BigDFT-suite Documentation

Release 1.8.3

BigDFT developers

Nov 19, 2018

Contents

The *BigDFT-suite* project regroup the packages which are needed to install, run and employ the BigDFT code for production calculations.

CHAPTER 1

Overview of BigDFT

1.1 Publications

Here, you can find the links to papers describing and using BigDFT.

1.2 Talks

You can find some conference and workshop slides about BigDFT here.

1.3 Available Functionalities

Todo: insert list of functionalities, current status (i.e. works/under development) and compatibility issues, and link to notebook if appropriate

CHAPTER 2

Users’ instructions

2.1 Get the code

BigDFT is available on Launchpad, from where it can be downloaded as a tar file or via bzr using the command `bzr branch lp:bigdft`.

2.2 Install the code

2.2.1 Install via Docker

BigDFT may be installed via Docker, see instructions here.

Todo: insert some basic information about Docker

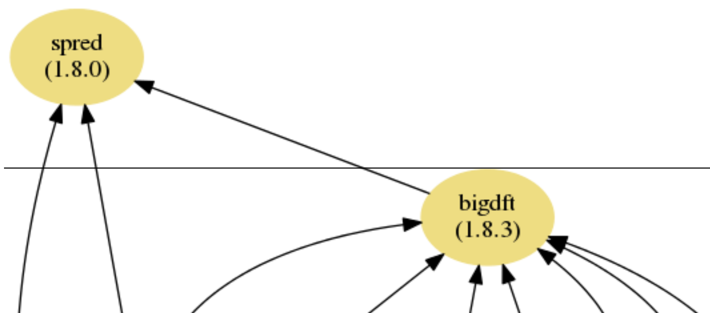
2.2.2 Install from sources

The BigDFT suite

From version 1.8.0, that can be downloaded either from the provided tarball or by having a launchpad account, via

```
bzr branch lp:bigdft
```

the build system of BigDFT has been modified. Instead of building the code with one single configure line, the code is now built as a suite of different packages.



In this scheme we might see how the BigDFT code is separated. This was also the same compiling procedure that has been used for the 1.7.x versions of the code. The figure describes the interdependencies among these packages. Let us describe each of the packages which are depicted here. The packages might be separated in *upstream* contributions and *native* contributions

Upstream packages

- `libyaml`: this library is used to parse the *yaml <http://yaml.org/>* Markup language, that is used in the BigDFT input files;
- *PyYaml <https://pyyaml.org/>*: this is a Python module which makes possible to convert Yaml into python objects. This part is mainly used for postprocessing purposes as BigDFT logfile also comes in yaml format;
- `libXC`: *this <http://www.tddft.org/programs/octopus/wiki/i* library handles most of the XC functionals that can be invoked from BigDFT runs;
- `GaIn`: this library handles analytic integrals of common operators between Gaussian Functions. It does not perform low-level operations and can be linked separately;

Native packages

- futile: a library handling most common FORTRAN low-level operations, like memory managment, profiling routines, I/O operations. It also supports yaml output and parsing for fortran programs. It also provides wrappers routines to MPI and linear algebra operations. This library is intensively used in BigDFT packages;
- `CheSS`: A module for performing Fermi Operator Expansions via Chebyshev Polynomials, released as a separate project on Launchpad

- `psolver`: a flexible real-space Poisson Solver based on Interpolating Scaling Functions. It constitutes a fundamental building block of BigDFT code, and it can also be used separately and linked to other codes. It also internally uses the `futile` library for the I/O.
- `libABINIT`: this is a subsection of files coming from ABINIT software package, to which BigDFT has been coupled since the early days. It handles different parts like symmetries, ewald corrections, PAW routines, density and potential mixing routines and some MD minimizers. Also some XC functionals, initially natively implemented in the `ABINIT` code, are also coded in this library. Also this library uses the `futile` code, through the (experimental) PAW section.
- BigDFT: the core routines of this package
- `spred`: a library for structure prediction tools, that is compiled on top of BigDFT routines.

In the previous versions, all these different packages were compiled with the same configuration instructions. With the present version, each of the code sections described above can be considered as a separate package (some more are upcoming), which improves modularity between code sections and reduces side-effects. In addition, each package can now be compiled with different installation instructions.

We have used a building suite tool based on the *Jhbuild <https://wiki.gnome.org/action/show/Projects/Jhbuild?action=show&redirect=J* which is regularly used by developers of `gnome` project. We have re-adapted/added some of the functionality of the `jhbuild` package to meet the needs of our package. Let us now present how the installation should work. We have prepared a script, called `Installer.py`, which should take care on the main actions related to BigDFT suite compilation and installation. Let us investigate how it works.

Usage of the `Installer.py` script

As mentioned above the BigDFT suite is compiled by means of instructions from the Python script `Installer.py`. Such script triggers the usage of the `jhbuild.py` Python file which is at the basis of the `jhbuild` project mentioned above. There are various actions available in addition to the `build` command. To know them, just type

```
$ ./Installer.py help
Parsing arguments with method argparse...
Quick overview of the BigDFT suite Installer program
--------------------------------------------------
USAGE: Installer.py <action> <package>
--------------------------------------------------Available actions
autogen :
      Perform the autogen in the modules which need that. For developers only.
build :
      Compile and install the code with the given configuration.
buildone :
      Build a single module of the suite
check :
      Perform check in the bigdft branches, skip external libraries.
clean :
      Clean the branches for a fresh reinstall.
cleanone :
      Clean a single module of the suite
dist :
      Creates a tarfile for the suite tailored to reproduce the compilation options␣
↪specified.
dry_run :
      Visualize the list of modules that will be compiled with the provided␣
↪configuration in the 'buildprocedure.png' file.
link :
      Show the linking line that have to be used to connect an external executable to␣
↪the package (when applicable)
```

```
make :
      Recompile the bigdft internal branches, skip configuring step.
startover :
      Wipe out all the build directories and recompile the important parts
update :
      Useful to update a pre-compiled branch after a merge
--------------------------------------------------
Available packages: ['futile', 'chess', 'psolver', 'bigdft', 'PyBigDFT', 'spred']
--------------------------------------------------
QIFI-QIFI-QIFI-QIFI-QIFI-QIFI-QIFI-QIFI-QIFI-QIFI- (Quick Instructions For the␣
↪Impatient)
Ideally, there are two different policies:
Developer: From a development branch, start by "autogen", then "build"
     User: From a tarball, start by "build"
Perform the "dry_run" command to have a graphical overview of the building procedure
```

So for example, to build the tarball of bigdft-suite out of a valid branch, you may type

```
Installer.py dist bigdft
```

You should have eventually a tarfile named `bigdft-suite.tar.gz` in the build tree. Such tarfile may be used to build the suite in another machine.

Few important informations:

- This script is intendent to provide the **end-user** with a functional set of executables coming from the suite packages. It has to be used to (re-)work on the entire suite, not a single package only.
- It does not replace the traditional `make` commands. A developer of a single package, say `futile` for example, should first compile *and install (`make install`) the package in its build directory, then rebuild the dependencies. In such a case, it is advised to run `Installer.py clean` first, then the `build` command would work.

Installing from a `configure` line

As written above, packages were already configured and compiled with a previous BigDFT version. Therefore we have prepared a compilation method to compile the 1.8.x build system from a configure line. See in the examples page some of the configure lines which were already tested on different machines.

The principle of this installer is to execute, in a build directory different of the source one, instead of the configure script, the following command:

`<path_to_sources>/Installer.py build -c`

Let us consider the example of the `pilipili` machine (internal L_Sim lab machine). Clearly, environment modules still have to be loaded:

`module load intel/13.0.1 impi/4.1.0.024`

Then the installer script can be used with the following command:

```
<path_to_sources>/Installer.py build -c 'FCFLAGS=-O2 -openmp' \
'--with-ext-linalg=-L/opt/intel/composer_xe_2013.1.117/mkl/lib/
intel64 -lmkl_rt -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64 -liomp5 -lm' \
'--enable-opencl' 'CC=mpicc' \
CFLAGS='-openmp' 'CXX=mpicxx' 'FC=mpifc' 'F77=mpif77' 'FCLIBS= '
```

The following message dialog will appear:

```
Configuration chosen for the Installer:\
 Hostname: pilipili
 Source directory: /home/athelas/genovese/work/BigDFT/1.8\
 Compiling from a branch: True\
 Build directory: /local/genovese/binaries/1.8-ocl\
 Action chosen: build\
 Verbose: False\
 Jhbuild baseline: <path_to_sources>/jhbuild.py \
 Configuration options:\
   Source: Environment variable 'BIGDFT_CONFIGURE_FLAGS'\
   Value: '"FCFLAGS=-O2 -openmp" "--with-ext-linalg=-L/opt/intel/
composer_xe_2013.1.117/mkl/lib/
intel64 -lmkl_rt -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64 -liomp5 -lm" "--enable-openc
Do you want to continue (Y/n)?
```

The Installer script has detected the different compilation options. It has filled the environment variable `BIGDFT_CONFIGURE_FLAGS` with the options passed after the `-c` option in the command line. By typing `Y` the bigdft bundle will build.

As we did not specified the `-v` option (type `./Installer.py help` for the available commands and options), the code will be built in silent mode (this would correspond to the `tinderbox` option of JhBuild. You should have the following information in the output:

```
List of modules to be treated: ['libyaml', 'futile', 'psolver', 'libxc',
'libABINIT', 'GaIn', 'bigdft', 'spred']
libyaml : ['checkout', 'configure', 'build', 'install']
futile : ['checkout', 'configure', 'build', 'install']
psolver : ['checkout', 'configure', 'build', 'install']
libxc : ['checkout', 'configure', 'build', 'install']
libABINIT : ['checkout', 'configure', 'build', 'install']
GaIn : ['checkout', 'configure', 'build', 'install']
bigdft : ['checkout', 'configure', 'build', 'install']
spred : ['checkout', 'configure', 'build', 'install']
```

Then in the directory named `buildlogs` of the build tree you might find the `index.html` file that contains the status of the compilation.

At the end of a successful compilation, you find in the build directory a file named `buildrc` that may be used for future compilation and to specify more flexible configurations options. See next section for the details.

Using a configuration file (`rcfile`)

The environment variable `BIGDFT_CONFIGURE_FLAGS` is a way to indicate some general options for all modules. A more powerful method is to use a `rcfile` configuration file which indicates all possible option for each module.

Some examples are provided in the directory `rcfiles`. For advanced features, the different possible options are detailed in 1.

The default behaviour (no information)

Working with a configuration file is the default behaviour of `jhbuild`. Therefore it is normally expected to provide a file to the `Installer.py` script (see next section on how to do that). If no files is provided in the command line, the script search for (priority order):

- A file named `buildrc` in the current build directory;
- A file in the directory `rcfiles/` of the source tree that contains the hostname string (or a part if it) in its basename. If multiple files satisfy this condition, it offers a choice.

Therefore when asked to proceed for the installation, it is advised to pay attention in the initial message which is the file chosen for the configuration.

How to invoke a configuration file

The name of the configuration file might be specified with the `-f` option of the installer. the file might be either specified via its absolute path, or by its name. In this case, it is searched for in (priority order):

- The current working directory;
- The directory `rcfiles/` of the source tree.

Manipulating the configuration file

The principle of the configuration file is to provide configure options which are different for each o the packaged of the suite (called modules in the `jhbuild` spirit). Therefore, to each of the package one must associate a configure line. Such information is provided in the dictionary `module_autogenargs` of jhbuild, and might be specified as follows (see e.g. the file `dynamic.rc`)

```
module_autogenargs['libxc'] = "CC=gcc --enable-shared"
```

or, alternatively

```
module_autogenargs.update({'libxc': "CC=gcc --enable-shared"})
```

depending on your taste. If the BigDFT suite is compiled from a configure line, at the end of the first compilation a `buildrc` file is produced, that can be then used in the following compilations.

The Python syntax of the configuration file

An rcfile is invoked inside the collection of python modules provided by `jhbuild`. Therefore within this file the python syntax is necessary. This adds extra features that would otherwise be difficult to implement. For example, one might define functions that indicate common configuration options, or that retrieve the current working directory to define more elaborated configuation lines. For example, in a rcfile we may found (see for example the file `mira.rc` of the distribution):

```
def fcflags_short():
 return """'FCFLAGS= -g -O3'"""
[...]
```

```
module_autogenargs.update({
  'libxc': fcflags_short(),
 [...]
 }
```

We here prefer to use return values of functions rather that to define extra variables in the script as `jhbuild` warns if unknown variable names are found in the configuration file.

Building the executables

There are some practical examples of compilations on different architectures where you might find useful information on how the code has been compiled on different platforms and for different options.

Linking external software with BigDFT packages

From version 1.8.0 on the build system of BigDFT is "generic" in the sense that it does not only allow the compilation of the main BigDFT software, but also of various sub-packages. This is useful if one is only interested in some of the packages distributed with BigDFT.

As an example we will show the compilation of the CheSS package, which itself depends on futile. It can be downloaded here: 2 After downloading the tar.gz execute the following steps:

```
tar -xzvf CheSS-0.1.1.tar.gz
cd CheSS-0.1.1
mkdir Build
cd Build
../Installer.py build chess -d -c FC= CC= FCFLAGS= --with-ext-linalg=
```

A dialogue similar to this one should appear:

```
Configuration chosen for the Installer:
  Hostname: stephan-Latitude-E7450
  Source directory: /home/stephan/Documents/BigDFT/stablebranch
  Compiling from a branch: True
  Build directory: /home/stephan/Documents/BigDFT/stablebranch/Build-gnu_debug
  Action chosen: dist
  Verbose: True
  Jhbuild baseline: ../jhbuild.py -f buildrc
  Configuration options:
    Source: Configuration file '/home/stephan/Documents/BigDFT/stablebranch/
Build-gnu_debug/buildrc'
Do you want to continue (Y/n)?
```

Confirm and wait until the compilation in complete. In order to link now another software with CheSS, run the command

```
../Installer.py link chess
```

which should give you an output similar to this one:

```
--------- Linking line to build with package "chess":
  -I/home/stephan/Downloads/CheSS-0.1.1/Build/install/include-L/home/stephan/
Downloads/CheSS-0.1.1/Build/install/
lib -lCheSS-1 -lfutile-1 -lblacs-openmpi -lblacsF77init-openmpi -llapack -lblas -lyaml -lrt
--------------------------------------------------
```

This is the link line that you can now use in your other software to link with CheSS.

The BigDFT Installer class

2.3 Run the code

We recommend running BigDFT using a jupyter notebook. Various features have been implemented in PyBigDFT for the straightforward pre- and post-processing of calculations, as demonstrated in these tutorials: pybigdft_tutorials, with further examples available on github.

Todo: add some brief text and a link to explain what a jupyter-notebook is; tips for using notebooks remotely (link to script); how to run without using a notebook, i.e. the key ingredients of a calculation and where to find variables - should be at a very basic level.

2.4 Frequently encountered problems

Todo: add here any problems (and how to avoid them) which occur on a frequent basis

CHAPTER 3

Developers' instructions

3.1 BigDFT-suite manifesto

The code is not a monolithic piece of software but a collection of *independent* packages that **may** be installed independently. The *Installer* script has been designed for the purpose.

3.2 Tips for developers

3.2.1 Choose the correct package in which to insert the developments

The first question to ask yourself is the *generality* of the functionality you are going to implement. The spirit is to work at the lowest possible level for a given task. The idea is to make available the functionality also to other potential users of the `BigDFT-suite` subpackages. This will also help in a better structure of the API of each package.

For instance, suppose you would like to implement a continuum solvent cavity determination for a particular DFT run of a molecular system. The correct level of development in this case would be the `psolver` package, as this is presently dealing with continuum solvents and cavities.

For a general overview one might say that:

- `futile` deals with low-level functionalities like `stdlib` (but for FORTRAN). New MPI wrappers, strategies for memory copy and allocations should be implemented there.
- `at_lab` library (will) deal with all the operations which are associated to position
- <to_B_continued>

3.2.2 Read the coding rules

For some inspiration on coding style and strategies, read this.

3.2.3 Document the API of the high-level routines

Todo: write something here

3.2.4 Create a test for the functionality

Each of the packages has its own continuous integration procedure, refer to it for a suitable implementation.

- `futile`, `psolver`: F_REGTEST_INSTRUCTION (to be documented)
- `bigdft` see here.

3.2.5 Make a notebook which demonstrates the functionality in PyBigDFT

For each new high level functionality, you should create a jupyter notebook which demonstrates the new capability. The idea is to ensure continuity and to help acquaint users with the new feature. Some examples of notebooks can be found on github.

3.2.6 Insert the notebook as a tutorial in the PyBigDFT documentation

Once an appropriate notebook has been written, this should be added to the tutorial directory (`BIGDFT_ROOT/PyBigDFT/source/tutorials`), so that the documentation will be automatically generated and available as a tutorial at pybigdft_tutorials.

Example of link to futile_index, followed by exemple to pybigdft_tutorials, actualized.

Example of link `zipfile.ZipFile` to python class or to `f/f_precisions` or maybe `futile.Utils.find_files()` this, or again `BigDFT.Logfiles`. If all these links are not broken, we may reach the following conclusion: *intersphinx* seems to work.

CHAPTER 4

Indices and tables

- genindex
- modindex
- search