This file describes how to install ATOMPAW on Mac OS X

- 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 (http://brew.sh)

Tested with mac OS X v10.9 (Mavericks), v10.10 (Yosemite), 10.11 (El Capitan).

A Homebrew official formula for ATOMPAW is available (author: M. Torrent).

----- Prerequisites -----  
* Homebrew installed (see: http://brew.sh/#install)

* Notes:  
  - Homebrew needs Xcode and "Xcode command line tools" to be installed; just type:  
    xcode-select --install

----- Installing ATOMPAW -----  
* Just type:  
  brew install homebrew/science/atompaw

* ATOMPAW should install smoothly... with its dependencies (gfortran, libXC, ...).

----- Comments -----  
* LibXC exchange-correlation library is used by default.  
  To build ATOMPAW without libXC support, use the --without-libxc option.

2- USING MACPORTS (http://www.macports.org)

Tested with mac OS X v10.10 (Yosemite), v10.11 (El Capitan).

There is an available port in the MacPorts system for ATOMPAW, originally created by ATOMPAW developers.

----- 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:  
  sudo port selfupdate  
  sudo port upgrade outdated

* Notes:  
  - It is recommended to completely reinstall MacPorts after a MacOS upgrade.  
  - MacPorts needs Xcode and "Xcode command line tools" to be installed; just type:  
    xcode-select --install

----- Installing ATOMPAW -----
* Install official ATOMPAW port:
  sudo port install atompaw

----- ATOMPAW port variants -----

* By default, ATOMPAW is installed with the following dependencies:
  libXC, vecLibFort (linear algebra)

* Linking ATOMPAW to Atlas library:
  sudo port install atompaw @X.Y.Z +atlas

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

* Linking ATOMPAW to vecLibFort library:
  sudo port install atompaw @X.Y.Z +veclibfort

* Other options available by typing:
  port info atompaw

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= 3- COMPILING ATOMPAW BY YOURSELF under MacOSX =
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----- Prerequisites -----

* Mac OSX

  * Xcode installed with "Xcode command line tools"; just 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 installed.
    By default the 'accelerate' Framework is included in MacOSX.

  * Optional, but recommended:
    libXC exchange-correlation library installed.
    To be found at: http://www.tddft.org/programs/octopus/wiki/index.php/Libxc

----- Installing ATOMPAW -----

* Create a working directory:
  cd atompaw_src_dir
  mkdir build && cd build

* Configure:
  With libXC support:
  ../configure FC=gfortran --enable-libxc \
    --with-libxc-incs="-Ipath_to_libxc/include" \
    --with-libxc-libs="-Lpath_to_libxc/lib -lxc -lxcf90"

  Without libXC support:
  ../configure FC=gfortran

* Compile:
make

* Install (optional):
  make install

----- Comments -----

* The Linear Algebra library should be automatically found.
  If not, try to add the following option to the configure line:
    --with-linalg-libs="-L/usr/lib -lblas -llapack"

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