions and/or ensembles of different components, a proper averaging of the single parameters (efficiency factors etc.) is implemented as well.

3 Long Write-up

3.1 Mie scattering

In the following, a brief overview of the scattering process and the different quantities which can be derived with **miex** is given. For a more detailed description of the Mie scattering solution we refer to the books of van de Hulst (1957) and Bohren & Huffman (1983).

Let the radiation be described by the four-component Stokes vector $\hat{I} = (I, Q, U, V)^{T}$. The scattering of radiation by a spherical particle is described by the scattering (Müller) matrix \hat{F} of special type

$$\hat{I}_1 \propto \hat{F}\hat{I}_0,$$
 (2)

where \hat{I}_0 (\hat{I}_1) is the Stokes vector before (after) the scattering and

$$\hat{F}(\Theta) = \begin{pmatrix} F_{11}(\Theta) & F_{12}(\Theta) & 0 & 0 \\ F_{12}(\Theta) & F_{11}(\Theta) & 0 & 0 \\ 0 & 0 & F_{33}(\Theta) & F_{34}(\Theta) \\ 0 & 0 & -F_{34}(\Theta) & F_{33}(\Theta) \end{pmatrix}.$$
(3)

Here, Θ is the angle between the direction of the incident and the scattered radiation (scattering angle). The elements of the scattering matrix F_{ik} can be derived from the complex amplitude functions (the asterisk denotes the complex conjugation) S_1 , S_2 :

$$F_{11}(\Theta) = \frac{1}{2} \left[|S_2(\Theta)|^2 + |S_1(\Theta)|^2 \right], \quad F_{12}(\Theta) = \frac{1}{2} \left[|S_2(\Theta)|^2 - |S_1(\Theta)|^2 \right],$$

$$F_{33}(\Theta) = \frac{1}{2} \left[S_2^*(\Theta) S_1(\Theta) + S_2(\Theta) S_1^*(\Theta) \right],$$

$$F_{34}(\Theta) = \frac{i}{2} \left[S_1(\Theta) S_2^*(\Theta) - S_2(\Theta) S_1^*(\Theta) \right].$$

$$(4)$$

The amplitude functions can be calculated as follows:

$$S_1(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_n \pi_n(\Theta) + b_n \tau_n(\Theta) \right]$$
 (5)

and

$$S_2(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_n \tau_n(\Theta) + b_n \pi_n(\Theta) \right].$$
 (6)

The complex scattering (Mie) coefficients a_n and b_n depend on the size parameter x and the refractive index m of the material. The angular functions π_n and τ_n depend on $\cos \Theta$ only and can be found from recurrence relations (Wiscombe 1980; $n \geq 2$)

$$\pi_n(\Theta) = \frac{2n-1}{n-1}\cos\Theta \,\pi_{n-1}(\Theta) - \frac{n}{n-1}\pi_{n-2}(\Theta) \tag{7}$$

and

$$\tau_n(\Theta) = n\cos\Theta\pi_n(\Theta) - (n+1)\pi_{n-1}(\Theta). \tag{8}$$

The initial values are

$$\pi_0(\Theta) = 0, \qquad \pi_1(\Theta) = 1. \tag{9}$$

The coefficients

$$a_n = \frac{\psi_n'(mx)\psi_n(x) - m\psi_n(mx)\psi_n'(x)}{\psi_n'(mx)\zeta_n(x) - m\psi_n(mx)\zeta_n'(x)}$$

$$(10)$$

and

$$b_n = \frac{m\psi_n'(mx)\psi_n(x) - \psi_n(mx)\psi_n'(x)}{m\psi_n'(mx)\zeta_n(x) - \psi_n(mx)\zeta_n'(x)}$$

$$\tag{11}$$

are usually transformed to a form convenient for calculations. Following Deirmendjian (1969) and Loskutov (1971), we replace the Riccati-Bessel functions $\psi_n(x)$ and $\zeta_n(x)$ and their first derivatives $\psi'_n(x)$ and $\zeta'_n(x)$ by spherical Bessel functions of the first and second kind $J_{n+1/2}(x)$ and $Y_{n+1/2}(x)$. With the aid of recursive relations for these functions (see, e.g., Abramowitz and Stegun 1964) we obtain:

$$a_n = \frac{\left[\frac{A_n}{m} + \frac{n}{x}\right] J_{n+1/2}(x) - J_{n-1/2}(x)}{\left[\frac{A_n}{m} + \frac{n}{x}\right] J_{n+1/2}(x) - J_{n-1/2}(x) + i \left\{\left[\frac{A_n}{m} + \frac{n}{x}\right] Y_{n+1/2}(x) - Y_{n-1/2}(x)\right\}} (12)$$

and

$$b_n = \frac{\left[m\mathcal{A}_n + \frac{n}{x}\right] J_{n+1/2}(x) - J_{n-1/2}(x)}{\left[m\mathcal{A}_n + \frac{n}{x}\right] J_{n+1/2}(x) - J_{n-1/2}(x) + i\left\{\left[m\mathcal{A}_n + \frac{n}{x}\right] Y_{n+1/2}(x) - Y_{n-1/2}(x)\right\}}, (13)$$

where

$$A_n \equiv \frac{\psi_n'(mx)}{\psi_n(mx)} = -\frac{n}{mx} + \frac{J_{n-1/2}(mx)}{J_{n+1/2}(mx)}.$$
 (14)

The logarithmic derivative to the Bessel functions of a complex argument A_n is calculated via backward recursion using the relation

$$\mathcal{A}_n = -\frac{n}{mx} + \left(\frac{n}{mx} - \mathcal{A}_{n-1}\right)^{-1}.\tag{15}$$

The starting number (variable "num" in the program) for $x \leq 50000$ ($\mathcal{A}_n = 0$) is chosen according to the recommendation of Loskutov (1971). It is smaller for large arguments than that given by Wiscombe (1980).

According to Voshchinnikov (2004), the calculation of the Bessel functions of a real argument is based on the upward recursion for the functions of the second kind $Y_{n+1/2}(x)$, which is known to be stable. This is given by the relation (Abramowitz and Stegun 1964; $n \ge 0$):

$$Y_{n+5/2}(x) = \frac{2n+1}{x} Y_{n+3/2}(x) - Y_{n+1/2}(x)$$
(16)

with the initial values

$$Y_{1/2}(x) = -\sqrt{\frac{2}{\pi x}}\cos x, \qquad Y_{3/2}(x) = \sqrt{\frac{2}{\pi x}}\left(-\frac{\cos x}{x} - \sin x\right).$$
 (17)

The Bessel functions of the first kind $J_{n+1/2}(x)$ $(n \ge 1)$ are determined by the relation

$$J_{n+1/2}(x) = \left[\frac{2}{\pi x} + Y_{n+1/2}(x)J_{n-1/2}(x)\right]/Y_{n-1/2}(x),\tag{18}$$

where

$$J_{1/2}(x) = \sqrt{\frac{2}{\pi x}} \sin x. \tag{19}$$

We want to remark that equation (18) gives wrong results if $n \gg x$, but this is not the case for standard Mie calculations. In order to avoid an overflow in the forward recursion, a normalization is used. The description of the general method of calculations of Bessel functions can be found in Loskutov (1971).

The extinction, scattering, backscattering and radiation pressure efficiency factors $(Q_{\text{ext}}, Q_{\text{sca}}, Q_{\text{bk}})$ and Q_{pr} are given by the relations

$$Q_{\text{ext}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}\{a_n + b_n\},$$
 (20)

$$Q_{\text{sca}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2), \tag{21}$$

$$Q_{\rm bk} = \frac{1}{x^2} \left| \sum_{n=1}^{\infty} (2n+1)(-1)^n (a_n - b_n) \right|^2, \tag{22}$$

and

$$Q_{\text{pr}} = Q_{\text{ext}} - gQ_{\text{sca}}$$

$$= Q_{\text{ext}} - \frac{4}{x^2} \left\{ \sum_{n=1}^{\infty} \left[\frac{n(n+2)}{n+1} \text{Re}(a_n a_{n+1} + b_n b_{n+1}) + \frac{2n+1}{n(n+1)} \text{Re}(a_n b_n) \right] \right\}.$$
(23)

Following quantities can be derived from the above efficiency factors:

Absorption efficiency :
$$Q_{abs} = Q_{ext} - Q_{sca}$$
,
Albedo : $\Lambda = Q_{sca}/Q_{ext}$, (24)
Asymmetry parameter : $g = (Q_{ext} - Q_{pr})/Q_{sca}$.

The asymmetry parameter g (or "mean cosine" $\langle \cos \Theta \rangle$) describes the distribution of the scattered radiation in the forward / backward direction. It is defined as

$$g = \langle \cos \Theta \rangle = \frac{\int_{4\pi}^{\pi} F_{11} \cos \Theta \, d\omega}{\int_{4\pi}^{\pi} F_{11} \, d\omega} = \frac{\int_{0}^{\pi} F_{11} \cos \Theta \, \sin \Theta \, d\Theta}{\int_{0}^{\pi} F_{11} \, \sin \Theta \, d\Theta}$$
(25)

and can be also found from the integration of the element F_{11} of the scattering matrix.

The corresponding cross sections can be derived from the relation

$$C = GQ, (26)$$

where $G = \pi a^2$ is the geometrical cross section of the particle.

For the description of scattering by an ensemble of particles consisting of several species and particles sizes, weighted mean values of the different quantities described above can be defined. They are obtained as the sums of the corresponding quantity averaged over the corresponding size distribution. Assuming "J" different species in the mixture having the fractional abundances f_j and a particle number density with some size distribution n(a), we can formulate the following normalization condition:

$$\sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) da = 1, \qquad \sum_{j=1}^{J} f_j = 1,$$
(27)

where a_{\min} and a_{\max} are the minimum and maximum particle radius. The Stokes parameters as well as all cross sections are additive. Therefore, the ensemble averaged values can be derived from their weighted contributions (see, e.g., Martin 1978, Šolc 1980):

$$\langle C_{\text{ext, sca,...}} \rangle = \sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) C_{\text{ext, sca,...,j}}(a) \, da, \qquad (28)$$

$$\langle F_{ik} \rangle = \sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) \hat{F}_{ik,j}(a) da.$$
 (29)

For the albedo Λ and the asymmetry parameter g the following expressions must be used:

$$\langle \Lambda \rangle = \frac{\sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) C_{\text{sca},j}(a) da}{\sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) C_{\text{ext},j}(a) da} = \frac{\langle C_{\text{sca}} \rangle}{\langle C_{\text{ext}} \rangle},$$
(30)

$$\langle g \rangle = \frac{\sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) C_{\text{sca},j}(a) g_j(a) da}{\sum_{j=1}^{J} f_j \int_{a_{\min}}^{a_{\max}} n(a) C_{\text{sca},j}(a) da}.$$
(31)

3.2 Code description

The presented Mie scattering code is written in Fortran 90/95. The main program regulates the input / output of data, calls the routine for the calculation of Mie scattering characteristics for a single size parameter and particle composition (embedded in the *module mie_routines*), and performs the averaging in case of a polydisperse ensemble.

The calculations are performed with double precision accuracy using the internally defined data type r2

integer, parameter, public ::
$$r2 = selected_real_kind(9)$$
 (32)

in the module datatype. Changing the definition of this data type allows one to adapt the variables to any required number of significant digits.

The routines shexqnn2 and aa2 are adaptations of the Mie scattering code published by Voshchinnikov (2004). They were extended in order to calculate the amplitude functions (see Eqs. (5), (6)) and to satisfy Fortran 90/95 standards. The numerical realization for calculation of the scattering amplitude functions follows the standard approach (Eqs. (7)–(9)). We also successfully tested the implementation of a direct calculation of the Legendre functions, based on the routine mlpmn.for provided by Zhang & Jin (1996), but decided not to include it in the presented version of the code because it resulted in longer runtimes. The runtime of the code is inversely proportional to the step of the scattering angles Θ for which the amplitude functions and, based on them, the scattering matrix elements are calculated. The angular step size $\Delta\Theta$ is an input parameter.

The calculation of Mie series for a single particle radius for a given material is finished as soon as the relative contribution of the current term to the extinction efficiency becomes smaller than 10^{-15} . If the default maximum number of terms (2×10^7) is too small to achieve this accuracy, it may be increased in subroutine shexqnn2:

! Maximum number of terms to be considered nterms = 20000000

In order to derive the optical properties of the particle ensemble weighted over a size distribution, an arbitrary number of particle radii to be considered can be defined. The considered radii are equidistantly distributed on a logarithmic scale within the radius interval $[a_{\min}, a_{\max}]$. In the published version, the size distribution follows a power-law

$$n(a) \propto a^q,$$
 (33)

where n(a) is the relative number of particles with the radius a and q is a constant, usually negative quantity for a given component of the mixture. This size distribution was introduced by Mathis et al. (1977) for silicate—graphite mixture with q = -3.5 in the process of the interpretation of the interstellar extinction curve and has been frequently used in different astrophysical applications. The code may be easily adapted to other particle size distributions by modification of the following program line (representing the Eq. (27) combined with Eq. (33))

```
weight = abun(jcomp) * rad * *q * delrad,  (34)
```

where weight is the weight for the component #jcomp with the radius rad and relative abundance abun. The quantity delrad is the radius step width at the current particle radius rad during the numerical integration stated in Eq. (27).

An arbitrary number of chemically different components in the ensemble can be considered. Beside the optical properties, each component is characterized by its relative abundance in the particle ensemble. The complex refractive index as a function of wavelength has to be provided in tabular form for each component in a separate file in the directory ./ri-data/ (see Tabl. 1):

```
Column 1 : Wavelength \lambda [\mum],
Column 2 : Re{m(\lambda)},
Column 3 : Im{m(\lambda)}
```

The results are stored in the directory ./results/ (see Tabl. 1, 2).

The order of the scattering matrix elements in the respective files (see Table 2) is defined by the following algorithm:

```
do for all wavelengths \lambda [\mum], in increasing order write \lambda do for all angles \Theta; in increasing order write \Theta [^{\mathrm{o}}], F_{ik}(\Theta,\lambda) end do end do
```

Table 1 Directory Structure.

Directory	Contents
./	Executable (<i>miex</i>), Source code, Makefile
./ri-data	Tables with optical data
./results	Output files (see Tab. 2)

Table 2 Output files (project is the project name).

Filename	Contents
project	Main file containing all results
	(see Appendix A for an example)
project.qext	$\lambda \; [\mu \mathrm{m}], Q_{\mathrm{ext}}$
project.cext	$\lambda \ [\mu \mathrm{m}], \ C_{\mathrm{ext}} \ [\mathrm{m}^2]$
project.qsca	$\lambda \; [\mu \mathrm{m}], \; Q_{\mathrm{sca}}$
$project.\mathtt{csca}$	$\lambda \ [\mu \mathrm{m}], \ C_{\mathrm{sca}} \ [\mathrm{m}^2]$
$project.\mathtt{qbk}$	$\lambda \; [\mu { m m}], Q_{ m bk}$
$project.\mathtt{cbk}$	$\lambda~[\mu \mathrm{m}],C_{\mathrm{bk}}~[\mathrm{m}^2]$
$project.\mathtt{qabs}$	$\lambda \ [\mu \mathrm{m}], Q_{\mathrm{abs}}$
$project.\mathtt{cabs}$	$\lambda \ [\mu \mathrm{m}], \ C_{\mathrm{abs}} \ [\mathrm{m}^2]$
$project. exttt{alb}$	λ [μ m], albedo
project.g	λ [µm], asymmetry parameter g
project.qpr	$\lambda \; [\mu { m m}], Q_{ m pr}$
project.f11	Θ [°], $F_{11}(\lambda [\mu m], \Theta [°])$
project.f12	Θ [°], $F_{12}(\lambda [\mu m], \Theta [°])$
project.f33	Θ [°], $F_{33}(\lambda \ [\mu \mathrm{m}], \Theta \ [$ °])
project.f34	Θ [°], $F_{34}(\lambda \ [\mu \mathrm{m}], \Theta$ [°])

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A Test Run

In the following, **miex** is used to calculate scattering matrix elements, efficiency factors, cross sections, the albedo and the asymmetry parameter for a particle ensemble typical for astrophysical applications (see Table A.1 and A.2):

- (1) Three components:
 - (a) Astronomical silicate (relative abundance: 62.5%; input file: silicate)
 - (b) Graphite; refractive index for the electric field vector parallel to the crystallographic c axis (relative abundance: 25%; input file: grap-per)
 - (c) Graphite; refractive index for the electric field vector perpendicular to the crystallographic c axis (relative abundance: 12.5%, input file: grap-par)
- (2) Grain size distribution:
 - minimum/maximum grain size: $a_{\min}=0.005 \,\mu\text{m}$, $a_{\max}=100 \,\mu\text{m}$
 - $n(a) \propto a^{-3.5}$
 - number of considered, logarithmically equidistantly distributed radii: 100
- (3) Calculation of the scattering matrix elements for the angles 0°, 2°, 4°, ..., 180°

Input files (with the dust properties) must be located in the directory "./input/", while the results ared stored in the directory "./results/".

In a second example, documented in Table A.3 and A.4, a dust grain ensemble with the chemical components as before but with a single grain size of 10 cm is considered.

The calculations are carried out for 100 wavelengths distributed equidistantly on a logarithmic scale within the interval $[0.05\mu\text{m}, 2000\mu\text{m}]$. The optical constants have been interpolated at the particular wavelengths using the data from Weingartner & Draine (2001) and Laor & Draine (1993).

We want to remark, that a large variety of refractive indexes can be found in the Jena – Petersburg Database of Optical Constants (Henning et al. 1999, see also Voshchinnikov 2004). The provided dust parameter files are presented in the format required by **miex**.

Table A.1 Input dialog for "example1". The runtime of the code on an Intel XEON CPU 3.0 GHz, using the Intel Fortran Compiler 8.0, amounts to 19 seconds (required memory: 1.5 MByte).

1.0 Real refractive index of the surrounding medium Number of wavelengths 100 Number of components 3 Name of the dust data files (lambda/n/k data) 001. component : silicate 002. component : grap-per 003. component : grap-par Relative abundances of the different components [%] 001. component : **62.5** 002. component : **25** 003. component : **12.5** -1- Single grain size -2- Grain size distribution 2 Minimum grain size [micron] 0.005Maximum grain size [micron] 100.0 Size distribution exponent -3.5Number of size bins 100 Calculate scattering matrix elements (0=n/1=y)1 Number of scattering angles in the interval $[0^{\circ},180^{\circ}]$; odd number! [example: '181' \rightarrow step width = 1°] 91Project name (8 characters) example1

1

Save results in separate files (0=n/1=y)

```
Table A.2
Program output. File: ''./results/example1''
```

```
# *** PROJECT PARAMETERS ***
# Number of wavelengths: 100
# *** RESULTS ***
# 1. Wavelength [micron], Extinction efficiency factor / cross section [m**2]
5.0000000000000000E-002 1.32305406861068 4.681097343048097E-016
. . .
# 2. Wavelength [micron], Scattering efficiency factor / cross section [m**2]
5.00000000000000000 0.587523440006963 2.078716568917760 E-016
# 3. Wavelength [micron], Backscattering efficiency factor / cross section [m**2]
5.000000000000000E-002 6.859423237184992E-002 2.426932402252230E-017
# 4. Wavelength [micron], Absorption efficiency factor / cross section [m**2]
# 5. Wavelength [micron], Albedo
5.00000000000000000E-002 0.444066084633951
# 6. Wavelength [micron], Scattering asymmetry factor g
5.000000000000000E-002 0.800843488171790
# 7. Radiation pressure efficiency factor Qpr
5.00000000000000000E-002 0.852539747532814
# 8. Wavelength [micron], theta [degree], F11-F12-F33-F34
5.0000000000000000E-002 0.00000000000000E+000 105571.611539073
5.0000000000000000E-002 0.00000000000000E+000 -5.641242912656195E-012
5.0000000000000000E-002\ 0.00000000000000E+000\ 105571.611539073
5.000000000000000E-002 0.00000000000000E+000 7.328649202947496E-011
```

Table A.3 Input dialog for "example2". The runtime of the code on an Intel XEON CPU $3.0\,\mathrm{GHz}$, using the Intel Fortran Compiler 8.0, amounts to 129 seconds (required memory: $\sim\!240\,\mathrm{MByte}$).

Real refractive index of the surrounding medium : 1.0

Number of wavelengths : 100

Number of components : 3

Name of the dust data files (lambda/n/k data)

001. component : silicate

002. component : grap-per

003. component : grap-par

Relative abundances of the different components [%]

001. component : **62.5**

002. component : **25**

003. component : **12.5**

-1- Single grain size

-2- Grain size distribution : 1

Grain size [micron]: 100000

Calculate scattering matrix elements (0=n/1=y) : 0

Project name (8 characters) : example2

Save results in separate files (0=n/1=y) : 1

```
Table A.4
Program output. File: ''./results/example2''
```

```
# *** PROJECT PARAMETERS ***
# Number of wavelengths: 100
# *** RESULTS ***
# 1. Wavelength [micron], Extinction efficiency factor / cross section [m**2]
# 2. Wavelength [micron], Scattering efficiency factor / cross section [m**2]
# 3. Wavelength [micron], Backscattering efficiency factor / cross section [m**2]
# 4. Wavelength [micron], Absorption efficiency factor / cross section [m**2]
# 5. Wavelength [micron], Albedo
# 6. Wavelength [micron], Scattering asymmetry factor g
5.00000000000000E-002 0.904868766536477
# 7. Radiation pressure efficiency factor Qpr
5.00000000000000E-002 0.682100777197063
```