MOMAP

Tutorial 05

QM/MM Calculation

Version 2019

October, 2019

MOMAP Tutorial 05

Version 2019 edited by:

Dr. Qikai Li

Dr. Yingli Niu

Ms. Lu Wang

Ms. Lihui Yan

Released by Hongzhiwei Technology (Shanghai) Co., Ltd
and Z.G. Shuai Group
The information in this document applies to version 2019 of MOMAP

MOMAP Tutorial 05

- QM/MM Calculation

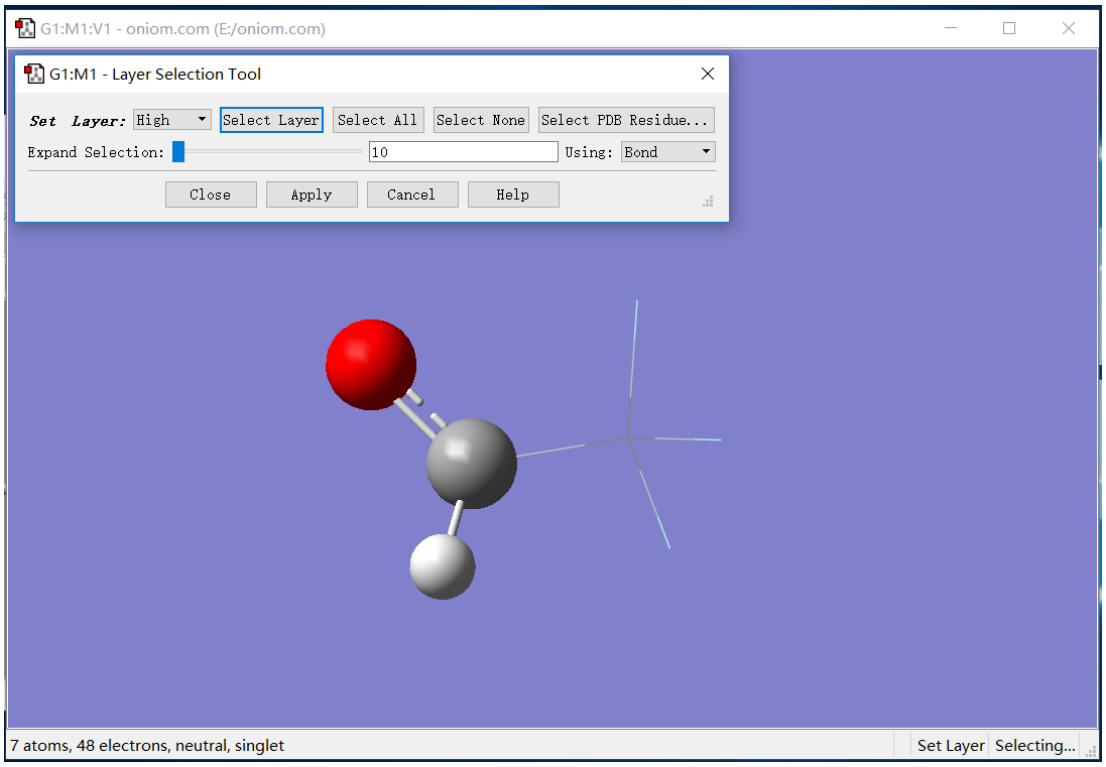
The basic steps involved in the calculations are as follows:

1) Prepare QM/MM input files
2) Carry out QM/MM calculations
3) Do evc calculation etc.

Contents

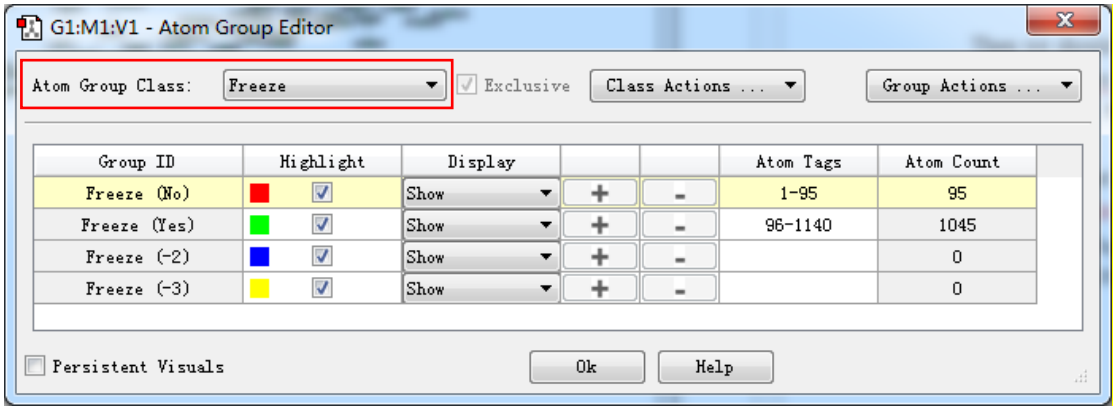
Prepare QM/MM input files

GaussView would be the fastest option to prepare input files for QM/MM calculations. Before we can do QM/MM calculations, we have to first select which atoms are in which layer, by using **`Tools->Select Layer`**... option. For example, we first put everything into the Low layer (**`Set Layer -> Low`**, **`Select All`**, **`Apply`**), then choose the ligand + perhaps some nearby residues, and then move them to High layer.



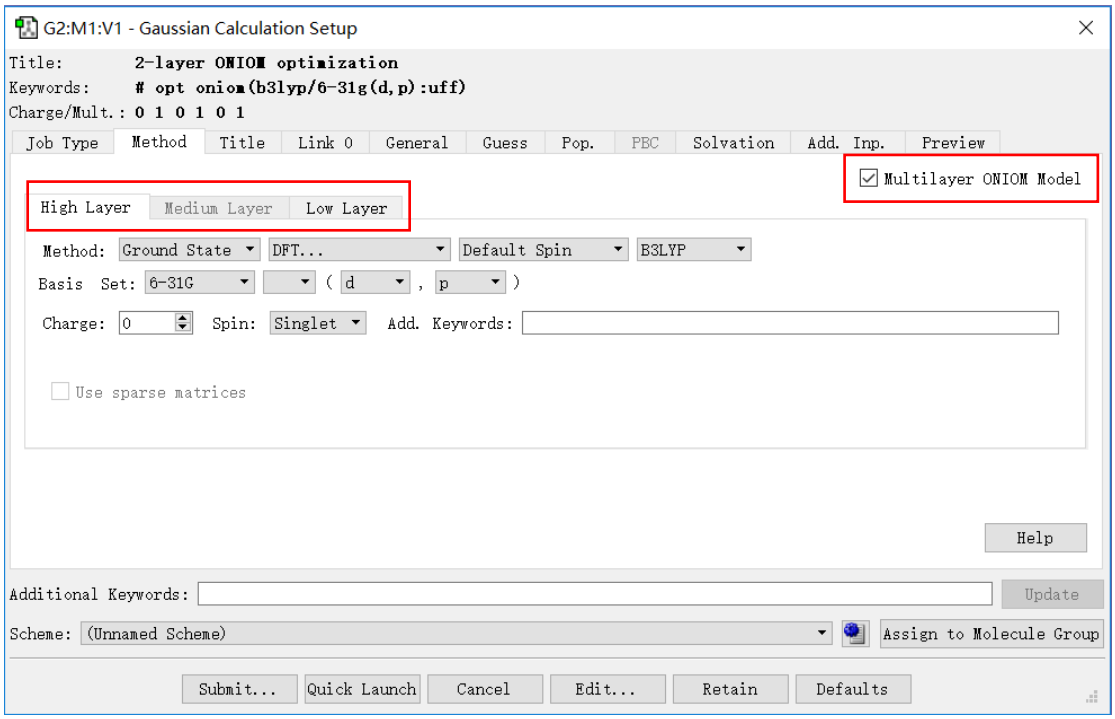
The High Layer consists of the final three atoms (as QM atoms). The other atoms are placed into the Lower Layer (as MM atoms). A link atom is defined for the first carbon atom.

Once we have set up the layers, then we would have to decide which atoms should be set as **Freeze (Yes, -1)** and which atom should be set as **Freeze (No, 0)** during the optimization process, by operating from the GaussView menu **`Tools -> Atom Groups -> Freeze`** as follows:

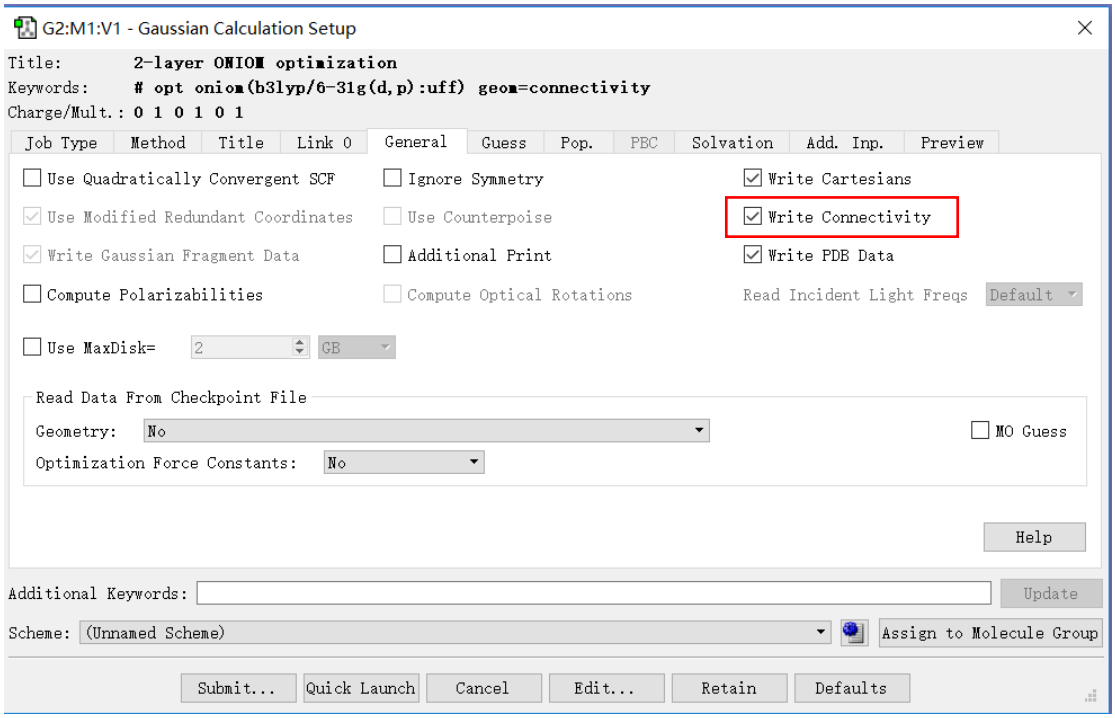


GaussView would normally set this value to 0, that is, all atoms are set as **Freeze (No)**, if we do not do anything. With GaussView 5 and 6, operation on freezing with Atom Group Class can be done from the GaussView menu **`Tools -> Atom List -> Freeze`** as show above.

Afterwards just choose **`Calculate->Gaussian calculation Setup`**..., in the **`Method`** tab select **`Multilayer Oniom Model`** and then define the Method separately for the **`Low Layer`** and **`High Layer`** (in the Method tab we will have Low Layer and High Layer tabs active if one selected the layers properly).



Click the **General** tab, and tick the **Write Connectivity:**



Note: One should carefully check the correctness of atom connectivity which was generated by GaussView automatically if one would like to use MM method (UFF, AMBER *et al.*) to do the Low Layer calculation, especially the bond order in benzene ring.

The Gaussian input file may look like:

```
%chk=s0.chk
%nprocs=24
%mem=60GB
# opt oniom(b3lyp/6-31g(d,p):uff) geom=connectivity

2-layer ONIOM optimization

0 1 0 1 0 1
 F-F_           -1   -1.04150621    0.00000000   -2.12610949 L
 F-F_           -1   -2.03368194   -1.14289207   -0.41221877 L
 F-F_           -1   -2.03368194    1.14289207   -0.41221877 L
 C-C_3          -1   -1.29903811    0.00000000   -0.75000000 L H-H_ 5
 C-C_2           0    0.00000000    0.00000000    0.00000000 H
 H-H_            0    0.00000000    0.00000000    1.10000000  H
 O-O_2           0    1.12583302    0.00000000   -0.65000000 H

 1 4 1.0
 2 4 1.0
 3 4 1.0
 4 5 1.0
 5 6 1.0 7 1.5
 6
 7
```

The 6th column is used to judge which atoms belong to the QM layer, normally the atoms marked with **H** are treated as QM (or free) atoms, which is later used in MOMAP to do the `evc` calculation.

In MOMAP, the 2nd column of data (in red box) can be omitted, that is, both 5 columns and 6 columns of data are supported.

Carry out QM/MM calculations

Once the input files are prepared, we can use QM program to do the calculations. Here we use Gaussian g16 to do the calculations, and the Gaussian log output file (segment related to QM) may look like:

```
------------------
Title Card Required
------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1 for low   level calculation on real  system.
Charge =  0 Multiplicity = 1 for high  level calculation on model system.
Charge =  0 Multiplicity = 1 for low   level calculation on model system.
C-C_R                -1    0.7315   -9.7969   -7.57692  L
C-C_R                -1    0.3898   -11.20542  -11.61389  L
C-C_R                -1    0.49442  -12.11868  -10.58599  L
H-H_                 -1    0.47497  -13.05064  -10.76799  L
C-C_R                -1    0.62992  -11.66088  -9.27435  L
H-H_                 -1    0.70805  -12.28647  -8.56401  L
C-C_R                -1    0.64988  -10.29488  -8.99592  L
C-C_R                -1    0.53102  -9.38892  -10.05365  L
H-H_                 -1    0.52456  -8.45499  -9.87672  L
C-C_R                -1    0.42363  -9.83959  -11.35136  L
H-H_                 -1    0.37178  -9.21709  -12.06743  L
```

However, there exist other cases where the output formats may differ, for example, if the **geom=check** is used in the Gaussian input file, the Gaussian input file may look like:

```
%chk=s1.chk
%nprocs=24
%mem=60GB
# oniom(b3lyp/6-31g(d) td(nstates=7):uff=qeq)=embed opt geom=check guess=read

2-layer ONIOM optimization

0 1 0 1 0 1
```

Then, the Gaussian log output file (segment related to QM) may look a bit different from those as shown above:

```
------------------
Title Card Required
------------------
Structure from the checkpoint file:  "s1.chk"
Charge =  0 Multiplicity = 1 for low   level calculation on real  system.
Charge =  0 Multiplicity = 1 for high  level calculation on model system.
Charge =  0 Multiplicity = 1 for low   level calculation on model system.
Redundant internal coordinates found in file.  (old form).
C,-1,-1.995,-7.384,-21.16
C,-1,-1.587,-7.947,-19.948
C,-1,-2.555,-8.168,-18.948
H,-1,-2.31,-8.584,-18.13
C,-1,-3.863,-7.774,-19.164
C,-1,-4.231,-7.199,-20.398
H,-1,-5.126,-6.916,-20.535
C,-1,-3.309,-7.042,-21.409
H,-1,-3.572,-6.707,-22.26
C,-1,0.429,-7.982,-21.156
C,-1,-0.186,-8.3,-19.939
C,-1,0.532,-8.93,-18.915
H,-1,0.128,-9.131,-18.078
```

Here, the data are separated by comma, rather than by empty spaces.

Note: The above three output data formats are supported by MOMAP.

Do evc calculation etc.

Once the Gaussian log files are prepared, we can do the `evc` calculated as usual, for example, the `momap.inp` may look like:

```
do_evc            = 1

&evc
  ffreq(1)        = "freq.log"
  ffreq(2)        = "freqes.log"
  proj_reorg      = t
/
```

Finally do the `evc` calculation:

```
momap -input momap.inp -np 1
Or
momap.py -i momap.in -n 1
```

Later on, we can use MOMAP to carry out other calculations.