

1 Executive Summary

In the context of WP5 – Promoting software availability, the ETSF distributes a suite of nine applications related to ab initio modeling theory. This report describes the actions that have been taken in order to build the several variants of binary packages and to distribute them by means of the ETSF website. The formal title of this deliverable does not clearly embody the actual tasks involved; hence, the scope of this report is wider than its formal title would imply.

Starting from the individual components' source code, this deliverable aims at publishing on-line an “easy to obtain, install and use” collection of applications designed to be inter-operable, compatible and up to date. The binaries have been produced with recent versions of the relevant compilers for efficiency; the stability and accuracy have been tested on a computing farm with a wide selection of hardware and on several virtual machines. The collection comes with extensive documentation, samples and tutorials. This suite of free (of rights) applications can be installed on many Linux distributions supporting the Debian or RedHat package standards; the liveCD version can operate on any adequate x86 hardware.

The binary packages may be downloaded from <http://www.etsf.eu/resources/software>. Both the packages and the on-line information are updated when new production versions are released, meeting the objective of the D5.2. They provide an illustration of ETSF achievements to the scientific community in the area of software engineering and user interaction.