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Chapter 1

Biased simulation I

1.1 Corrections in analysis

1.1.1 Abstract

A biased simulation was run as per the CV explained in section 1.1.2. QM calculations on the resulting configurations were done using CP2K (quickstep) to calculate the energy. The same was compared with the energy reported from the n2p2 run (reported in the standard output of the simulation run). However the values were seen to be differing by a factor of approximately 27. The same has been resolved by applying the units correction on the values extracted from n2p2 output(the values were in eV and were being compared with a.u. hartree values from CP2K). The graphs from earlier and the new graphs are compared in section 1.1.3 of this report.

1.1.2 Simulation

We ran a biased simulation of water with the following Collective variable:

- For every oxygen, find the closest H.
- Find the longest such O-H bond (in the statement above).

The details of the simulation run are in Table 1.1

Ensemble	dt(fs)	Steps	T(K)	N	Box(x,y,z)$\mathring{A}$	ρ (g/cm^3)	outfile
NVT	0.5	10,000	300	64	46.937,44.121,45.182	0.0204	out7.xyz

Table 1.1 Simulations for H_2O system using N2P2
Bias column can be decoded from Table 1.2. Not all outfiles may be present on the git repo due to size exceeding 100MB.

1.1.3 Correction

The output from n2p2 reported energies in eV whereas the training energies as well as the cp2k energies were in atomic unit (Hartree). In our earlier report we were comparing there eV values against the hartree values without correction for units. Fig 1.1 compares the graphs post the correction. There seem to be some outliers in plot a and b.

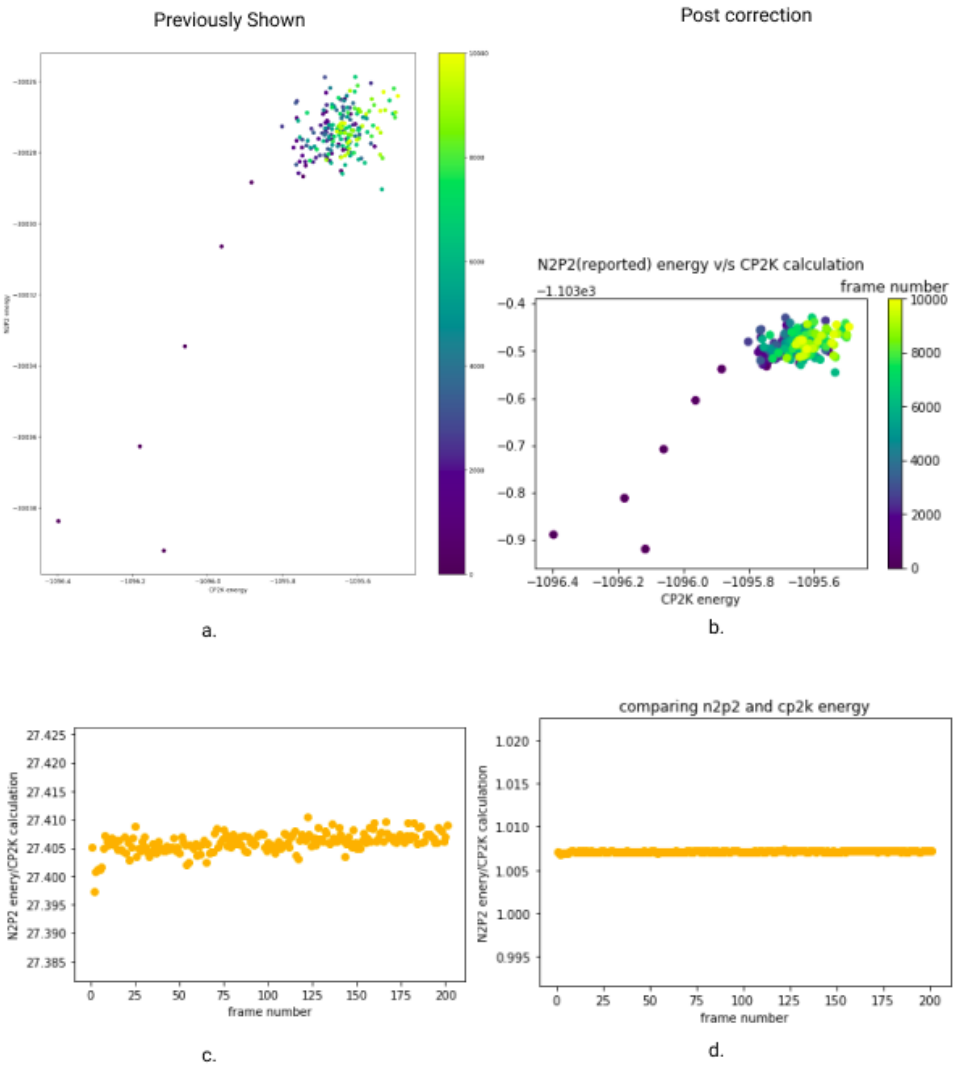

Figure 1.1 Comparing previously shown graphs with the corrected graphs

1.1.4 Analysis

There is small difference (approx 8 a.u.) in the values from cp2k calcualtions and n2p2 energies. The difference can be due to lack of precision from multiple unit conversions or approximations in simulation runs. However, this difference is small when compared with the absolute values of the energies themselves. The positives are:

- similar shape of energy profile
- small separation between profile values

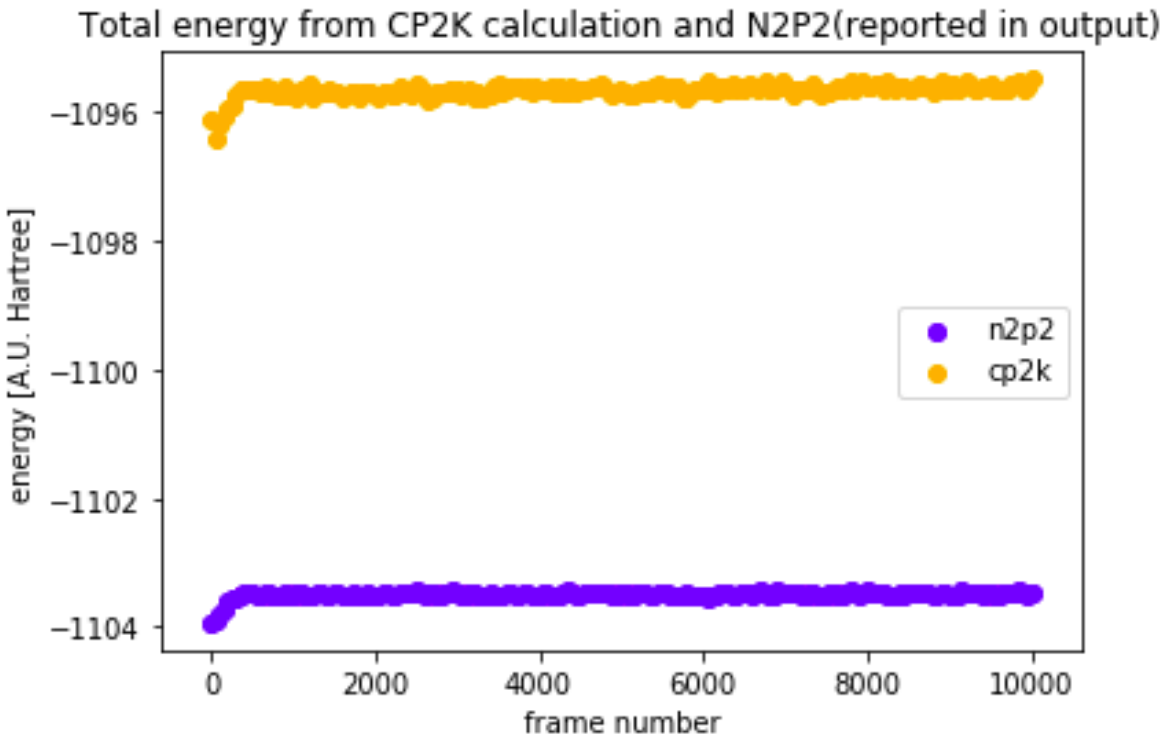

Figure 1.2 Comparing Energies from n2p2 and cp2k

Relative energies in Fig1.3 and Fig1.4 are calculated by subtracting the pivot energy values from all the values. The pivot value is the minimum/median energy in the respective profile(separate for n2p2 profile and cp2k profile). There seems to be a good overlap in the case when median is used as the pivot. Similar values might be visible for minimum value as the pivot if the initial few frames are discarded.

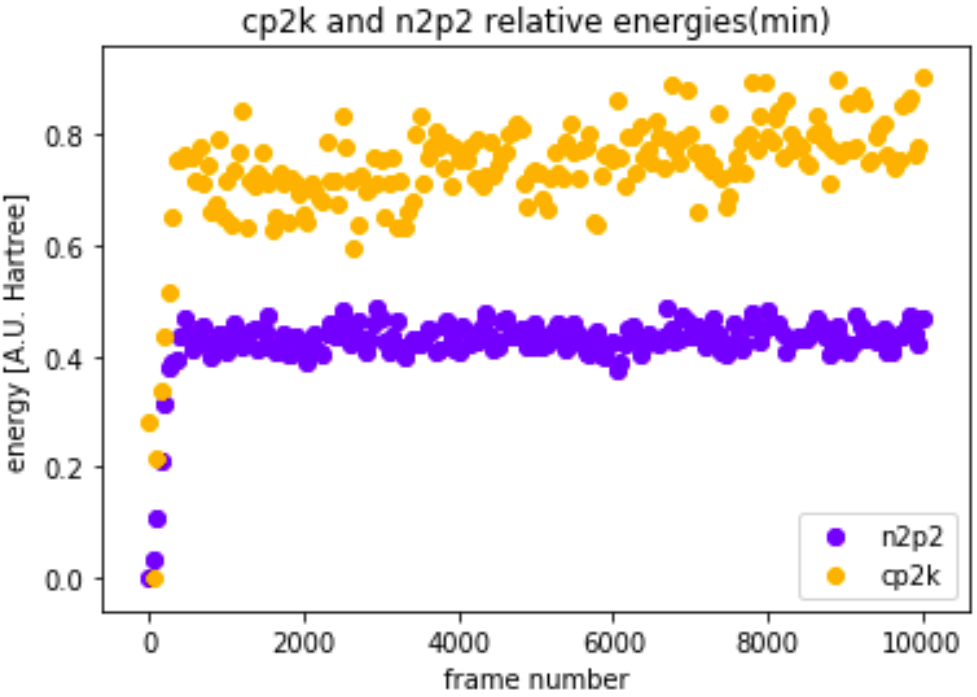

Figure 1.3 comparing relative(by median) energies

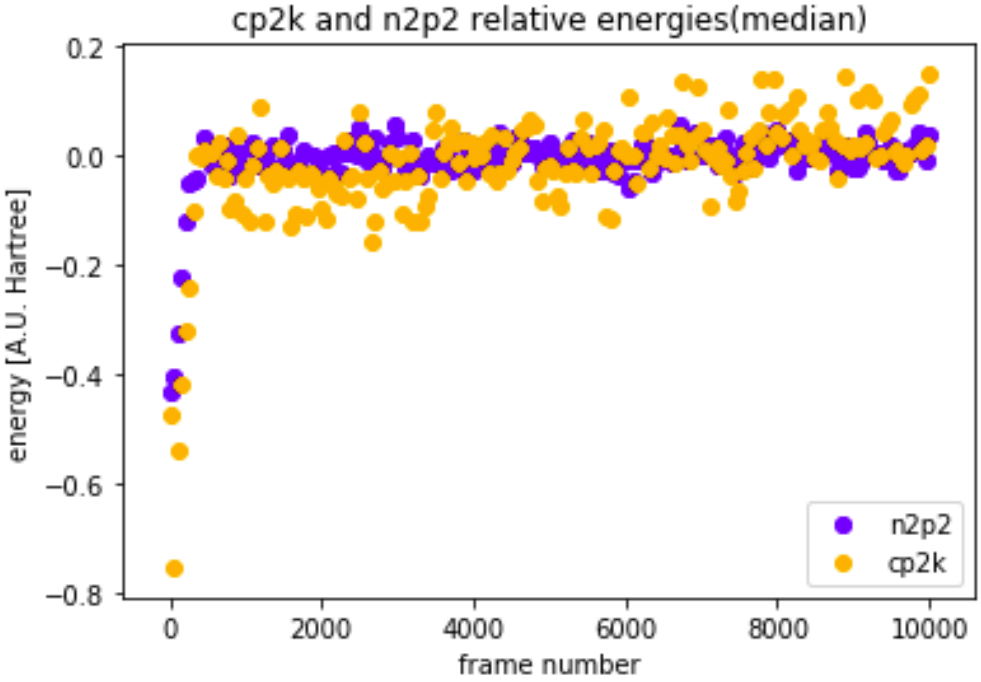

Figure 1.4 comparing relative(by minimum) energies