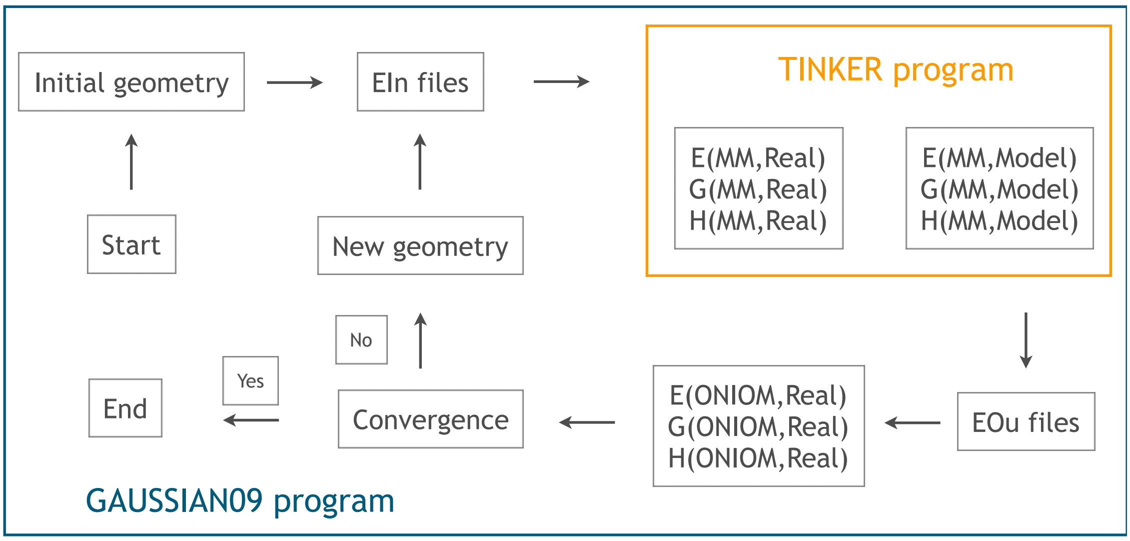
Introduction

This tutorial provides a quick guide to use Gaussian09 standardized interface to perform ONIOM(QM:MM) calculations with an external MM program. With this implementation, you can use Gaussian 09 to perform QM calculation and an external program for MM calculation. Present implementation uses Tinker6.1 program package as the external MM program, and allows you to use the Tinker force filed parameter sets for ONIOM(QM/MM) calculations, specifically Amber (ff94, ff96, ff98 and ff99), CHARMM (CHARMM19 and CHARMM27), Allinger (MM2-1991 and MM3-2000) and OPLS (OPLS-UA, OPLS-AA and OPLS-AA/L). I encourage you to read the Tinker6.1 manual that can be found at;
http://dasher.wustl.edu/ffe/downloads/guide.pdf

Implementation

Following scheme shows the software implementation for Gaussian09 standardized interface to run Tinker6.1 program. There are three scripts, namely `external_tinker`, `make_input`, and `make_output` automate this mechanism.



This process starts with Gaussian09 to provide text files (`EIn`) with the current structure (real system and model system). Then, `make_input` script refers the `EIn` files to setup input files for Tinker. Thereafter, `ext_tinker` script runs Tinker modules, and `make_output` script can convert functional values and derivatives into a standard text file (`EOu`) for the recovery by Gaussian09 program.

`ext_tinker` script

This `bash` script performs the following tasks;

- Identify the file name of `EIn` files that Gaussian09 generates.
- Execute `make_input` and `make_out` scripts.
- Execute `analyze`, `testgrad`, and `testhess` modules of Tinker.

`Make_input` script

This `Perl` script refers Gaussian09 `EIn` files to prepare input files for Tinker program. The "atom types section" of the `make_input` script is very important, and this section has to be defined by the user. General format of the `Perl` script is;

```
if($atom[$lnum] eq "UFF type") {$atomc[$lnum] = "TINKER type"};
```

The "`UFF type`" section of above `Perl` script can be filled with the UFF atom types. Detailed information about the UFF atom types can be found in literature. [1] Corresponding TINKER atom type goes to the "`TINKER type`" section, where you can check the TINKER parameter files (`prm`) from the following link;

http://dasher.wustl.edu/ffe/distribution/params/

`Make_output` script

This `Perl` script extracts functional values and derivatives from Tinker MM calculations, and report them into a standard text file (`EOu`) in the following order;

- Energy and dipole moment.
- Gradients.
- Polarizability.
- Dipole derivatives.
- Force constants.

Present implementation calculates MM gradients and MM hessian analytically. In case of frequency (or force constant) calculations, reporting polarizability and dipole derivatives in the `EOu` file is mandatory. However, these parameters are set to zero for simplicity, and therefore present implementation does not calculate these properties or properties derived from them.

`inp.key` file

The `inp.key` file always has the extension `key`, and this file has to be in the working directory. The `inp.key` file contains full path for the Tinker parameter files (`prm`). You can also include a wide variety of switches and missing potential parameters in this file.

How to submit calculations on kimik2.iciq.es

This section uses $OsO_4(NR_3)$ model complex (Figure 2)[2] to setup an ONIOM(DFT:MM3) calculation and run on kimik2.iciq.es

Step 1: Use Gaussview software to set up the ONIOM(QM:MM3) calculation – refer Figure 2 to assign QM and MM partitions, and copy this to your home directory on kimik2.iciq.es

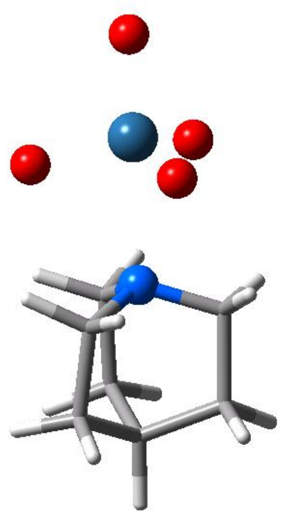


Figure 2. QM/MM molecular model of $OsO_4(NR_3)$ model ('ball and stick' model represents the QM region and 'tube' model represents the MM region). Note: In the QM region, Os-N and Os-O bonds were removed for simplicity.

Input file is shown below;

```
%nproc=4
%Mem=4000MB
%Chk=test
#p opt(nomicro) freq oniom(b3lyp/genecp:external="./ext_tinker")
# geom=connectivity nosymm scf(maxcyc=100)

QM - GAUSSIAN09 and MM – TINKER6.1 with MM3

0 1 0 1 0 1
 Os-X              0    0.00000000    0.00000000    0.00000000 H
 O-O_3             0   -1.68425000   -0.37872000    0.00000000 H
 O-O_3             0    1.02911000   -0.37784000   -1.33378000 H
 O-O_3             0    0.00000000    1.71880000    0.00000000 H
 O-O_3             0    0.64048000   -0.37670000    1.55831000 H
 N-N_3             0    0.00105000   -2.46450000   -0.00018000 H
 C-C_3             0    1.36710000   -2.90190000    0.19808000 L H-H_ 6
 C-C_3             0   -0.85424000   -2.90221000    1.08315000 L H-H_ 6
 C-C_3             0   -0.50994000   -2.89997000   -1.28312000 L H-H_ 6
 C-C_3             0   -0.08705000   -4.99145000   -0.00439000 L
 C-C_3             0   -0.46997000   -4.43901000   -1.38395000 L
 C-C_3             0    1.31129000   -4.45668000    0.33223000 L
 C-C_3             0   -1.08657000   -4.43308000    1.02690000 L
 H-H_              0    1.96740016   -2.62659086   -0.64378970 L
 H-H_              0    1.57222000   -4.78184000    1.35975000 L
 H-H_              0    2.06715000   -4.92296000   -0.34041000 L
 H-H_              0   -0.09992000   -6.10606000   -0.01149000 L
 H-H_              0   -1.45703000   -4.83698000   -1.71029000 L
 H-H_              0    0.27668000   -4.76102000   -2.14472000 L
 H-H_              0    0.07293000   -2.45572000   -2.11786000 L
 H-H_              0   -1.55474000   -2.54342000   -1.41521000 L
 H-H_              0   -1.84301000   -2.40079000    1.02931000 L
 H-H_              0   -0.42478000   -2.60740000    2.06036000 L
 H-H_              0   -2.08900855   -4.64059714    0.71552628 L
 H-H_              0   -0.90324368   -4.86729000    1.98750040 L
 H-H_              0    1.76575158   -2.46958518    1.09199320 L

 1
 2
 3
 4
 5
 6 7 1.0 8 1.0 9 1.0
 7 12 1.0 14 1.0 26 1.0
 8 13 1.0 22 1.0 23 1.0
 9 11 1.0 20 1.0 21 1.0
 10 11 1.0 12 1.0 13 1.0 17 1.0
 11 18 1.0 19 1.0
```

```
 12 15 1.0 16 1.0
 13 24 1.0 25 1.0
 14
 15
 16
 17
 18
 19
 20
 21
 22
 23
 24
 25
 26

Os 0
LanL2DZ
****
O C H N 0
6-31G*
****

Os 0
LanL2DZ
```

Important notes:

- In order to minimize the problems associate with EIn files, the UFF arom type symbol of Os, (Os6+6), was changed to a different character, "X".
- `Opt(nomicro)` option is mandatory.
- `external="./ext_tinker"` keyword commands Gaussian09 to perform the MM calculation externally.

Step 2: Keep `external_tinker`, `make_input`, `make_output`, `inp.key` scripts and above input file in your working directory.

Step 3: Edit the `make_input` script.

Update `make_input` script with the following atom type conversions;

```
# ******************************************************
#    Convert UFF atom types to TINKER MM3 atom types
# ******************************************************
# Following format is required
# if($atom[$lnum] eq "UFF_atom_type")  {$atomc[$lnum] = Tinker_atom_type};
#
   if($atom[$lnum] eq "X")  {$atomc[$lnum] = 165};
   if($atom[$lnum] eq "C_3") {$atomc[$lnum] = 1};
   if($atom[$lnum] eq "H_")  {$atomc[$lnum] = 5};
   if($atom[$lnum] eq "O_3") {$atomc[$lnum] = 7};
   if($atom[$lnum] eq "O_R") {$atomc[$lnum] = 6};
   if($atom[$lnum] eq "C_R") {$atomc[$lnum] = 2};
   if($atom[$lnum] eq "N_3") {$atomc[$lnum] = 8};
   if($atom[$lnum] eq "N_R") {$atomc[$lnum] = 37};
```

Step 4: Edit the `inp.key` script.

Enter the full path for the Tinker MM3 parameter file (`mm3.prm`) at the Tinker home directory, and assign the missing potential parameters as shown below;

```
#
# This script was written by W. M. C. Sameera
#
# The keyword parameter file always has the extension key.
# This file contains full path for the Tinker parameter
# files (prm).
# You can also include a wide variety of switches and
# missing potential parameters.
#
# ******************************************************
#     Path for the TINKER force field parameter file
# ******************************************************
#
parameters /mnt/data/applications/TINKER/v6.1/install_dirs/params/mm3
#
# ******************************************************
#         Define missing potential parameters
# ******************************************************
#
# Define atoms
atom    165    X    "Os atom"    76    190.23    4 # X is Os
```

```
# Define bond parameters
bond   7   165   0.3     1.67
bond   8   5     6.420   1.0150

# Define bond angle parameters
angle   7   165  7    0.5     90.0
angle   6   2    37   0.6     120.0
angle   5   8    5    0.605   106.40   107.10   0.00

# Define torsion parameters
torsion  2  1  6  2   0.0  0.0  1  0.0  180.0  2  0.403 0.0  3
torsion  6  2  37 37  0.0  0.0  1  12.0 180.0  2  0.0   0.0  3
torsion  1  6  2  37  1.05 0.0  1  7.5  180.0  2 -0.2   0.0  3
#
```

Step 5: Submit calculation to the queue system

Use the following script (`test.sub`) to submit calculations to c4m8 machines;

```
#!/bin/bash

#$ -cwd
#$ -pe c4m8_smp 4
#$ -m ae
#$ -r n
#$ -masterq c4m8.q

### APPLICATION ENVIRONMENT VARIABLES ###

. /etc/profile.d/modules.sh
module load tinker/6.0r1
module load gaussian/g09

. $g09root/g09/bsd/g09.profile

mkdir $TMPDIR/$JOB_NAME.$JOB_ID
unset $GAUSS_SCRDIR
export GAUSS_SCRDIR=$TMPDIR/$JOB_NAME.$JOB_ID

### USER VARS & EXEC ###

DIRECTORY=`echo  $PWD`
cd $TMPDIR/$JOB_NAME.$JOB_ID

### Input file name ###
SCRIPT=test
```

```
### Input file name ###
SCRIPT=test

cp $DIRECTORY/* ./
time g09 < $SCRIPT.in > $DIRECTORY/$SCRIPT.out
cp -rf * $DIRECTORY/
```

For c8m24 machines, change the lines 3-7 for:

```
#$ -cwd
#$ -pe c8m24_smp 8
#$ -m ae
#$ -r n
#$ -masterq c8m24.q
```

For c12m24 machines, change the lines 3-7 for:

```
#$ -cwd
#$ -pe c12m24_smp 12
#$ -m ae
#$ -r n
#$ -masterq c12m24.q
```

Calculations can be submitted with the following command;

```
qsub test.sub
```

Step 6: Check the output files.

In the job is sent with new version of ".sub" file, the ".out" file is saved automatically in your work directory and it is not necessary to login in the computer node and check the output file.

After submission, your calculation will be running in the /scratch directory of a computer node. You can check your queue and identify the node where your calculation is running. You can manually login to this computer node and check the output files.

Result of the external MM calculation, will be reported in the Gaussion09 output file at each geometry;

```
External calculation of energy, first and second derivatives.
 Running external command "./ext_tinker R"
         input file       "/scratch/test.sub.85322/Gau-1732.EIn"
         output file      "/scratch/test.sub.85322/Gau-1732.EOu"
         message file     "/scratch/test.sub.85322/Gau-1732.EMs"

--------------------------------- EXTERNAL PROGRAM STARTED ----------------------

TINKER program started .....
TINKER program finished ....
Information recovery ...........

--------------------------------- EXTERNAL PROGRAM FINISHED ---------------------

 Recovered energy= 0.281332248859     dipole=     -0.018097795778
1.310909902876     -0.930069330852
 External forces:
 I=    1 X=  -2.676624678000D-04 Y=  -6.582776382000D-04 Z=  -1.017016182000D-04
 I=    2 X=   2.353009454250D-02 Y=  -1.897097797140D-02 Z=  -7.264413347100D-03
 I=    3 X=   1.982085268800D-03 Y=   2.898496118700D-03 Z=   5.352406059000D-03
 I=    4 X=   3.387186730200D-02 Y=   7.342586979000D-03 Z=  -8.887507083000D-04
 I=    5 X=   1.619636218200D-03 Y=   4.199366070900D-03 Z=  -2.339896185900D-03
 I=    6 X=   2.440838836800D-03 Y=  -8.662599773100D-03 Z=  -6.354411554400D-03
 I=    7 X=  -1.583458776900D-02 Y=   5.585080134270D-02 Z=   2.637833016000D-03
 I=    8 X=  -7.391278947780D-02 Y=  -5.672605929900D-03 Z=  -5.811555976590D-02
 I=    9 X=   9.399472691700D-03 Y=   5.636850137100D-03 Z=   1.367406085500D-02
 I=   10 X=  -1.267559720700D-03 Y=  -9.138556599900D-03 Z=  -1.331633426760D-02
```

When the job is finished, all files will be copied back to the home directory, and you can find the total ONIOM(DFT:MM3) energy in the *.out file.

```
 ONIOM: calculating energy.
 ONIOM: gridpoint  1 method:  low   system:  model energy:     0.005747003286
 ONIOM: gridpoint  2 method:  high  system:  model energy:  -448.482418984184
 ONIOM: gridpoint  3 method:  low   system:  real  energy:     0.047110032762
 ONIOM: extrapolated energy =    -448.441055954708
```

Appendix

Names of the files:

If you want to change the name of the input file (test.in is the default name) it is necessary to change in the *.sub (by default is test.sub but it can be changed without problems) the value of the SCRIPT variable (by default is test).

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[1] A. K. Rappé, C. J. Casewit, K. S. Colwell, W. A. G. III, and W. M. Skiff, *J. Am. Chem. Soc.*, **114** (1992) 10024-35.

[2] G. Ujaque, F. Maseras, A. Lledos *Theor. Chem. Acc.* 1996, *94*, 67-73.