

grid2cube utility : How to Use

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In order to use *grid2cube* use the instructions given in the top of *grid2cube.f* i.e.

The program *grid2cube* needs three input files:

(i) Main input text file (i.e. *Input.bader*), read by standard input. A sample of input file is:

C --- begin input file ---

h2o # The label of the system, as in SIESTA SystemLabel

rho # the task viz rho, toch, bader drho, ldos, vh or vt (in lowercase!!).

4.0 6.0 5.0 # a shift of the origin of coordinates (in bohr).

2 an integer (nskip) that specifies the density of grid points in the output. F

unformatted

C --- end input file ---

(ii) *SystemLabel.XV* file: this is a file generated by SIESTA i.e. in example above: *h2o.XV*. You should copy it from the directory with your SIESTA output files.

(iii) *SystemLabel.TASK* file: this is a file generated by SIESTA, with the values of the appropriate quantity on the grid. In example above: *h2o.rho*. You should copy it from the directory with your SIESTA output files.

Now use a single command :

./grid2cube<input.bader

```
drmohonlv@localhost:~/paper1-gga/paper1-agisystem-gga/peo5-  
File Edit View Search Terminal Help  
[drmohonlv@localhost bader]$ ./grid2cube<input.bader  
  
Reading grid data from file peorel5-agi-lda.BADER  
  
Cell vectors  
  
9.4486343890000004      0.0000000000000000      0.0000000000000000  
0.0000000000000000      18.897268778000001      0.0000000000000000  
0.0000000000000000      0.0000000000000000      22.676722533000000  
  
Grid mesh:           60 x           120 x           144  
  
nspin =              1  
  
Writing CUBE file peorel5-agi-lda.BADER.cube  
[drmohonlv@localhost bader]$ █
```

This will generate *.CUBE file for further use.

All the best.

Please give the feedback in drmohanlv@gmail.com
