Session 2: pseudopotential development

A discussion developed around the deliberately provocative question: "Can this community afford to continue building ever more pseudopotential libraries? Shouldn't we focus more on all-electron methods instead?" Some arguments that play a role:

- Having multiple approaches (pseudopotentials vs. all-electron, one pseudolibrary vs. another, …) is an asset. It shows this community is healthy, and it offers a biodiversity on which we can draw when confronted with new situations.
- In all-electron methods, the challenge is shifted from creating a good pseudopotential to creating a good basis set. This is a kind of conservation law of hard work.
- It is not such that all-electron codes are static and stable, while pseudopotentials keep developing. Also in all-electron codes new evolutions are happening (cfr. HDLOs in LAPW).
- The value of pseudopotentials depends to some extent of the property one is interested in. As a corollary, benchmark sets that are focusing on a particular property could be useful for pseudopotential development.

Benchmark sets that are specifically designed for testing pseudopotentials require different features. It could help, for instance, to keep the k-mesh coarse. As long as the all-electron reference uses the same coarse k-mesh, this is fine. It would make rapid testing much easier. More generally, for future test sets there should be more strict instructions on which k-mesh to use, and which type and amount of Fermi surface smearing.

Apart from the precision by which a pseudopotential calculations reproduces an all-electron result, the execution time for both calculations matters as well. If pseudopotentials do not lead to smaller execution times, there is no reason using them. Their precision will often be a trade-off with speed. Benchmarking speed is not straightforward and can probably not be done in a machine-independent way. Nevertheless, efforts in this respect would be welcome.

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).