Aesp

Amesp’s electrostatic potential program

Program Manual

https://github.com/978142355/aesp

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1. Overview

Aesp is a program that uses density-fitting (DF) method to rapidly gain the molecular electrostatic potential (ESP) under Linux operating system, which is freely available at https://github.com/978142355/aesp.

2. Usage

There are two main programs, one is the **pfdmdf**, which is used to gain the density-fitting file (*.df) as the input file of aesp; the other is the **aesp**, which is to obtain the DF-ESP

a. Prepare the formatted checkpoint file (.fchk) from the Gaussian calculation, then use the command:

```
pfdmdf test.fchk def2-J -aesp 4
```

where test.fchk is the Gaussian formatted checkpoint file, def2-J is the auxiliary base set and def2-JK, cc-pvtz-jk, and cc-pvqz-jk auxiliary basis sets are provided to use, and number 4 denotes the parallel number. After that, the test.df can be yielded.

b. Build an input file (.inp) whose default value for asep is

```
npara 1
file filename(amo file or df file)
task esp
esp on
unit angs
read type1
Points Set
```

where the **1st** line is the parallel number;
the **2nd** line is the filename;
the **3rd** line is the task name, including molecular electrostatic potential and electron density;
the **4th** line is the keyword for ESP calculation, including “on”, ”ne”, “grad”, “hess”, and “off” five keywords, which controls the nuclear and electronic part in the ESP calculation; “on” is to calculate the ESP; “ne” means negative value of ESP, “grad” controls the analytical gradient of ESP calculation, “hess” controls the analytical hessian of the ESP calculation, and “off” denotes no calculation for ESP;
the **5th** line is the unit comprising “angs” and “bohr” two keywords, which

specifies the units used for input;

the **6th** line includes “type1”, “type2” and “type3” three keywords that must be written;

the **7th** line must follow this line

If read=“type1”, the structure of Points Set is:

```
Nx    Shiftx
Ny    Shifty
Nz    Shiftz
```

Nx, Ny, Nz are the point numbers of x, y, z directions, Shiftx, Shifty, Shiftz are the length of extended boundary of x, y, z and -x, -y, -z directions, and the unit of Shiftx, Shifty, Shiftz is Bohr.

If read=“type2”,the structure of Points Set is:

```
dx    Shiftx
dy    Shifty
dz    Shiftz
```

dx, dy, dz are the steps of x, y, z directions.

If read=“type3”,the structure of Points Set is:

x_1 y_1 z_1

x_2 y_2 z_2

……

x_n y_n z_n

For instance,

```
npara  4
file  CH4.df
task   esp
read  type1
50   0.5
40   0.5
45   0.6
```

Type1

```
file  CH3I.amo
task   esp
ecp    on
vxc    blyp
read  type2
0.01   0.5
0.01   0.5
0.01   0.6
```

Type2

```
npara  1
file  CH4.df
task   den
read   type3
   -1.06938851    3.37227536    0.09351981
   -1.25642813    3.37227536    0.09351981
   -1.06938851    3.18523574    0.09351981
   -1.25642813    3.18523574    0.09351981
   -1.06938851    3.37227536   -0.09351981
   -1.25642813    3.37227536   -0.09351981
   -1.06938851    3.18523574   -0.09351981
   -1.25642813    3.18523574   -0.09351981
```

Type 3

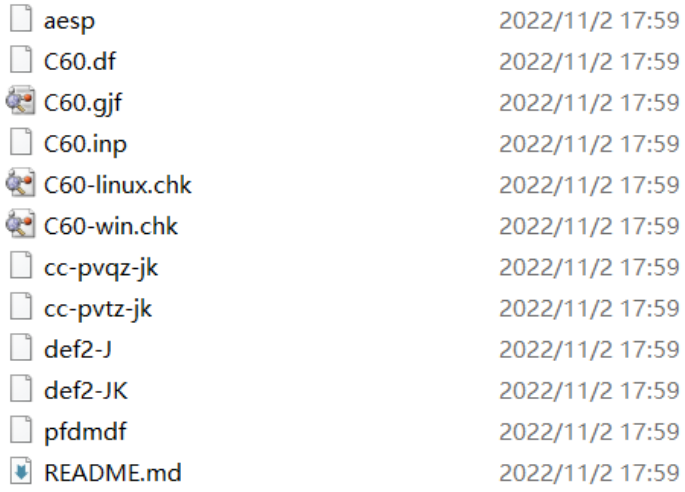
After setting the keywords for test.inp file, just run the command:

```
aesp test.inp
```

finally, the test.cub file that has the ESP from DF-ESP method generates.

3. Example

When one downloads the program from github, it comprises the following files:



The reason why uploads the chk file is the restriction on the file size at github. The .chk files at Windows and Linux systems are provided, where one can convert them to .fchk file.
Assume that we have the C60-linux.fchk file, then

```
pfdmdf C60-linux.fchk def2-J -aesp 4
```

the C60-linux.df generates, and

```
aesp C60-linux.inp
```

the C60-linux.cub obtains. One can use that cub file to present at GaussView or VMD, etc.