MOMAP

Tutorial 13

Reorganization Energy Calculation by Using
the Four-Point Method with MOMAP

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Reorganization Energy Calculation by Using the Four-Point Method with MOMAP

Here we take `naphthalene` as an example to show how to do the reorganization energy calculations by using the four-point method with MOMAP. In this tutorial, we assume the gaussian QC package (g09 or g16) is properly installed and the scheduling system SLURM is used.

Prepare the files

Suppose we initially have the file `mol1.mol` for `naphthalene`, we can use Jmol tool to generate a template gaussian input file `mol1.com`.

```
$ cat mol1.com
```

```
# HF/3-21G** opt pop=full gfprint

Title: Created by Jmol version 14.32.5  2022-04-18 16:19

0 1
C    -0.93840    0.11050    2.34410
C    -0.17480    0.97530    1.59120
C     0.20711    0.62610    0.26510
C     0.99060    1.49910   -0.54130
C    -1.35140   -1.13230    1.81760
H    -1.22030    0.35060    3.25100
H     0.12200    1.81920    1.93540
H     1.26370    2.32580   -0.16851
H    -1.88910   -1.75730    2.36510
C    -0.20711   -0.62610   -0.26510
C     0.17480   -0.97530   -1.59120
C     0.93840   -0.11050   -2.34410
C    -0.99060   -1.49910    0.54130
C     1.35140    1.13230   -1.81760
H     1.22030   -0.35060   -3.25100
H    -0.12200   -1.81920   -1.93540
H    -1.26370   -2.32580    0.16851
H     1.88910    1.75730   -2.36510
```

Note: This is just a template, only the coordinates are used in following generated Gaussian `.com` files. The converted file lacks an empty line at the end of the file, this will be corrected in the generated `.com` files.

Next we use the MOMAP `momap_geninp.exe` with the option `-reorg4p` to generate the file `momap.inp` for reorganization energy calculation by using the four-point method:

```
$ momap_geninp.exe -reorg4p
```

or

```
$ momap_geninp.exe -reorg4p -triplet
```

```
$ ls

mol1.com  mol1.mol. momap.inp  run.sh

$ cat momap.inp

&transport
  queue_name      = X16Cv3
  sched_type      = slurm       !  pbs, slurm, lsf, or local

  compute_engine = 1            !  1 = Gaussian, 2 = ORCA, 3 = QCHEM
  qc_exe          = g16         !  g09/g16 or fullpath/orca or qchem

# module_qc = gaussian/g16.c01-avx2

  qc_method       = b3lyp       !  ignored for g09/g16
  qc_basis        = b3lyp 6-31g(d)
  qc_basis_re     = b3lyp 6-31g(d)

  #  UDFT is recommended to use for T1 optimization by setting qc_es_mult = 3
  qc_es_opt       = TD          !  TD, TD(nstates=n); TD(triplets), TD(triplets,nstates=n)
  qc_gs_tddft     = TD          !  n is default to 3, change the number as needed
  qc_es_mult      = 1           !  default to 1, set to 3 for T1 optimization by UDFT
  qc_es_tddft     = TD(triplet) !  used only when qc_es_mult = 3 for T1 optimization

  qc_memory       = 54096       !  MB
  qc_nodes        = 1
  qc_ppn          = 16
/
```

Users may need to make changes according to one's specific situation. For example, change the `queue_name`, uncomment the `module_qc` line, and adjust `qc_ppn` *etc*. Once the modifications are done, we can continue use the MOMAP tool `momap_prep_reorg4p.exe` to generate the needed files for reorganization energy calculations by using the four-point method:

```
$ momap_prep_reorg4p.exe -input mol1.com
```

Note: If the option `-input` is not specified, the tool will search the current directory and use the first found Gaussian `.gjf` file as the Gaussian input file.

Then quite a few of files will be generated, as shown below:

```
[reorg_by_4p]$ tree ./

./
├── RE_run.py
├── jobs
│   ├── gaussian_log_check.py
│   ├── re-es.py
│   ├── re-es.slurm
│   ├── re-gs.py
│   ├── re-gs.slurm
│   ├── re-gs-tddft.py
│   └── re-gs-tddft.slurm
├── mol1.com
├── mol1.mol
├── momap.inp
```

```
├── re-es.com
├── re-gs.com
├── re-gs-tddft.com
└── run.sh

1 directory, 15 files
```

Run the job

Once the above preparations are done, we can simply launch the `run.sh` bash script to carry out the reorganization energy calculations by using the four-point method. It actually calls the python script `RE_run.py` to do the calculations.

```
$ sh run.sh
```

or

```
$ ./run.sh
```

If the calculations are finished successfully, then the final files are shown as below:

```
[reorg-by-4p]$ ls
```

```
jobs        re-es.chk  re-gs.log            RE_run.py
log         re-es.com  re-gs-tddft.chk      run.sh
mol1.com    re-es.log  re-gs-tddft.com      stdout-es
mol1.mol    re-gs.chk  re-gs-tddft.log      stdout-gs
momap.inp   re-gs.com  reorg_lambda_4P.dat  stdout-gs-tddft
```

The final reorganization energy data are put in the file `reorg_lambda_4P.dat`.

The results are also output to the `log` file as shown below:

```
[reorg-by-4p]$ cat log
```

```
 __  __   ___   __  __     _     ____
|  \/  | / _ \ |  \/  |   / \   |  _ \
| |\/| || | | || |\/| |  / _ \  | |_) |
| |  | || |_| || |  | | / ___ \ |  __/
|_|  |_| \___/ |_|  |_|/_/   \_\|_|       Version 2022A

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Job <892> is submitted to queue <normal>.
Job <893> is submitted to queue <normal>.
Job <894> is submitted to queue <normal>.

Energy definitions:
         2         2
          2       2
           2     2
       E2 |2   2
          |  2  E4
          |  |
          |  |
```

```
      1     |  | 1
       1    |  |1
        1   |  1
         1  | 1  E3
           1
          E1

Parsing re-gs.log...
  E1 =     -385.892706528 a.u.

Parsing re-gs-tddft.log...
  E2 =     -385.728779049 a.u.

Parsing re-es.log...
  E3 =     -385.882505594 a.u.
  E4 =     -385.739039325 a.u.

Reorganization energies:
  lam1 = E3 - E1
  lam2 = E2 - E4
  lam  = lam1 + lam2
  lam1 =     431.658901 meV (   3481.760694 cm-1)
  lam2 =     391.452942 meV (   3157.459428 cm-1)
  lam  =     823.111843 meV (   6639.220122 cm-1)

Successfully done at 2022-04-18 07:39:24.359745
DURATION: 0 days 0 hours 11 minutes 52 seconds.
```