This file describes how to install ATOMPAW on MacOS

- Using Homebrew package manager
- Using MacPorts package manager
- Compiling by yourself

This manpage is available as ~atompaw_src_dir/doc/README.MacOSX

1- USING HOMEBREW PACKAGE MANAGER

A ***`Homebrew`*** *third-party Formula for ATOMPAW is available*
Tested with macOS v10.9 to v10.14.

Prerequisite: Homebrew installed (see: http://brew.sh/#install)

To install ATOMPAW just type:

```
brew install atompaw/repo/atompaw
```

Note: **`libxc`** library is used by default.
This can be disabled by passing `--without-libxc` option to `brew install`.

2- USING MACPORTS PACKAGE MANAGER

ABINIT is available on ***`MacPorts`*** *project, not necessarily in its latest version.*
Tested with mac OS v10.8 to 10.14.

Prerequisites:

- MacPorts installed (see: https://www.macports.org/install.php)
- gcc (last version) port installed with Fortran variant (Fortran compiler),
- Before starting, it is preferable to update MacPorts system:

To install ABINIT just type:

```
sudo port install atompaw
```

By default, ATOMPAW is installed with the following **`libxc`** and **`accelerate`** (linear algebra) dependencies.

Variant:
Linking to **`OpenBLAS`** library: `port install atompaw @X.Y.Z +openblas`

3- COMPILING ATOMPAW BY YOURSELF under MacOSX

Prerequisites:

- `MacOS` (10.8+)
- `Xcode` installed with `command line tools` (type: `xcode-select --install`)
- A Fortran compiler installed. Possible options:
  - `gfortran` binary from: http://hpc.sourceforge.net
  - `gfortran` binary from: https://gcc.gnu.org/wiki/GFortranBinaries#MacOS
  - `gfortran` installed via a package manager (MacPorts, Homebrew, Fink)
  - `Intel Fortran compiler`
- A Linear Algebra library. By default `accelerate` is included in MacOS.
- By default the accelerate Framework is installed on MacOSX and ATOMPAW build system should find it.
- `libxc` library installed [optional but recommended] (https://tddft.org/programs/libxc)

Installing ATOMPAW:

- Create a working directory:

```
cd atompaw_src_dir
mkdir build && cd build
```

- Configure:

With libXC support

```
../configure =gfortran \
--prefix=where_to_install_atompaw \
--enable-libxc \
--with-libxc-incs="-Ipath_to_libxc/include" \
--with-libxc-libs="-Lpath_to_libxc/lib -lxc -lxcf90"
```

Without libXC support:

```
../configure FC=gfortran \
--prefix=where_to_install_atompaw
```

- Compile and install [optional]:

```
make
make install
```

Help available by typing: `../configure --help`