

# Building BigDFT

To link ABINIT with BigDFT, BigDFT must be compiled as a library.

## Building dependencies

Before compiling, one should compile or provide its dependencies :

- libXC ;
- libYAML ;
- linear algebra (Lapack and Blas or equivalents) ;
- a subset of ABINIT called later on libABINIT.

libXC, libYAML and the linear algebra are official packages provided by upstream. Refer to the different project pages for compilation indications.

To compile libABINIT, download it from [abinit.org](http://abinit.org). It works with the Autotools. So configure it with :

```
./configure FC=mpif90 --with-libxc-incs="-I/path/to/libXC/install/includes"
--with-libxc-libs="-L/path/to/libXC/install/lib -lxcf90 -lxc"
```

Mind that it depends on libXC itself that should be compiled before.

## Building BigDFT as a library

BigDFT is using the Autotools. One can download it from [abinit.org](http://abinit.org). To configure it, one needs to provide access to all dependencies. Besides, one should disable the building of binaries and of Python bindings :

```
./configure FC=mpif90 --with-libxc-incs="-I/path/to/libXC/install/includes"
--with-libxc-libs="-L/path/to/libXC/install/lib -lxcf90 -lxc" --with-
libabinit-incs="-I/path/to/libABINIT/install/includes" --with-libabinit-
libs="-L/path/to/libABINIT/install/lib -labinit" --disable-binaries --
disable-bindings --without-gobject --enable-libbigdft
```

## Linking everything into ABINIT

Add bigdft to the dft flavor in ABINIT configuration : `--with-dft-flavor=bigdft+...`

From:

<https://wiki.abinit.org/> - **Tips for ABINIT users and developers**

Permanent link:

[https://wiki.abinit.org/doku.php?id=build:install\\_bigdft&rev=1474549488](https://wiki.abinit.org/doku.php?id=build:install_bigdft&rev=1474549488)

Last update: **2016/09/22 15:04**

