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

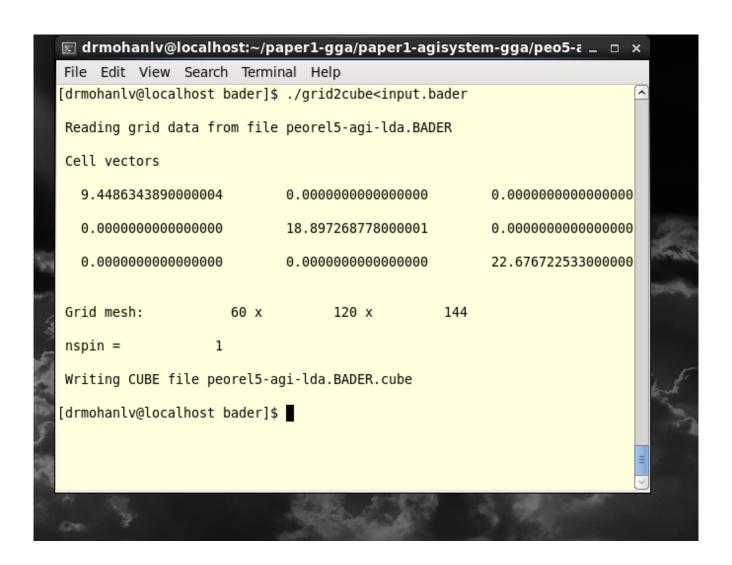
rho # the task viz rho, toch, bader drho, ldos, vh or vt (in lowercase!!).

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

- 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



This will generate *.CUBE file for further use.

All the best.

Please give the feedback in <u>drmohanlv@gmail.com</u>
