SIGMA : Simple Icy Grain Model for Aggregates User Guide

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1 Introduction

SIGMA is a code that computes the standard opacities for a given dust composition, size distribution and shape. SIGMA is able to provide dust properties for spherical and aggregate shapes. The code makes use of the Effective Medium Theory (EMT) applied to a Distribution of Hollow Spheres (DHS) to mimic aggregate made of n components. Thanks to polynomial solver, SIGMA is not limited in terms of number of components to made the dust mixture. SIGMA offers famous dust models from the literature and allows the user to tune the dust parameters.

1.1 Terms of use

The user agrees to cite the papers below in any publication using SIGMA:

- DOI associated to Zenodo registration of SIGMA: http://doi.org/10.5281/zenodo.2573887
- Lefèvre, C., Min, M., Pagani, P., et al. 2020, A&A (subm.), SIGMA: Simple Icy Grain Model for Aggregates
- The distribution of Hollow Spheres as defined in Min, M., Hovenier, J. W., and de Koter, A. 2005, A&A, 432, 909
- The agreement between approximate methods ans DHS: Min, M., Rab, C., Woitke, P., Dominik, C., & Ménard, F. 2016, A&A, 585, A13, Multiwavelength optical properties of compact dust aggregates in protoplanetary disks
- Any references associated to the refractive index data taken by the user.

2 Installation

SIGMA is a FORTRAN 90 code. It can be compiled either with gfortran or ifort. The code itself is delivered via github. Please make sure that you have

git and a fortran compiler installed. For the compilation to work, the cfitsio library must be installed on the system. This library can be downloaded from: http://heasarc.gsfc.nasa.gov/ fitsio/fitsio.html. Please try to solve software installation with your computer support before reporting problems.

To install SIGMA please do:

```
>git clone https://github.com/charlenelefevre/SIGMA.git
>cd SIGMA
>make clean
>make test
>make
```

By default gfortran is used, if you want to use ifort please do

```
>make ifort=true
```

or make sure to add in your configuration file:

```
export ifort="true" !for bash
setenv ifort "true" !for csh
```

Please update SIGMA on a regular basis and recompile if necessary.

```
>git pull
Already up-to-date.
```

To check if the instllation is successful you can do:

```
>cp DATA/input/COMPO_S03_NRM.dat DATA/input/COMPO.dat
>SIGMA -nm 6 -na 100 -v
```

3 Using SIGMA

All input or output ASCII files should use .dat extension.

3.1 Inputs

3.1.1 Dust composition

The dust composition is set according to DATA/input/COMPO.dat. The different components could be mixed or added (rule). The keyword *mix* is the default behavior for SIGMA i.e. to mix all components together into a composite aggregate. The keyword *add* allows to reproduce dust grain models from the literature for which the different grain populations are distinct from one another (e.g. Weingartner and Draine 2001, see example 2 below).

For the mix option, the different volume fractions of each component is defined by vfrac. The sum of vfrac for all components in COMPO.dat does not necessarily have to be equal to one because the code will normalize it to unity for all refractory components. For ice mantles, we consider vfrac as the additional volume on top of the refractory component. The total volume is $V_{tot} = V_{refractory}$ + vfrac(ices). amin and amax are given for the refractory component and also has to be identical Mdust/(100*MH) has to be identical for all individual components. Mdust/(100*MH) equal to 1 corresponds to a total dust-to-gas mass ratio Mgas/Mdust = 136 assuming Mgas/MH = 1.36.

For the add option, vfrac is used to distribute the proportions between two subvarieties of grains that sums up for the same type of grain (e.g. perpendicular and parallel refractive indexes of graphite). With the add option, Mdust/(100*MH) has to be set carefully by the user for each individual dust population with the total dust-to-gas mass ratio defined by $\sum$ vfrac $\times$ Mdust/(100 $*$ MH).

Two examples of COMPO.dat are provided below:

```
! Example 1
! # name ref_index vfrac rule sizedistrib Mdust/(100*MH) amin amax
1 silicates Mg70Fe30_2_SiO4_Henning 0.075 mix plaw 1.0 5.0E-03 5.0
2 iron Fe_Henning 0.002 mix plaw 1.0 5.0E-03 5.0
3 silicates Mg70Fe30SiO3_Henning 0.022 mix plaw 1.0 5.0E-03 5.0
4 iron_sulfides FeS_Henning 0.015 mix plaw 1.0 5.0E-03 5.0
5 carbonaceous CHON_Henning 0.291 mix plaw 1.0 5.0E-03 5.0
6 ices Water_ice_Henning 0.595 mix plaw 1.0 5.0E-03 5.0
```

```
! Example 2
! # name ref_index vfrac rule sizedistrib Mdust/(100*MH) amin amax
1 silicates Sil_WD01 1.0 add na_WD01_3.1_sil 8.2600E-01 3.1E-04 2.0
2 carbonaceous graphite_Epara_Draine2003 0.333 add
    na_WD01_3.1_gra_plaw-ed-cv 2.3300E-01 3.1E-04 2.0
3 carbonaceous graphite_Eperp_Draine2003 0.667 add
    na_WD01_3.1_gra_plaw-ed-cv 2.3300E-01 3.1E-04 2.0
4 carbonaceous graphite_Epara_Draine2003 0.333 add
    na_WD01_3.1_gra_log 1.8000E-02 3.1E-04 2.0
5 carbonaceous graphite_Eperp_Draine2003 0.667 add
    na_WD01_3.1_gra_log 1.8000E-02 3.1E-04 2.0
```

Individual component refractive index tables are located in DATA in the following subdirectories:

- carbonaceous
- silicates
- iron
- iron_sulfides

- ices

New directories can be created and the second column in DATA/input/COMPO.dat should be consistent with the location of refractive index files, while the third column should indicate the file name without extension. **Only the ices directory cannot be renamed and ices must always be defined as the last component in the composition input file.** Refractive index files must contain an header line with the number of wavelengths and the bulk density of the material in g.cm^{-3}. Then the file content is the wavelength (in micron), n and k as provided by refractive index database.

```
Example for Sil_WD01.dat in DATA/silicates/:
1201 3.5
1.0000E-03 0.999565 9.7381E-05
1.0116E-03 0.999554 1.0162E-04
1.0233E-03 0.999543 1.0605E-04
1.0351E-03 0.999531 1.1063E-04
1.0471E-03 0.99952 1.1522E-04
1.0593E-03 0.999509 1.2005E-04
1.0715E-03 0.999498 1.2509E-04
1.0839E-03 0.999487 1.3036E-04
1.0965E-03 0.999476 1.3582E-04
1.1092E-03 0.999465 1.4149E-04
1.1220E-03 0.999453 1.4734E-04
...
```

Columns 3 to 8 in DATA/input/COMPO.dat correspond to the volume fraction of the material in the dust mixture (vfrac), the rule to compute dust properties: mixed or added opacities, the size distribution, the fraction of dust mass with respect to hydrogen normalized by 100, and the minimum and maximum size to be considered for the size distribution.

SIGMA checks the number of dust components and ask the user to provide it as an argument with -nm being the number of dust components apart from vacuum (porosity):

```
>SIGMA
ERROR: 6 components found in DATA/input/COMPO.dat
You should run SIGMA with -nm 6
```

3.1.2 Size distribution

The size distribution can be set individually for each component according to DATA/input/COMPO.dat. The keyword must be identical for mixture (mix) while it could be different for added opacities (add, see examples above). Either power law (plaw) or custom size distribution from ascii file can be used. For power laws,

the keyword plaw should be set and a_{min} and a_{max} will be used and the power spectral index is set by default to $a_{pow} = 3.5$. The number of dust by bin size (between a and a+da) is defined by: $n(a) = a^{(-a_{pow}+1)}$. The number of bin sizes is 50 by default. The last two parameters can be modified by calling SIGMA with the following arguments -apow and -na, respectively:

```
>SIGMA -nm 6 -apow 2.5 -na 100
```

Custom size distributions should be recorded inside DATA/sizedistrib folder. Please provide the filename without extension in DATA/input/COMPO.dat. The size distribution file must contain a(microns), n(a)×a, porosity. When porosity is set to -1, the value defined by -porosity is used (by default 0, see Sect. 3.1.3).

```
Example of DATA/sizedistrib/na_WD01_5.5B_sil.dat
3.100000E-004 1.42307e-22 -1
3.387218E-004 1.28747e-22 -1
3.701048E-004 1.16478e-22 -1
4.043954E-004 1.05379e-22 -1
4.418630E-004 9.53369e-23 -1
4.828021E-004 8.62517e-23 -1
5.275343E-004 7.80322e-23 -1
5.764109E-004 7.05957e-23 -1
6.298160E-004 6.38679e-23 -1
6.881691E-004 5.7781e-23 -1
7.519287E-004 5.22741e-23 -1
8.215957E-004 4.7292e-23 -1
8.977175E-004 4.27845e-23 -1
9.808919E-004 3.87065e-23 -1
...
```

3.1.3 Dust shape

Two dust shapes are offered by SIGMA by varying the maximum volume fraction of vacuum of the distribution of hollow spheres (f_{max}):

- spherical dust shape ($f_{max} = 0$)
- aggregates ($f_{max} = 0.8$)

For aggregates, porosity has also to be set consistently with aggregate shape: values close to 0.25 are expected for compact aggregates with a fractal degree $D_f \sim 3$ (Min et al. 2016), while values typically above 0.8 (Ormel et al. 2011, Tazaki et al. 2018) are expected for fluffy aggregates ($D_f \sim 2$).

Porosity can either be constant or vary as a function of dust grain size as defined inside the size distribution file. A constant porosity will be used by default if power law is used as size distribution or if -1 is set on the first line of the 3rd column of

the size distribution file (see example above). The default value is 0 (spherical compact dust), but porosity can be modified using -porosity as an argument when calling SIGMA:

```
>SIGMA -nm 6 -porosity 0.25 -fmax 0.8
```

3.1.4 Other parameters

Other options are available when calling SIGMA and listed below:
-v = verbose mode (recommended)
-lmin = $\lambda_{\min}$ in μm(0.3 μmby default)
-lmax = $\lambda_{\max}$ in μm(100 μmby default)
-nlam = number of wavelength bins (100 by default)
-lambda_ref = wavelength in micron to normalize the extinction, by default K_S band is used (2.2 μm)
-file or -filename = output filename, by default opacities
-non_norm_ice = opacities will be normalized by the average bulk density without ices like in Ossenkopf et al. 1994

For example, all options above can be used in a single command line like:

```
> SIGMA -nm 6 -lmin 0.1 -lmax 1000 -nlam 500 -lambda_ref 9.7 -file
    mytest -non_norm_ice
```

3.2 Outputs

By default output files are written in the output folder. All output files will be overwritten if a different filename is not given as an argument with -file or -filename.

By default, SIGMA provides the following outputs:

- filename.dat = ASCII file that contains the main output
  λ[μm], K_{abs}[cm^2/g], K_{sca}[cm^2/g], K_{ext}[cm^2/g], albedo, g, p
  where g is the asymmetry parameter and p the linear polarization
- Kext_filename.dat = extinction normalized by lambda_ref

Additionally, SIGMA is thought to provide custom outputs for the following radiative transfer codes:

- CRT (Juvela et al.):
  * *CRT_filename.nH2.dust*: Tabulated dust properties averaged over the size distribution: (frequency, g, Q_{abs}, Q_{sca}).
  * *CRT_DSC_filename.dat*: Tabulated scattering function instead of the Henyey-Greenstein approximation.

- HYPERION (Robitaille et al.):
  * *HYPERION_set_filename.py*: full parameters needed to build an equivalent hdf5 dust model that can be directly used by HYPERION. It also include the possibility to compute Rosseland and Planck mean extinctions.

- Debris Disk Simulator (et al.):
  * *dds_filename.dat*: Tabulated dust properties (Q_{abs}, Q_{sca}, Q_{ext}, albedo) as a function of wavelength for all the different dust grain radii

Parameters to create or not the output files for radiative transfer codes can be found and modified inside the code itself (in SIGMA.f90). In particular we recommend the user to update them to suit their needs, e.g.:

```
verbose   = .false.
crt       = .true.
hyperion  = .false.
dds       = .false.
```