

Replica exchange (REHMC)

1. Calculation setup

The following setup is used.

- Method: REHMC
- Replica exchange method: Temperature exchange
- Potential: MM (classical force field)
- System: enkephalin (Tyr-Gly-Gly-Phe-Met)
- Number of replicas: 4
- Temperature ranges: 300-450 K and 300-400 K

2. Results

The detection rate of replica exchange is shown in the `ratex` column in “standard.out”. The following result is for the temperature range 300-450 K.

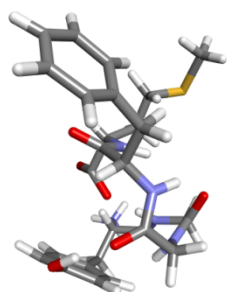
step	dt [fs]	ratio	ratex	potential [au]	wall clock time
0	2.00000	0.00000	0.00000	-0.20654849	2016-04-21 木 20:33:56.50
1000	2.00000	0.07475	0.21567	-0.19482228	2016-04-21 木 20:35:33.78
2000	2.00000	0.12200	0.18958	-0.19441402	2016-04-21 木 20:39:39.02
3000	2.00000	0.16908	0.17661	-0.21410624	2016-04-21 木 20:43:41.32
4000	2.00000	0.18975	0.17054	-0.20787744	2016-04-21 木 20:47:49.43
5000	2.00000	0.20365	0.17147	-0.21907792	2016-04-21 木 20:52:04.44
6000	2.00000	0.21125	0.16286	-0.21615655	2016-04-21 木 20:54:45.37
7000	2.00000	0.21596	0.16048	-0.21797942	2016-04-21 木 20:57:47.31
8000	2.00000	0.21875	0.15725	-0.21056090	2016-04-21 木 21:00:52.71
9000	2.00000	0.22006	0.16009	-0.21799798	2016-04-21 木 21:03:48.73
10000	2.00000	0.22212	0.15920	-0.20795958	2016-04-21 木 21:06:56.89
...omitted...					

The following result is for the temperature range 300 – 400 K.

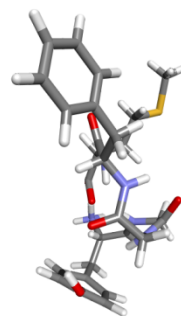
step	dt [fs]	ratio	ratex	potential [au]	wall clock time
0	2.00000	0.00000	0.00000	-0.20654849	2016-04-21 木 20:48:20.72
1000	2.00000	0.11975	0.32833	-0.20889803	2016-04-21 木 20:51:41.60
2000	2.00000	0.18250	0.30392	-0.20639404	2016-04-21 木 20:56:12.64
3000	2.00000	0.20367	0.30717	-0.21405550	2016-04-21 木 21:00:45.09
4000	2.00000	0.21481	0.30758	-0.21752652	2016-04-21 木 21:05:12.39
5000	2.00000	0.22430	0.31050	-0.22621834	2016-04-21 木 21:09:48.11
6000	2.00000	0.23017	0.31069	-0.21955134	2016-04-21 木 21:14:23.41
7000	2.00000	0.23418	0.30926	-0.22502032	2016-04-21 木 21:17:17.19
8000	2.00000	0.23522	0.30835	-0.22184941	2016-04-21 木 21:20:10.55
9000	2.00000	0.23733	0.30913	-0.21232836	2016-04-21 木 21:24:45.53
10000	2.00000	0.23670	0.31382	-0.22802106	2016-04-21 木 21:29:45.06

...omitted...

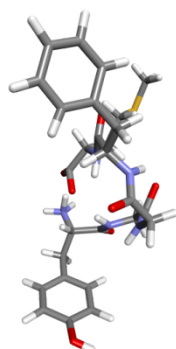
The initial structure and three snapshots at 300 K are shown.



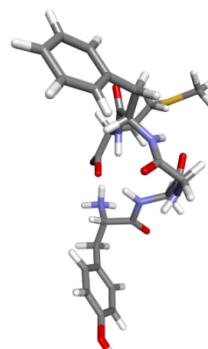
(Initial structure)



(Snapshot 1)



(Snapshot 2)



(Snapshot 3)

