i-EIP(improved Elastic Image Pair)方法是一种双端过渡态搜索方法,该方法使用反应物和产物结构作为输入,可以自动定位过渡态.

参考文献: Improved Elastic Image Pair Method for Finding Transition States. J. Chem. Theory Comput. 2023, 19 (8), 2410-2417.

Installation

环境: Python 3.X, numpy

步骤 1: 解压代码
步骤 2: 将代码目录路径添加到环境变量
步骤 3: 给 `run_iEIP` 文件添加可执行权限

(本代码使用Gaussian 09软件进行量化计算,请确保Gaussian 09被正确安装,且能正确使用 `g09` `formchk` `unfchk` 指令)

Input file

本软件使用 `.gjf` 文件作为输入文件,计算任务需要被设定为 `force` 且添加 `nosymm` 关键词,一般文件格式为:

```
%nproc=[N]
%mem=[M]
#p force nosymm [Method/BasisSet] [Solvent]

title

[charge spin]
[coord]
```

Run i-EIP

准备反应物和产物文件(如: A.gjf B.gjf, 文件中原子顺序需要一一对应)
执行 `run_iEIP A.gjf B.gjf`
程序正常结束后,目录下会生成 `ts` 开头的.log文件,该文件为最终过渡态文件.

Example

以 example 文件中1号反应为例,在该目录下执行 run_iEIP 1_A.gjf 1_B.gjf ,得到以下输出:

```
|-------------------------------------------------------------------|
|                                                                   |
|                  Improved Elastic Image Pair method               |
|                                                                   |
|         If this program benefitted your research please cite:     |
|                https://doi.org/10.1021/acs.jctc.3c00151           |
|                                                                   |
|-------------------------------------------------------------------|


                     ########################
                     ##     Read input     ##
                     ########################
Current directory: /home/lyq/code/test
Input files: 1_A.gjf 1_B.gjf
Number of atoms: 3
```

```
                    ############################
                    ##  Generate image pair   ##
                    ############################
Node number: 200
Running IDPP interpolation...
Interpolation finished
Path length: 2.1877

 cycle  index E/a.u.
     1      0 -93.4240719176
     2     50 -93.3437034972
     3    100 -93.3058843443
     4    150 -93.3385381038
     5    201 -93.3977203205
Index of maximum: 100
Selected index: 59 141
```

```
                     ############################
                     ##  i-EIP optimization  ##
                     ############################
Initial length of the image pair: 1.1480
Running i-EIP optimization
Maximum number of cycles: 300

Convergence thresholds:
                L <=  0.6
          max|Fv| <=  0.008
         |overlap| >=  0.8 (after i-EIP optimization)
(All quantities are given in a.u.)


cycle L   Lt    Fp(A)  Fp(B) max|Fv| rms(Fv)   d(E)  sum(E) ReGen
  6 1.15 1.15 -0.0980  0.0991 0.0776 0.0403  -0.0031 -186.6603  0
  7 1.15 1.15 -0.0667  0.0639 0.0499 0.0186   0.0011 -186.7094  0
  8 1.03 1.03 -0.0316  0.0370 0.0478 0.0150   0.0048 -186.7127  0
  9 0.93 0.93 -0.0529  0.0297 0.0112 0.0052   0.0007 -186.7114  0
 10 0.84 0.84 -0.0487  0.0304 0.0051 0.0022  -0.0001 -186.7080  0
 11 0.75 0.75 -0.0439  0.0305 0.0040 0.0016   0.0000 -186.7048  0
 12 0.68 0.68 -0.0406  0.0301 0.0012 0.0006   0.0000 -186.7021  0
 13 0.61 0.61 -0.0374  0.0289 0.0015 0.0006   0.0000 -186.6998  0
 14 0.57 0.57 -0.0355  0.0284 0.0003 0.0002   0.0000 -186.6985  0

Calculating Hessian matrix...
|overlap| is 0.996638
i-EIP optimization converged!
All force call (i-EIP):  23
Total Hessian: 1
```

```
                     ####################
                     ##   Search TS    ##
                     ####################
Running direct TS searching (read Hessian)...
!!   Finished   !!
```