

Optional packages

Overview

AtomPAW

AtomPAW is a generation library for PAW atomic data sets (like pseudopotentials). It is the reference package to generate datasets for ABINIT, but several others can be used as well.

You can download AtomPAW from its [Wake Forest University project page](#).

Our [Installing AtomPAW](#) page will give you useful instructions to install AtomPAW properly and make it work with Abinit.

Please note that AtomPAW depends on [linear algebra](#) and [LibXC](#), which must be installed before.



Useful tip

AtomPAW is not necessary to build Abinit but will let you execute more test cases from the test suite and create your own PAW datasets.

BigDFT

BigDFT is a DFT code, solving the Kohn Sham equations in a Wavelet basis set. It is adapted for large systems with multiresolution and many nice features (PAW, fancy Poisson solvers, QM/MM...). BigDFT is interfaced with and can be called from ABINIT, to exploit some features of the latter.

You can download BigDFT from its [Home page](#).

Our [Installing BigDFT](#) page will give you useful instructions to install BigDFT properly and make it work with Abinit.

Please note that BigDFT requires [linear algebra](#) and also depends on [ETSF_IO](#) and [LibXC](#), which must be installed before.

ETSF_IO

ETSF_IO is a Fortran library allowing the platform-independent storage and exchange of electronic-structure data. It is of great interest to restart a calculation on a different computer, as well as to perform multi-step calculations involving other software projects. Thanks to ETSF_IO, Abinit can for instance calculate the ground-state properties of a system and provide input data for a GW calculation with [Yambo](#).

You can download ETSF_IO from:

- the [Libraries and Tools](#) page of the [ETSF website](#);
- its [Launchpad project page](#).

Our [Installing ETSF_IO](#) page will give you useful instructions to install ETSF_IO properly and make it work with Abinit.

Please note that ETSF_IO depends on [NetCDF](#), which must be installed before.

GSL

GSL is the GNU Scientific Library, and implements many mathematical algorithms, optimization, minimization etc... Some of these features can be used by ABINIT if GSL is linked at make time.

You can download the GSL from the [GNU website](#) or your [nearest mirror](#).

Our [Installing GSL](#) page will give you useful instructions to install the GSL properly and make it work with Abinit.

Levmar

Levmar is a library implementing the Levenberg-Marquardt optimization algorithm, which ABINIT can call and use.

You can download Levmar from its [FORTH-ICS page](#).

Our [Installing Levmar](#) page will give you useful instructions to install Levmar properly and make it work with Abinit.

PAPI

PAPI is a library for instruction counting and profiling, to know where your code is spending time.

You can download PAPI from its [University of Tennessee page](#).

Our [Installing PAPI](#) page will give you useful instructions to install PAPI properly and make it work with Abinit.

PSML

PSML is a library pseudopotential file format in XML, with a corresponding library. PSML is supported by a number of codes, in particular ABINIT and SIESTA, to have inter-operable DFT calculations with different features.

You can download PSML from its [Launchpad project page](#).

Our [Installing PSML](#) page will give you useful instructions to install PSML properly and make it work with Abinit.

TRIQS

TRIQS is a library for the quantum Monte Carlo solution of a quantum correlated impurity problem (within DMFT).

You can download TRIQS from its [CNRS page](#).

Our [Installing TRIQS](#) page will give you useful instructions to install TRIQS properly and make it work with Abinit.

Wannier90

Wannier90 implements the maximally localized Wannier Function scheme from Marzari and Vanderbilt. It allows interpolation and post-processing of many electronic quantities, and is interfaced with most modern DFT codes.

You can download Wannier90 from:

- its [home page](#) for the pristine version;
- the [Launchpad project page](#) for the patched version that works directly with Abinit.

Our [Installing Wannier90](#) page will give you useful instructions to install Wannier90 properly and make it work with Abinit.

Please note that Wannier90 requires [linear algebra](#), which must be installed before.



Warning!

The pristine version of Wannier90 has some bugs and must be patched to work with Abinit. If you decide to use it, please download our patches from the [Installing Wannier90](#) page.

YAML

YAML is a human readable yet easy to parse file format, for some input and output files of ABINIT.

You can download YAML from the [PyYAML repository](#).

Our [Installing YAML](#) page will give you useful instructions to install YAML properly and make it work with Abinit.

Libpspio

Libpspio is a library for interchange (input and output) of different pseudopotential file formats. It supports a number of them for many different codes.

You can download Libpspio from its [Launchpad project page](#) and soon from its [ESL wiki page](#).

Our [Installing Libpspio](#) page will give you useful instructions to install Libpspio properly and make it work with Abinit.

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