CODES FOR CHAPTER 12

mmmie.f, mmmiea.f

Fortran77 programs `mmmie` and `mmmiea` calculate Mie coefficients (scattering coefficients a_n and b_n, efficiencies $Q_{\rm sca}, Q_{\rm ext}$ and $Q_{\rm abs}$, see Section 12.2 for definitions), and relate them to particle cloud properties (extinction coefficient β, absorption coefficient κ, scattering coefficient σ_s, scattering phase function Φ for specified scattering angles. In addition, program `mmmiea` also calculates the asymmetry factor g, and phase function expansion coefficients A_n, as defined in Section 12.3), but at a severe penalty in cpu time.
The input for both programs is the same, and is done via a data file `MIE.DAT`:

Input:

`IDSTF`	=	1: single particle size; =2: modified gamma distribution
`IETA`	=	1: single wavenumber; =2: wave number spectrum
`IPRNT`	=	1: print only final results; =2: also intermediate integrations
`CIR`	=	complex index of refraction
`RMIN`	=	minimum particle size in gamma distribution (in μm)
`RMAX`	=	maximum particle size in gamma distribution (in μm)
`AMG`, `BMG`, `ALMG`, `GAMG`	=	constants in gamma distribution, equation (12.34), `FR(R) = AMG*R**ALMG*DEXP(-BMG*R**GAMG)`; units: `AMG` [cm$^{-3}\mu$m$^{\rm ALMG+1}$], `ALMG` [-], `BMG` [μm^{-1}], `GAMG`[-]
`NPV`	=	number of particles per unit volume (in particles/cm^3)
`ETA`	=	wavenumber if single wavenumber is considered (in cm^{-1})
`ETMIN`	=	minimum wavenumber to be considered
`ETMAX`	=	maximum wavenumber to be considered
`NETA`	=	number of wavenumbers to be considered (equally spaced between `ETMIN` and `ETMAX`)
`ERRP`	=	maximum error allowed for absorption/scattering coefficients (and also the asymmetry factor for `mmmiea`)(in %)
`ERRA`	=	maximum absolute error desired for phase function values (`mmmie`) or expansion coefficients A_n (`mmmiea`) (in $10^{-\rm digits}$)

Note: to allow running the program on machines with relatively little RAM, array sizes have been declared fairly small, limiting calculations to (i) a maximum of 10 different wavenumbers, (ii) relatively small size parameters ($x \lesssim 300$), and (iii) relatively coarse integration intervals (< 500 nodes). More involved problems can be calculated by carefully increasing array limits as indicated in the programs.

Example:

The input file `MIE.DAT` as given in this directory, contains the following data:

```
  2, 1, 2
  (1.30149,-0.1620E-05)
   1.-10   1.+10,
   1.619424-4, 0.740741, 7.6,  1., 74.
10000.
  1.    .005
```

stating that a gamma-distribution of particles is to be considered for a single wavenumber, with detailed output (including intermediate integrations) (first line).
The complex index of refraction of the particles is $m = 1.30149 - 0.1620 \times 10^{-05} i$ (second line).

Particle sizes range from $10^{-10}\,\mu$m to $10^{+10}\,\mu$m (third line).
Gamma-function parameters in equation (12.34) are $A = 1.61942410^{-4}, B = 0.740741, \gamma = 7.6, \delta = 1$. The number of particles is given as $N(T) = 74/\text{cm}^3$ (this number is really not necessary for a gamma distribution, since it can be calculated from equation (12.35), and is only read and printed, but not used) (fourth line).
Since only a single wavenumber is considered, the fifth line contains only one number, $\eta = 100000\,\text{cm}^{-1}$.
Finally, the last line specifies to calculate κ, σ and β to an accuracy of 1% or better, and that the values for Φ or A_n should be calculated to an absolute accuracy of 0.005.

Running `mmmie` produces the following self-explanatory output, placed into file `MIE.RES`:

```
   PARAMETERS FOR PARTICLE DISTRIBUTION/SINGLE WAVENUMBER
   ******************************************************

   WAVENUMBER             = 0.100E+05 CM-1
   MINIMUM PARTICLE RADIUS= 0.100E-09 MICROM
   MAXIMUM PARTICLE RADIUS= 0.100E+11 MICROM
   REFRACTIVE INDEX       = 1.3015-0.0000i
   PARTICLE DENSITY       = 0.740E+02 PER CM**3
   DISTRIBUTION FUNCTION: N(R)=0.16194E-03*R**7.6*EXP(-0.74074E+00*R**1.0)


   MIE-PARAMETERS ARE CALCULATED FOR  16.00000  < X < 216.00000


   INTEGRATION WITH   9 NODES, AND A DX =25.000


ETA (CM-1)      1.000E+04
KAPPA (CM-1)    1.250E-07
SIGMA (CM-1)    3.675E-04
BETA  (CM-1)    3.676E-04


PHASE FUNCTION
DEG.              PHI
  0             4.835E+03
  1             1.943E+03
  2             2.093E+02
  3             5.329E+01
.
.
.
176             2.264E-01
177             1.503E-01
178             2.086E-01
179             3.508E-01
180             1.364E+00

   INTEGRATION WITH  17 NODES, AND A DX =12.500

ETA (CM-1)      1.000E+04
KAPPA (CM-1)    9.997E-08
SIGMA (CM-1)    3.667E-04
BETA  (CM-1)    3.668E-04


PHASE FUNCTION
DEG.              PHI
  0             4.634E+03
```

```
  1            1.851E+03
  2            2.304E+02
  3            4.943E+01
 .
 .
 .
 177           2.428E-01
 178           3.551E-01
 179           3.691E-01
 180           9.224E-01

    INTEGRATION WITH  65 NODES, AND A DX = 3.125

 ETA (CM-1)      1.000E+04
 KAPPA (CM-1)    1.023E-07
 SIGMA (CM-1)    3.684E-04
 BETA  (CM-1)    3.685E-04


 PHASE FUNCTION
 DEG.             PHI
   0           4.617E+03
   1           1.847E+03
   2           2.331E+02
   3           6.044E+01
   .
   .
   .
    INTEGRATION DID NOT CONVERGE: MAXIMUM ERROR = 0.18%


    ERROR FOR SIGMA : 0.18%, ERROR FOR BETA : 0.18%
    ERROR FOR
PHASE(  1): 2.84309
PHASE(  2): 2.45336
PHASE(  3): 1.56688
PHASE(  4): 0.47940
PHASE(  5): 0.23725
.
.
.
PHASE(179): 0.03003
PHASE(180): 0.05414
PHASE(181): 0.10000


 ETA (CM-1)      1.000E+04
 KAPPA (CM-1)    9.785E-08
 SIGMA (CM-1)    3.677E-04
 BETA  (CM-1)    3.678E-04


 PHASE FUNCTION
 DEG.             PHI
   0           4.614E+03
   1           1.845E+03
   2           2.347E+02
   3           6.092E+01
   4           3.153E+01
```

```
  5            2.034E+01
  6            1.511E+01
  7            1.234E+01
  8            1.066E+01
  9            9.560E+00
 .
 .
 .
170            7.660E-02
171            1.032E-01
172            1.213E-01
173            1.069E-01
174            9.150E-02
175            1.214E-01
176            1.629E-01
177            2.179E-01
178            2.986E-01
179            2.761E-01
180            7.212E-01
```

Running `mmmiea`, on the other hand produces the following output, placed into file `MIEA.RES`:

```
   PARAMETERS FOR PARTICLE DISTRIBUTION/SINGLE WAVENUMBER
   ******************************************************

   WAVENUMBER             = 0.100E+05 CM-1
   MINIMUM PARTICLE RADIUS= 0.100E-09 MICROM
   MAXIMUM PARTICLE RADIUS= 0.100E+11 MICROM
   REFRACTIVE INDEX       = 1.30149-1.62000E-06i
   PARTICLE DENSITY       = 7.400E+01 PER CM**3
   DISTRIBUTION FUNCTION: N(R)=1.61942E-04*R**7.6*EXP(-0.74074E+00*R**1.0)



   MIE-PARAMETERS ARE CALCULATED FOR  16.00000  < X < 216.00000


INTEGRATION WITH   9 NODES, AND A DX =25.000

 ETA (CM-1)      1.000E+04
 KAPPA (CM-1)    1.250E-07
 SIGMA (CM-1)    3.675E-04
 BETA  (CM-1)    3.676E-04
 GCOS  ( -- )    8.691E-01
       A(  1)    2.60744
       A(  2)    4.02359
       A(  3)    4.85462
       A(  4)    5.53582
       A(  5)    6.29942
       A(  6)    6.88010
       A(  7)    7.63828
       A(  8)    8.43823
       A(  9)    9.15186
       .
       .
       .
       A(449)    0.00000
       A(450)    0.00000
       A(451)    0.00000
       A(452)    0.00000
```

```
INTEGRATION WITH  33 NODES, AND A DX = 6.250

 ETA (CM-1)      1.000E+04
 KAPPA (CM-1)    1.015E-07
 SIGMA (CM-1)    3.681E-04
 BETA  (CM-1)    3.682E-04
 GCOS  ( -- )    8.716E-01
       A(  1)    2.52586
       A(  2)    3.88357
       A(  3)    4.68158
       A(  4)    5.32619
       A(  5)    6.04063
       A(  6)    6.59512
       A(  7)    7.31633
       A(  8)    8.08751
       A(  9)    8.72379
       A( 10)    9.58797
          .
          .
          .
       A(449)    0.00000
       A(450)    0.00000
       A(451)    0.00000
       A(452)    0.00000


 PHASEFUNCTION
 DEG.              PHI
   0             4.260E+03
   5             1.758E+01
  10             8.615E+00
  15             5.157E+00
  20             4.088E+00
  25             3.059E+00
  30             2.206E+00
  35             1.287E+00
  40             1.089E+00
  45             6.978E-01
  50             7.122E-01
  55             3.592E-01
  60             2.251E-01
  65             1.581E-01
  70             1.343E-01
  75             9.730E-02
  80             8.906E-02
  85             6.900E-02
  90             5.605E-02
  95             4.968E-02
 100             5.518E-02
 105             5.099E-02
 110             4.992E-02
 115             5.291E-02
 120             5.204E-02
 125             8.062E-02
 130             5.287E-02
 135             2.674E-01
 140             2.485E-01
```

```
145            1.552E-01
150            1.190E-01
155            1.194E-01
160            1.216E-01
165            1.328E-01
170            1.030E-01
175            1.690E-01
180            9.319E-01
```

`coalash.f90, coalash.exe`

This Fortran90 program determines absorption and extinction coefficients κ^*, β^* for the Rayleigh limit, from the Buckius and Hwang [1] model, as well as from the Mengüç and Viskanta [2] model. The user is prompted to input the complex index of refraction n and k as well as the nondimensional size parameter x of the coal/ash particles; results are then printed to the screen.

References

1. Buckius, R. O., and D. C. Hwang: "Radiation properties for polydispersions: Application to coal," *ASME Journal of Heat Transfer*, vol. 102, pp. 99–103, 1980.
2. Mengüç, M. P., and R. Viskanta: "On the radiative properties of polydispersions: A simplified approach," *Combustion Science and Technology*, vol. 44, pp. 143–159, 1985.