

The i-EIP (improved Elastic Image Pair) method is a double-ended transition state search method, which uses reactant and product structures as input and can automatically locate the transition state.

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

Installation

Require: Python 3.X, numpy

Step 1: Unzip the code.

Step 2: Add the code directory to enviroment variable.

Step 3: Add execute permission to `run_iEIP` file.

(This program uses Gaussian 09 software for quantitative calculations, please ensure that Gaussian 09 is installed correctly, and the `g09` `formchk` `unfchk` commands can be used correctly)

Input file

This program uses `.gjf` files as input. The calculation task needs to be set to `force` and the `nosymm` keyword should be added. The general file format is:

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

title

[charge spin]
[coord]
```

Run i-EIP

Prepare reactant and product files (such as: A.gjf B.gjf, the order of atoms in the files needs to be corresponding)

Excute `run_iEIP A.gjf B.gjf`

After the program ends normally, a `.log` file beginning with `ts` will be generated in the directory, which is the final transition state file.

Example

Take reaction 1 in the `example` file as an example, execute `run_iEIP 1_A.gjf 1_B.gjf` in this directory, and following output will be get:

```
-----
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  !!

```