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================================================================================
=         This file describes how to install ATOMPAW on Mac OS X               =
=          - Using Homebrew package manager                                    =
=          - Using MacPorts package manager                                    =
=          - Compiling by yourself                                             =
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This manpage is available as ~atompaw_src_dir/doc/README.MacOSX


================================================================================
=  1- USING HOMEBREW    (http://brew.sh)                                       =
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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).

----- Prerequesites -----

* 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.


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

----- Prerequesites -----

* 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    sudo port upgrade outdated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 -----
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* 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


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

* 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:
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    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"



================================================================================
Author: M. Torrent, Feb. 2016
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