ADAPTIVE AND LOCALIZED BASIS FUNCTIONS FOR LINEAR SCALING, LARGE SYSTEMS AND COMPLEX QM SIMULATIONS

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Since 2008, the BigDFT project consortium has developed an ab initio DFT code based on Daubechies wavelets. In recent articles, we presented the linear scaling version of BigDFT code[1], where a minimal set of localized support functions is optimized in situ for systems in various boundary conditions. We will present how the flexibility of this approach is helpful in providing a basis set that is optimally tuned to the chemical environment surrounding each atom. In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, without reoptimization, for charge-constrained DFT calculations within a fragment approach[2]. We demonstrate the interest of this approach to express highly precise and efficient calculations of systems in complex environments[3].

In a second part, we show that these exascale-oriented capabilities need to build complex input files but also to pre- and post-process output files; more generally we would like to handle complex computational laboratory notebooks. We conclude with some ideas about reproducibility and continuity of the computational research.

[1] JCP 140, 204110 (2014), PCCP 17, 31360 (2015)
[2] JCP 142, 23, 234105 (2015)
[3] JCTC 11, 2077 (2015)