general actions and recommendations (after PQ-DFT 2019)

Action: towards more diverse test sets. Future steps should focus on creating and documenting a series of relatively small test sets, each of them built for a specific feature/property/purpose. Having all-electron reference data for each set is mandatory. Users can use as many or as few of those sets as they wish for their benchmarking, depending on their need. A sketch list of such sets could be:

- The initial Delta set (mainly because data from many other codes and methods are available to compare with)
- The Delta set for structural variety (fcc/bcc/simple cubic/diamond) (*)
- The Delta set for chemical variety (6 artificial oxides per element) (*)
- The Delta set for experimentally relevant crystals (handpicked list of simple binaries, every element appearing multiple times) (*)
- The GBRV set (combinations of various oxidations states and structures, for experimentally relevant crystals)
- Low-symmetry sets (molecules, surfaces, vacancies)
- A set with crystals where all atoms are randomly displaced, to inspect forces
- A set with all free atoms (to get cohesive energies for all other test sets)
- A set with all elementary crystal ground states (=completion of the initial Delta set) for formation energies of all other test sets
- A set with magnetic materials
- …

When these test sets are used for the sole purpose of pseudopotential development, it would be sufficient to run them with a coarse k-mesh (this requires all-electron data at the same coarse k-mesh). Enforcing more strictly than before which k-mesh is to be used for every crystal in the set is a good strategy (e.g. one coarse k-mesh and one that is very dense, yet not unreasonably dense).

(*) currently under construction at Ghent University, to be delivered during 2019.

Action: work flow managers for benchmarking and convergence testing. It is recommended that the different work flow management packages on the market implement procedures (1) to carry out the benchmark tests for the codes they work with, and (2) to perform the convergence testing that one should do at the beginning of every new project. The former will make it easier to carry out decent benchmarks with many codes/methods. The latter will help ensuring that at least a minimal amount of convergence testing is performed by all/most users.

Action: databases and libraries. Concerted actions and stimulating the development of joint libraries (libxc, ESL,…) as well as databases (Nomad, Materials Cloud, Materials Project, aflowlib, oqmd, Optimade,…) are very much needed.

Action: expert panels and recommendations. More efforts should be done to make the knowledge explicit that is implicitly known and used by some experts in the field. This can be done by implementing this knowledge in workflow managers (particularly suitable for procedures), and/or by community expert panels that review the literature and formulate recommendations for procedures and user input choices (e.g. selecting the XC-functional that is most appropriate for a given case). There might be a task for Psi-k here. The Psi-k 2020 conference could be a place to make progress on this.

Action: accuracy assessment for more properties and more functionals. Documenting the systematic bias and the random scatter for the prediction of properties for a given XC-functional compared to experimental values, remains a useful task. It should be performed for more properties and more functionals, on sets of crystals that are relevant for the property studied. This is a task on which collaboration with experimentalists is relevant (providing better/more experimental data).

This action list was distilled from the talks and discussion sessions at PQ-DFT 2019. For videos of all talks and discussion digests per topic, 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).

THE NEXT STEPS … (WRAPPING UP)

PQ-DFT

May 23-24 2019

Louvain-la-Neuve, Belgium

UNIVERSITEIT GENT

CENTER FOR MOLECULAR MODELING

Beyond the elemental crystals

- Tier2 and Tier3 test sets: binaries with diverse oxidation states and bonding types
- need to go beyond perfect crystals:
  surfaces, defects, random structures
- unbiased test set vs focus on cases that are most likely to be wrong

WARNING: modular test set needed, avoid monolithic single set that nobody wants to do

2

beyond the equation of state

- formation energies follow naturally from unary and binary test set
- many properties boil down to energy differences
- some properties need to be tested explicitly (e.g. electronic band structure), but be careful of combinatorial hell: all properties for all materials -> use proxies
- choose next property from application needs?

3

beyond DFT-PBE

- making new pseudopotentials for other functionals is (in most cases) not that difficult
- need to go beyond PBE as a default
- dedicated test sets might be needed
- reliable reference values are crucial:
  curated experimental data? high-level theoretical data?
- automatic correction is dangerous, but expert opinion would be useful (review, expert panel, …)

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all videos and discussion digests:
https://pqdft2019.abinit.org/

beyond current pseudopotentials

- aim for better pseudopotentials or go for all-electron all the way? important of biodiversity in codes
- the (N-th) elephant in the room: speed! benchmarking needed
- suitable pseudopotentials depend on property of interest

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numerical settings

- artificial test set for Delta with low k-grids? low cost + comparability
- numerical precision should not go several orders of magnitude beyond accuracy?
- convergence issues worse of complex properties, expert users needed to benchmark
- automatic convergence tools are an advantage
- not all numerical issues can be converged straightforwardly, e.g. minima in electronic cycle

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data and workflows

- availability of data is crucial
- cross database communication for data searching and curation
- data context is important, but not too much to scare off users

- automation important to reduce human time
- be careful of too many defaults (user abuse!)
- workflows ideal to increase reproducibility

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