Comparison of K-point selection methods.

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May 2016

Description of plot

The plot displayed in Fig. 1 is a representation of the "speed-up" that the Mueller K-point method offers over the Froyen method and the methods employed by AFLOW. By speed-up we mean the ratio of the irreducible K-points used by either the Froyen or AFLOW method to the Mueller method (i.e., Froyen or AFLOW/Mueller irreducible K-points). The data was generated from three systems; pure Co, pure W, and pure V with cell sizes ranging from 1 to 11 atoms per cell for each system. The tests were also run over different K-point densities ranging from 1 to 22^3 K-points per reciprocal atom The K-points used for each method were generated as follows, for the Froyen method only K-point density that were commensurate with the cell size were used. The K-point grids for the Froyen method were generated by dividing the number cubed root of K-points per reciprocal atom by each lattice vector to create a uniform K-point grid for each cell and K-point density. The K-points grids for AFLOW were generated by putting the desired number of K-points per reciprocal atom into the correct location in the AFLOW aflow.in script, AFLOW was then allowed to generate the K-points using whichever methods it would use by default. For the Mueller method r_min was found using the following equation:

$$r\_min \ = 2.8074(k_n^{1/3}) - 3.4008 \tag{1}$$

where k_n is the number of K-points per reciprocal atom. The database of Mueller K-point grids was then queried for a system with the desired r_min and a KPOINTS file generated. The program VASP was used to calculate

the energy of each system for each cell size and K-point density available to determine the energy of the systems.

Once all VASP calculations were complete, for the Froyen and Mueller methods only 20 NSW steps were permitted however the default value of NSW=52 for AFLOW could not be overwritten so the AFLOW tests used more ionic steps in some cases, the resulting energies were divided by the number of atoms in the cell in order to easily compare the values. The converged energy was then taken to be the energy of the largest system with the highest K-point density. The difference between each systems energy per atom and the converged energy per atom was taken as a measure of the accuracy of the calculation, i.e., the systems error.

In order to generate Fig. 1 the range of the errors, roughly 10^{-6} to 10^{2}, was discretized into steps of size 0.001 on a log scale (10^{x} with $-6 <= x <= 2$) to make an discrete error space. For each point in this error space the K-point methods were searched for the largest error that was >= to the point (this was done for each system Co, W, and V and each cell size separately). Once the K-point density whose error meant these conditions was found for each method the ratio of the Froyen and Mueller irreducible K-points and the ration of the ALFOW and Mueller irreducible K-points were found and saved for that error value. This process produced 33 different speed-up data sets for each method comparison. Fig. 1 shows the results of averaging those 33 data sets by adding together all the runs at each error and dividing by the number of runs.

The plot itself shows that, on average, the Mueller method is always better than the Froyen method by nearly a factor of 10. The comparison with the AFLOW method shows that, on average, the Mueller method can be faster except when accuracies smaller than 10^{-5} are desired[1].

[1]The fact that AFLOW outperformed the Mueller method in the small error region could partially be explained by the fact the AFLOW runs didn't converge to the same energy for the different cell sizes. As a result only a few of the AFLOW runs achieved accuracy to this level while most of the Mueller and Froyen runs reached the small error region.

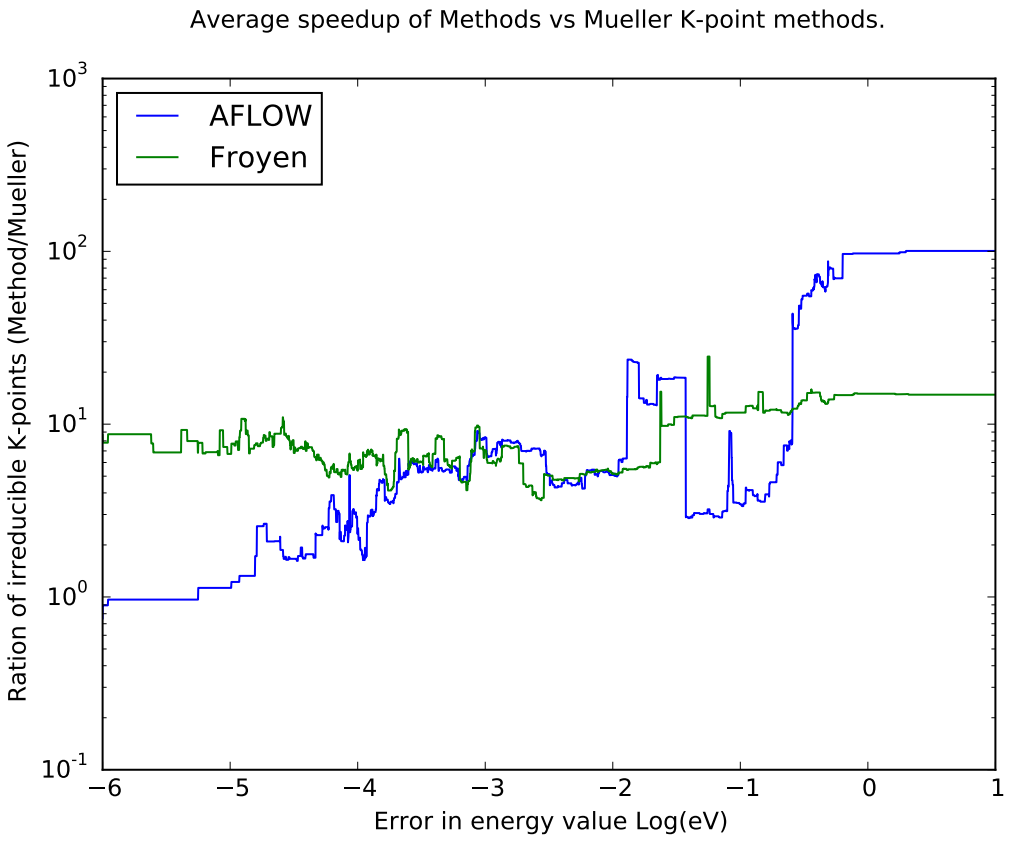

Figure 1: The ratio of irreducible K-points vs error in calculated energy for each method vs the Mueller method. Both axis are on log scales.