

INSTRUCTIONS TO USING SHIVA CODE

To run:

The SHIVA code calculates the change of dust size distribution and aromatisation level of dust grains in time under different conditions. The dust evolution model, on which SHIVA is based, is described in the paper of Murga et. al. 2019. For any questions please write to e-mail: murga@inasan.ru.

To work with the code you should have installed any C++ compiler and the CVODE package that can be downloaded from the SUNDIAL website <https://computation.llnl.gov/projects/sundials/cvode>. The version 2.8.2 is attached to the model. Please follow the instructions for the CVODE installation in «INSTALL_GUIDE.pdf».

To run the SHIVA code you should edit the Makefile where instead of PATH_TO you with specify the path to the CVODE libraries. Also you should specify your C++ compiler after «CXX = », usually it is g++.

After the makefile and all initial data were modified you can type:

```
$ make
```

```
$./run.out
```

Depending on the initial data the calculation time may take from several seconds to tens of minutes. Please be patient to get a result.

Initial data:

There are some optional files where you can change parameters of outer conditions and choose a type of dust grains. As the dust evolution is a multi-parameter problem we give possibility to change many of them. Files with initial parameters are stored in **_ini/** directory, namely there are: **__parameters.ini**, **__processes.ini**, **filenames.ini** and **__program_param.ini**. Below the contents of these files are described.

1) **__parameters.ini**

File **__parameters.ini** includes a number of parameters that influence on the evolution of dust grains. Namely parameters are:

1. Nbin_a - number of bins by radius (mass). It shouldn't be less than 15, but the numbers higher than 32 will lead to long time of calculations but not significantly precise the results.
2. Nbin_e - number of bins by the band gap energy (hydrogen fraction). We adopt this value equal to 5. And this more than enough to follow the aromatisation level evolution.
3. graintype - it should be one of the three: gra (graphite + PAHs.), hac (HAC), sil (silicates). Mainly SHIVA was developed to calculate the evolution of HAC grains, but you can also calculate the evolution of graphites, PAHs and silicates if you specify this.
4. nH - hydrogen density nH, cm⁻³
5. T - temperature of gas, K
6. fieldfactor - factor scaling the radiation field flux (MMP83)
7. ne - electron density, cm⁻³
8. chi_he - number of helium atoms per H atom
9. chi_c - number of carbon atoms per H atom
10. incharge = 1 or 0. It shows whether you consider or not consider grain charge. If you consider the charge you should give the file with charges (see below).
11. vgas - gas velocity, cm/s
12. arom_init = 1 or 0 - initial aromatisation state, 1 - dust is aromatised, 0 - dust is aliphatic
13. fi_h - fraction of ionised hydrogen in nH
14. fi-he - fraction of ionised helium in nHe
15. fi_c - fraction of ionised carbon in nC
16. disp, grain velocity dispersions are pre-calculated

2) **__processes.ini**

In file **__processes.ini** you can choose processes that you want to consider in the evolution (1 means that a process is included, 0 - not included):

aromatisation due to photodestruction
aromatisation due sputtering
photodestruction (loss of carbon atoms)
sputtering (loss of carbon atoms)
shattering

For silicate grains only sputtering and shattering processes are available. For graphite material no aromatisation may occur.

3) **__filenames.ini**

It's possible to calculate the dust evolution taking into account the charge. Actually the charge only little changes the results (mostly photodestruction). Now the charge is calculated for WNM conditions, but you can also give your own charges in a file. To do this you should put the file in directory ini and insert the name of your «charge» file in **__filenames.ini**, and you should also modify the parameter #15 (n_ini_charge) in **__par_arrays.ini**, that means the number of radii in your «charge» file.

ISRF is given in flux values in [ergs/cm²/cm/s] in the file [**__par_photons.ini**]. This ISRF corresponds to the MMP83 field. You can rescale the field by any factor changing the parameter #6 in **__parameters.ini**. You can also modify the file and add more photons or extend the ISRF to shorter wavelengths. To do this you should put the file in directory ini and insert the name of your «fieldflux» file in **__filenames.ini**, and you should also modify the parameter #6 (nla) in **__par_arrays.ini**, that means the number of wavelengths in your «fieldflux» file. However you should estimate how many times your field roughly differ from the MMP83 and indicate this value as «fieldfactor» in **__parameters.ini**.

You can change the initial size distribution. Now 3 dust models are included in the code: MRN, WD01, J13. For them there are the prepared files with size distributions for carbonaceous grains and silicates. To choose one of the model you should insert one of the names in the file **__filenames.ini** in line #2. You should also indicate the minimum and maximum grain size in **__parameters.ini** in lines #16 and #17 correspondingly.

Velocities of dust grains may have two components in the code: thermal and non-thermal (i.e. turbulent). Actually thermal velocities are almost negligible for shattering process, but we still use them. Non-thermal velocities may be set through the file that consists of three columns: radius, velocity, dispersion. If you do not specify velocity dispersions it will be equalled to velocity. You can see in the paper how the velocity of grain-grain collision is calculated in the code. The file should be inserted in **__filenames.ini** in line #4, and you should also modify the parameter #13 (n_ini_vel) in **__par_arrays.ini**, that means the number of radii in your «dust velocity» file. The file with «WIM» velocities from the work Yan et al. 2004 is included in our data.

4) **__program_param.ini**

In this file you should specify the time of calculations (in kyr) including the total duration time (line #1), integration time step (line #2) and the output time step (line #3). Actually the integration time step without any consequences can be equalled to the output time step.

Output data:

The output file **result.dat** is stored in **_dat/** directory. It consists of Nbin_a*Nbin_e*Ntimes blocks like:

```
0 0
5.599838e-08 3.570000e-01 0.000000e+00
1.007926e-07 3.570000e-01 0.000000e+00
1.814185e-07 3.570000e-01 0.000000e+00
3.265386e-07 3.570000e-01 0.000000e+00
5.877430e-07 3.570000e-01 0.000000e+00
1.057890e-06 3.570000e-01 0.000000e+00
1.904116e-06 3.570000e-01 0.000000e+00
3.427255e-06 3.570000e-01 0.000000e+00
6.168782e-06 3.570000e-01 0.000000e+00
1.110331e-05 3.570000e-01 0.000000e+00
1.998506e-05 3.570000e-01 0.000000e+00
3.597149e-05 3.570000e-01 0.000000e+00
6.474577e-05 3.570000e-01 0.000000e+00
```

```
1.165372e-04 3.570000e-01 0.000000e+00
2.097575e-04 3.570000e-01 0.000000e+00
3.775465e-04 3.570000e-01 0.000000e+00
```

where the first line has 2 numbers: number of aromatisation bin (from 0 to Nbin_e-1) and the number of time step (from 0 to Ntimes = the total duration time/the output time step). Then there are Nbin_a lines with mean radius of a bin, the band gap energy of these bins and number density of a bin.