Minima Hopping Tutorial

Sandip De

October 7, 2011

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3. Input & Output files
4. Input files
   - input.dft & mdinput.dft
     - Tuning the parameters
     - Fine tuning input.dft
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     - Effect of Rotation: Direct verification of expected energy accuracy
   - input.geopt & mdinput.geopt
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   - psppar.Mg & rand.inp
5. Input/Output files
   - earr.dat
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     - determining nsoften
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Introduction

In this Tutorial we will consider a Mg_7 cluster. Because of the small size and availability of a very soft pseudo-potential for Mg, these calculations are not very expensive.

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input.dft & mdinput.dft

input.dft and **mdinput.dft** have similar structures. **input.dft** controls the accuracy of the whole calculation and final results. Thus the parameters of **input.dft** are set for high accuracy. **mdinput.dft** file is used for MD-steps. From performance point of view it is suggested to choose the parameters for **mdinput.dft** file such that it gives reasonable accuracy and faster speedup.

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An example **input.dft** file

1.15 1.15 1.15	hx,hy,hz: grid spacing in the three directions
7.0 12.0	crmult, frmult: $c(f)rmult * radii_C f(*, 1(2))$ gives the coarse (fine)radius around each atom
1	ixc: exchange-correlation parameter ($LDA = 1$, $PBE = 11$)
0. 0.000 0.000 0.000	*ncharge* : *chargeofthesystem*, *Electricfield*
1 0	*nspin* = 1 non-spin polarization, *mpol* = *totalmagneticmoment*
1.E-05	gnrm_cv: convergence criterion gradient
50 2	itermax,nrepmax: maximum number of wavefunction optimizations and of re-diagonalised runs
5 8	*ncong*, *idsx* : CG iterations for the preconditioning equation, length of the diis history
0	dispersion correction functional (*values*1, 2, 3), 0 = *no* correction
0 0 0	InputPsiId, output-wf, output-grid
0.0 30	calc-tail, rbuf, ncongt: calculate tails,length of the tail (AU), tail CG iterations
0 0 0	davidson treatment, no. of virtual orbitals, no of plotted orbitals
2	verbosity of the output 0 = *low*, 2 = *high*
T	disable the symmetry detection

The parameters in the first two lines defines the basis set, thus affect the accuracy of the calculation.

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Expected Energy Accuracy

For choosing the parameters of **input.dft** and **mdinput.dft** file we need to have an idea of how the parameters of **input.dft** file affects the expected accuracy of the calculation. The accuracy of the BigDft energy calculation depends on the three parameters

- hgrid values (hx,hy,hz)[1st line of the file]
- crmult [1st number in 2nd line]
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THE RULE OF THUMB FOR TUNING

- High *h*grid $\rightarrow$ low accuracy (high speed).
- Low *crmult*, *frmult* $\rightarrow$ low accuracy (high speed).

"Expected accuracy" is only a rough prediction of the accuracy and should not be relied blindly.

Tuning the parameters

For the system in consideration: Mg_7 cluster we start several BigDft runs with different values for hgrid,crmult and frmult. At the starting of the calculation Bigdft writes the value of expected accuracy.

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hgrid	crmult	frmult	expected accuracy
0.5	5	10	2.08E-2
0.5	7	10	1.77E-4
0.5	8	10	1.37E-5
0.5	9	10	9.70E-6
0.7	9	10	2.75E-6
0.9	9	10	2.86E-5
1.0	9	10	7.90E-5
1.1	9	10	1.84E-4

Fine tuning input.dft

1. Set target energy accuracy for the calculation. In our example we will choose an accuracy of 5.0E-6 hartree .
2. Choose the set of parameters from the previous table for which we get similar accuracy.
3. Now we start from that set of parameters and fine tune it to obtain the target accuracy.

hgrid	crmult	frmult	expected accuracy
0.7	9	10	2.75E-6
0.75	9	10	4.95E-6
0.80	9	10	9.07E-6
0.75	8	10	1.39E-5
0.75	9	11	4.95E-6
0.75	9	12	4.95E-6

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0.80	9	10	9.07E-6
0.75	8	10	1.39E-5
0.75	9	11	4.95E-6
0.75	9	12	4.95E-6

Fine tuning mdinput.dft

1. Set target energy accuracy based on the accuracy set for **input.dft** . In our example we have 5.0E-6 hartree accuracy for **input.dft** file. So for **mdinput.dft** a reasonable target choice an accuracy would be 5.0E-4 hartree .
2. Choose the set of parameters from the following table for which we get similar accuracy.

hgrid	crmult	frmult	expected accuracy
0.5	5	10	2.08E-2
0.5	7	10	1.77E-4
0.5	8	10	1.37E-5
0.5	9	10	9.70E-6
0.7	9	10	2.75E-6
0.9	9	10	2.86E-5
1.0	9	10	7.90E-5
1.1	9	10	1.84E-4

3. Now we start from that set of parameters and fine tune it to obtain the target accuracy.

Fine tuning mdinput.dft

A careful selection of parameters for **mdinput.dft** is very important for performance of the code. As all the molecular dynamics part will be using this file we need to set the parameters such that a good balance of accuracy and performance speed is obtained.

hgrid	crmult	frmult	expected accuracy
1.1	9	10	1.84E-4
1.15	9	10	2.76E-4
1.15	8	10	2.83E-4
1.15	7	10	3.68E-4
1.15	6	10	1.33E-3
1.15	7	9	3.75E-4
1.15	7	8	4.32E-4
1.2	7	8	5.4E-4

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1.15	7	9	3.75E-4
1.15	7	8	4.32E-4
1.2	7	8	5.4E-4

Effect of Rotation: Direct verification of expected energy accuracy

After finalizing the parameters for **input.dft** file, we should check the numerical error in energy due to rotation of the system. This is direct confirmation test for the expected energy accuracy. We provide an utility program for rotating a cluster arbitrarily with respect to x, y and z axis. In this case we will note the **FINAL energy** of the system at the end of the calculation.

x	y	z	Total Energy
0	0	0	-5.990669**41648055362E+00**
10	30	40	-5.990669**40967330019E+00**
5	70	10	-5.990669**42374528999E+00**
20	5	90	-5.990669**39452840685E+00**

So we can see that the energy value is accurate up to 6th decimal place in the case of arbitrary rotation. As our expected accuracy was 5.0E-06, we can see that the condition is fulfilled.

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input.geopt & mdinput.geopt

input.geopt and **mdinput.geopt** files have almost same formats and parameters. These two files are for controlling the geometry optimization in the calculation. A typical **input.geopt** file is given below .

```
BFGS                    Geometry optimization method (BFGS/SDCG/VSSD)
200                     Maximum number of force evaluations
5.0     1.0E-4          fract-fluct,forcemax
0.0                     random displacement amplitude
4.0                     Stepsize for the geometry optimization
```

We generally use **BFGS** in **input.geopt** and **SDCG** in **mdinput.geopt**. The **stepsize** is system dependent and it has therefore to be determined for each system. If the VSSD method is used one can start with a small stepsize of around 1 and then **VSSD** will suggest a better value in the last line of the **geopt.mon** file. Please refer to Bigdft manual for more details.

VSSD should only be used to determine the optimal "stepsize" and should never be used in actual Minima Hopping runs.

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poscur.xyz

The **poscur.xyz** file contains the coordinates of the input cluster. The file is in the same xyz format as BigDft input file **posinp.xyz** Please refer to Bigdft manual for more details.

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- **psppar.Mg :** Pseudo potential file for Mg. Pseudo potential can be obtained from abinit website.

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- **rand.inp:** This file contains a single integer value which is used as random seed for the MD part.

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earr.dat

earr.dat file has the following structure.

```
3     13                    # of minima already found     # of minima to be found in consecutive run
-0.65000000000000000E+01    eref
0.50000000000000000E-04     accur
0.51510000000000000E+00     1.0000000000E+00
0.51775000000000004E+00     1.0000000000E+00
0.55890000000000006E+00     1.0000000000E+00
```

- 1st number indicates the number of minima already found. From the 4th line on the sorted energies of local minima are written. **For fresh runs it has to be** 0
- 2nd number in 1st line indicates the number of minima to be obtained.
- **eref**: The reference energy for the system has to be chosen such that the total energy with respect to **eref** is positive . In our example our total energy was -5.990669 hartree. So a reasonable choice of *eref* can be -6.5 hartree.
- **accuracy**: If two structures differ in energy by less than this value then the Minima Hopping code will consider them to be identical. In our example we have 5.0E-06 energy accuracy set by **input.dft** parameters. We could set the same value here. But it is recommended to choose the value of **accur** to be 5.0E-05 to stay absolutely on the safe side.
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ioput

The **ioput** file contains 4 parameters in one line .

5.0E-03	5.0E-03	1.0	10	ediff	ekinetic	dt	nsoften

The 1st three parameters are **automatically adjusted** by the program during the run.

- **ediff**: The criteria for accepting new minimum which is higher in energy than present one is $E_{new} - E_{present} \leq ediff$. As the typical energy gap between local minima in a given basin is of the order of milli-hartree, 5.0E-03 is a reasonable value as a starting point for most systems.
- **ekinetic**: The kinetic energy for the MD. In this case also a value of the order of milli-hartree is a reasonable choice.
- **dt:** time-step in atomic unit (2.418884326505E1017 s). As nucleus mass in MD simulation has been taken 1 where as the masses of even light atoms is a few thousand in atomic units, that means that if we would to do MD with real masses we would have time steps of the order of 1.0E-14 which is 10 fs. So in atomic unit a value between 0.5 to 1 is a reasonable choice for **dt**.
- **nsoften:** Number of iteration to find soft modes. This parameter is system dependent. We will see how to choose the value of nsoften in the next slide.

ioput

The **ioput** file contains 4 parameters in one line .

5.0E-03	5.0E-03	1.0	10	ediff	ekinetic	dt	nsoften

The 1st three parameters are **automatically adjusted** by the program during the run.

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nsoften

- Generally the value of **nsoften** lies between between 5 and 30.
- To accurately determine the necessary value of **nsoften** one should start the program with high value of **nsoften** depending on the system, *e.g* 20 in the present example

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  - After sometime if you use grep soften screenoutput you will get output of several sets like the following .

# soften it,	curv,	fd2,dE,res,epsvxyz:	1	0.02061	0.02044	0.00080	0.00361	0.28032
# soften it,	curv,	fd2,dE,res,epsvxyz:	2	0.01787	0.01781	0.00101	0.00438	0.33639
# soften it,	curv,	fd2,dE,res,epsvxyz:	3	0.01503	0.01521	0.00124	0.00513	0.40367
# soften it,	curv,	fd2,dE,res,epsvxyz:	4	0.01232	0.01267	0.00149	0.00578	0.48440
# soften it,	curv,	fd2,dE,res,epsvxyz:	5	0.00994	0.01040	0.00176	0.00628	0.58128
# soften it,	curv,	fd2,dE,res,epsvxyz:	6	0.00794	0.00847	0.00206	0.00665	0.69753
# soften it,	curv,	fd2,dE,res,epsvxyz:	7	0.00635	0.00693	0.00243	0.00693	0.83704
# soften it,	curv,	fd2,dE,res,epsvxyz:	8	0.00511	0.00568	0.00287	0.00718	1.00445
# soften it,	curv,	fd2,dE,res,epsvxyz:	9	0.00414	0.00471	0.00342	0.00746	1.20534
# soften it,	curv,	fd2,dE,res,epsvxyz:	10	0.00339	0.00392	0.00410	0.00779	1.4464
# soften it,	curv,	fd2,dE,res,epsvxyz:	11	0.00280	0.00328	0.00494	0.00824	1.7356
# soften it,	curv,	fd2,dE,res,epsvxyz:	12	0.00238	0.00279	0.00605	0.00883	2.0828
# soften it,	curv,	fd2,dE,res,epsvxyz:	13	0.00208	0.00238	0.00744	0.00962	2.4993
# soften it,	curv,	fd2,dE,res,epsvxyz:	14	0.00192	0.00207	0.00932	0.01063	2.9992
# soften it,	curv,	fd2,dE,res,epsvxyz:	15	0.00188	0.00186	0.01202	0.01190	3.5991
# soften it,	curv,	fd2,dE,res,epsvxyz:	16	0.00172	0.00169	0.01092	0.01132	3.5991
# soften it,	curv,	fd2,dE,res,epsvxyz:	17	0.00156	0.00153	0.00992	0.01073	3.5991
# soften it,	curv,	fd2,dE,res,epsvxyz:	18	0.00169	0.00144	0.01345	0.01246	4.3189
# soften it,	curv,	fd2,dE,res,epsvxyz:	19	0.00155	0.00132	0.01227	0.01186	4.3189
# soften it,	curv,	fd2,dE,res,epsvxyz:	20	0.00142	0.00120	0.01118	0.01128	4.3189

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# soften it,	curv,	fd2,dE,res,epsvxyz:	15	0.00188	0.00186	0.01202	0.01190	3.5991
# soften it,	curv,	fd2,dE,res,epsvxyz:	16	0.00172	0.00169	0.01092	0.01132	3.5991
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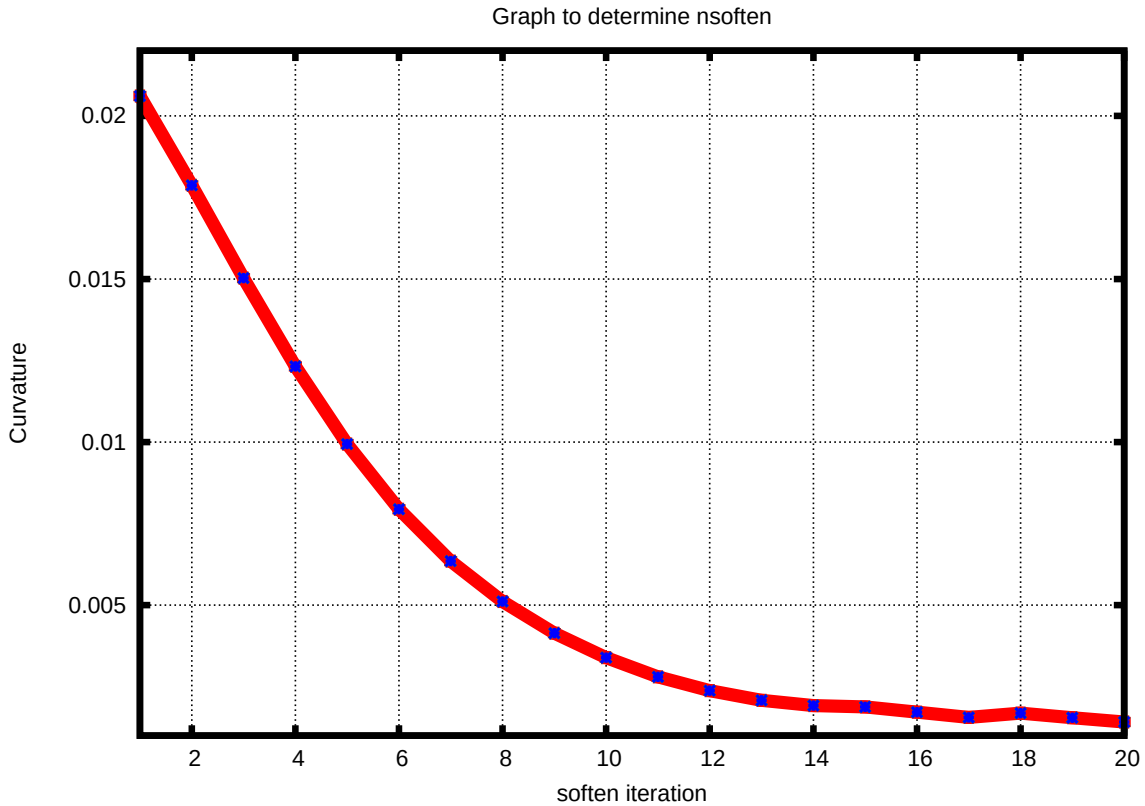
# soften it,	curv,	fd2,dE,res,epsvxyz:	20	0.00142	0.00120	0.01118	0.01128	4.3189

  - Now we plot 4th vs 5th column

nsoften determination



In this case *nsoften* = 8 will be a good choice.
CAUTION: High nsoften (eg in this case 16) can make the system ergodic which should be avoided in order to explore new minima.

Outline

1. Outline
2. Introduction
3. Input & Output files
4. Input files
   - input.dft & mdinput.dft
     - Tuning the parameters
     - Fine tuning input.dft
     - Fine tuning mdinput.dft
     - Effect of Rotation: Direct verification of expected energy accuracy
   - input.geopt & mdinput.geopt
   - poscur.xyz
   - psppar.Mg & rand.inp
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   - earr.dat
   - ioput
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   - global.mon file
7. Optional Input File

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poslow*****.xyz

The **poslow*****.xyz** files contain the xyz coordinates of the local minima obtained .

- **poslow00001.xyz**: The global minimum.
- **poslow00002.xyz**: 1st local minimum.
- **poslow00003.xyz**: 2nd local minimum.
- **poslow0000n.xyz**: (n-1)th local minimum.

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global.mon

A example of **global.mon** file.

0.	5.58926749358852E-01	5.500E-03	3.757E-03						
1.	5.17791609055973E-01	5.500E-03	3.415E-03	0.00	0.00	1.00	T	A	1
2.	5.15133746089417E-01	5.000E-03	3.105E-03	0.00	0.00	1.00	T	A	1
3.	5.15132445559042E-01	4.545E-03	3.415E-03	0.33	0.00	0.67	S		
4.	5.17792640238337E-01	4.545E-03	3.757E-03	0.25	0.25	0.50	F	A	2
5.	5.09330518019620E-01	4.132E-03	3.415E-03	0.20	0.20	0.60	T	A	1
6.	5.09330514596172E-01	3.757E-03	3.757E-03	0.33	0.17	0.50	S		
7.	5.17792535761185E-01	3.757E-03	4.132E-03	0.29	0.29	0.43	F	R	3
8.	5.17287417585399E-01	4.132E-03	3.757E-03	0.25	0.25	0.50	T	R	1
9.	5.17285614386745E-01	4.545E-03	4.132E-03	0.22	0.33	0.44	F	R	2
10.	5.09330579201748E-01	5.000E-03	4.545E-03	0.30	0.30	0.40	S		
11.	5.09330530782908E-01	5.000E-03	5.000E-03	0.36	0.27	0.36	S		
12.	5.09330475600953E-01	5.000E-03	5.500E-03	0.42	0.25	0.33	S		
13.	5.16119052438151E-01	5.000E-03	5.000E-03	0.38	0.23	0.38	T	R	1
14.	5.17285532541758E-01	5.500E-03	5.500E-03	0.36	0.29	0.36	F	R	3
15.	5.15132432040568E-01	6.050E-03	6.050E-03	0.33	0.33	0.33	F	A	2
16.	5.17285625602291E-01	5.500E-03	6.655E-03	0.31	0.38	0.31	F	A	4

global.mon

A example of **global.mon** file.

	energy	ediff	ekinetic		Fraction				
0.	5.58926749358852E-01	5.500E-03	3.757E-03	same	old	new			
1.	5.17791609055973E-01	5.500E-03	3.415E-03	0.00	0.00	1.00	T	A	1
2.	5.15133746089417E-01	5.000E-03	3.105E-03	0.00	0.00	1.00	T	A	1
3.	5.15132445559042E-01	4.545E-03	3.415E-03	0.33	0.00	0.67	S		
4.	5.17792640238337E-01	4.545E-03	3.757E-03	0.25	0.25	0.50	F	A	2
5.	5.09330518019620E-01	4.132E-03	3.415E-03	0.20	0.20	0.60	T	A	1
6.	5.09330514596172E-01	3.757E-03	3.757E-03	0.33	0.17	0.50	S		
7.	5.17792535761185E-01	3.757E-03	4.132E-03	0.29	0.29	0.43	F	R	3
8.	5.17287417585399E-01	4.132E-03	3.757E-03	0.25	0.25	0.50	T	R	1
9.	5.17285614386745E-01	4.545E-03	4.132E-03	0.22	0.33	0.44	F	R	2
10.	5.09330579201748E-01	5.000E-03	4.545E-03	0.30	0.30	0.40	S		
11.	5.09330530782908E-01	5.000E-03	5.000E-03	0.36	0.27	0.36	S		
12.	5.09330475600953E-01	5.000E-03	5.500E-03	0.42	0.25	0.33	S		
13.	5.16119052438151E-01	5.000E-03	5.000E-03	0.38	0.23	0.38	T	R	1
14.	5.17285532541758E-01	5.500E-03	5.500E-03	0.36	0.29	0.36	F	R	3
15.	5.15132432040568E-01	6.050E-03	6.050E-03	0.33	0.33	0.33	F	A	2
16.	5.17285625602291E-01	5.500E-03	6.655E-03	0.31	0.38	0.31	F	A	4

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0.	5.58926749358852E-01	5.500E-03	3.757E-03						
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3.	5.15132445559042E-01	4.545E-03	3.415E-03	0.33	0.00	0.67	S		
4.	5.17792640238337E-01	4.545E-03	3.757E-03	0.25	0.25	0.50	F	A	2
5.	5.09330518019620E-01	4.132E-03	3.415E-03	0.20	0.20	0.60	T	A	1
6.	5.09330514596172E-01	3.757E-03	3.757E-03	0.33	0.17	0.50	S		
7.	5.17792535761185E-01	3.757E-03	4.132E-03	0.29	0.29	0.43	F	R	3
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13.	5.16119052438151E-01	5.000E-03	5.000E-03	0.38	0.23	0.38	T	R	1
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15.	5.15132432040568E-01	6.050E-03	6.050E-03	0.33	0.33	0.33	F	A	2
16.	5.17285625602291E-01	5.500E-03	6.655E-03	0.31	0.38	0.31	F	A	4

- column 8: New minimum (T), Old minimum (F), Same as previous minimum (S).

global.mon

A example of **global.mon** file.

	energy	ediff	ekinetic		Fraction				
				same	old	new			
0.	5.58926749358852E-01	5.500E-03	3.757E-03						
1.	5.17791609055973E-01	5.500E-03	3.415E-03	0.00	0.00	1.00	T	A	1
2.	5.15133746089417E-01	5.000E-03	3.105E-03	0.00	0.00	1.00	T	A	1
3.	5.15132445559042E-01	4.545E-03	3.415E-03	0.33	0.00	0.67	S		
4.	5.17792640238337E-01	4.545E-03	3.757E-03	0.25	0.25	0.50	F	A	2
5.	5.09330518019620E-01	4.132E-03	3.415E-03	0.20	0.20	0.60	T	A	1
6.	5.09330514596172E-01	3.757E-03	3.757E-03	0.33	0.17	0.50	S		
7.	5.17792535761185E-01	3.757E-03	4.132E-03	0.29	0.29	0.43	F	R	3
8.	5.17287417585399E-01	4.132E-03	3.757E-03	0.25	0.25	0.50	T	R	1
9.	5.17285614386745E-01	4.545E-03	4.132E-03	0.22	0.33	0.44	F	R	2
10.	5.09330579201748E-01	5.000E-03	4.545E-03	0.30	0.30	0.40	S		
11.	5.09330530782908E-01	5.000E-03	5.000E-03	0.36	0.27	0.36	S		
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- column 8:New minimum (T), Old minimum (F), Same as previous minimum (S).
- column 9: Minima Accepted or Rejected

global.mon

A example of **global.mon** file.

	energy	ediff	ekinetic		Fraction				
				same	old	new			
0.	5.58926749358852E-01	5.500E-03	3.757E-03						
1.	5.17791609055973E-01	5.500E-03	3.415E-03	0.00	0.00	1.00	T	A	1
2.	5.15133746089417E-01	5.000E-03	3.105E-03	0.00	0.00	1.00	T	A	1
3.	5.15132445559042E-01	4.545E-03	3.415E-03	0.33	0.00	0.67	S		
4.	5.17792640238337E-01	4.545E-03	3.757E-03	0.25	0.25	0.50	F	A	2
5.	5.09330518019620E-01	4.132E-03	3.415E-03	0.20	0.20	0.60	T	A	1
6.	5.09330514596172E-01	3.757E-03	3.757E-03	0.33	0.17	0.50	S		
7.	5.17792535761185E-01	3.757E-03	4.132E-03	0.29	0.29	0.43	F	R	3
8.	5.17287417585399E-01	4.132E-03	3.757E-03	0.25	0.25	0.50	T	R	1
9.	5.17285614386745E-01	4.545E-03	4.132E-03	0.22	0.33	0.44	F	R	2
10.	5.09330579201748E-01	5.000E-03	4.545E-03	0.30	0.30	0.40	S		
11.	5.09330530782908E-01	5.000E-03	5.000E-03	0.36	0.27	0.36	S		
12.	5.09330475600953E-01	5.000E-03	5.500E-03	0.42	0.25	0.33	S		
13.	5.16119052438151E-01	5.000E-03	5.000E-03	0.38	0.23	0.38	T	R	1
14.	5.17285532541758E-01	5.500E-03	5.500E-03	0.36	0.29	0.36	F	R	3
15.	5.15132432040568E-01	6.050E-03	6.050E-03	0.33	0.33	0.33	F	A	2
16.	5.17285625602291E-01	5.500E-03	6.655E-03	0.31	0.38	0.31	F	A	4

- column 8:New minimum (T), Old minimum (F), Same as previous minimum (S).
- column 9: Minima Accepted or Rejected
- column 10: Number of times the minimum was visited.

Outline

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5. Input/Output files
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7. Optional Input File

Optional Input File

In addition to the optional input files for **Bigdft** there is one optional input file for **Minima Hopping** program:

CPUlimit_global

One can use a value of **n** in this file to limit the Minima Hopping run to **n** hours.

In case you are using openmp version of the program, you should put $n \times thread_{numbers}$ in the file to limit the run to **n** hours.

In both cases the time-limit is not strictly followed as the time checking is done only at the starting of a new MD part. So in case one want to stop the program definitely in 10 hours, he should give the input so that program stops in say 8 hours.

THANK YOU