

Reducing technical debt and complexity by promoting collaborations

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Technical debt and complexity are inevitable consequences of software growth. Most of the times, they can be mitigated by appropriate practices — such as periodic beautifications and core-developer coordination meetings — and do not necessarily become growing threats. Along the history of ABINIT, they have lead to the creation of a bunch of components and features which were solutions to specific problems at specific times: abilint, the ABINIT Fallbacks, the bindings, or the hierarchical block-structured user interface of the build system, to cite the most obvious ones. With time, the situation evolved significantly, and they stopped being adequate solutions.

Over the last few years, the build system of ABINIT has been redesigned to address the issues encountered in the current technological and social contexts of electronic structure. Its internals have been rewritten to allow non-expert developers to interact with it. This long and tedious restructuring process has lead to a noticeable simplification in the maintenance of the logical blocks of ABINIT. It has also permitted the split of the source tree and a multi-stage compilation. One of its main outcomes is a definitive end to the circular dependency that had been chaining ABINIT and BigDFT for nearly 10 years.

In the meantime, other collaborations have been established and/or strengthened to improve the overall quality of software developed within the electronic structure community and make progress on the complex topic of dependency management. Different solutions have been explored within the Electronic Structure Library (ESL) and the E-CAM Center of Excellence. Some of them, like the ESL Bundle, EasyBuild, and Spack, work together and are already used by some Electronic Structure codes. They constitute a growing number of superior alternatives to the ABINIT Fallbacks and will likely replace it in the near future.