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:

```sh
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 macOS 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:

```sh
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

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