Session 6: pushing numerical convergence

When it is about the limits of numerical convergence, one will run into the problem that the same code run on different computers will lead to (slightly) different results. In this respect, the toy DFT code programmed in the Julia language (https://julialang.org/), as presented by A. Levitt in his talk, can be relevant (apart from other advantages): it can work at quadruple precision, such that differences when run on different machines/architectures should essentially vanish.

The pitfall of multiple minima was touched during the discussion. Only very simple cases with simple functionals (LDA/GGA) have one unique minimum in the self-consist solution process. When studying f-electron systems or magnetic systems, multiple minima are common. Idem when using more complex functionals (HSE, SCAN). The differences can sometimes be subtle, and are not easily spot. This can interfere with precision studies, and the more so the higher the numerical precision is that one aims for. Two calculations might look different, whereas they are perhaps just two different local minima.

Another aspect that was discussed, is: when we do not look at ultimate precision but at 'normal' precision, for publication quality, how can we ensure that all users run their calculations at the required precision? Some argue that this is not a task that can be left to the user, the software should take care of this. Others argue that this task is too complex to implement in a fool-proof way, as the required precision often depends on the physical property one tries to predict. And even if it could be done for DFT, there are more complex methods (GW) where the 'flat' regime of converged values cannot be reached within a reasonable amount of time. Everything keeps changing, whatever input parameter one touches.

In any case, a more formal procedure to obtain the proper numerical settings for a given level of precision is desirable, be it via educating users or by automating the process.

This is a digest of a dedicated discussion session held at PQ-DFT 2019. For other digests, videos of all talks and summarizing recommendations, please visit https://pqdft2019.abinit.org/. To access the videos directly on Youtube, visit http://bit.ly/2XFKUCl. Any comments, thoughts or items you want to discuss? Feel free to contact Stefaan Cottenier (stefaan.cottenier@ugent.be) or Kurt Lejaeghere (kurt.lejaeghere@ugent.be).