

1 Executive Summary

The ETSF libraries and tools are pieces of software meant to greatly facilitate code reuse, providing enhanced portability and interoperability as well. They comprise:

- the ETSF_IO library, which implements the ETSF File Format specifications;
- the LibXC library, which provides a comprehensive set of exchange-correlation functionals;
- the pseudopotential converter PspConverter, to exchange and cross-check pseudopotential data between codes;
- the 3D renderer V_Sim, allowing for the visualization of solids, surfaces, and molecules, as well as their dynamical, electronic, and magnetic properties.

ETSF_IO provides a fully-documented reference implementation of the ETSF File Format specifications, which is mandatory to achieve a full deployment within the ETSF. Home-made implementations for each code would indeed be extremely difficult for most of the developers and result in a very low reliability. New versions of ETSF_IO are tightly bound to the evolution of the ETSF File Format specifications (see deliverable 8.1). None has been released during the current reporting period.

Creating LibXC was not as critical as for ETSF_IO, since there were many pre-existing implementations of exchange-correlation functionals. However such a situation was highly suboptimal, and rather of a “reinventing-the-wheel” kind, with the same endlessly repeated trial-and-error cycles, to finally end-up with very similar implementations in various codes. As each routine of LibXC is provided with a test case and deployed in several codes, its portability and robustness can only increase steadily with time, with the additional benefit that any bugfix applied to the library can be immediately propagated to all dependent codes. Many efforts have been undertaken to have LibXC working with Abinit in a pilot project, and to make it independent from Octopus, its parent code. They have resulted in a new version of LibXC, constituting a significant step in improving its usability.

A lot of efforts have been deployed among several communities a few years ago, in order to create a standard format for pseudopotential data. This resulted in a comprehensive XML-based set of specifications, which were unfortunately not released along with a reference implementation. PspConverter was thus developed as an alternative, with the aim of permitting the seamless exchange of pseudopotentials between codes, regardless of the existence of any standard.

V_Sim is an individual initiative that became popular within the ETSF because its features were matching the visualization needs of the researchers very well, and also because its developers are very open and responsive to bug reports and feature requests. V_Sim is indeed very helpful when it comes to analyze and interpret the results of many kinds of calculations. A new version has been produced, improving its user interface and its portability.

Last but not least, the efforts conducted for WP5 and WP8 have attracted the attention of packagers from several Linux distributions. Their involvement will constitute a precious resource to improve the deployment, portability, and interoperability of all ETSF tools, libraries, and codes. Their huge user base will also greatly facilitate the expansion of the visibility of the ETSF way beyond its current limits.