MOMAP

Installation Guide

Version 2019B

Molecular Material Property Prediction Package

Version 2019B

September, 2019

MOMAP Installation Guide

Version 2019B edited by:

Dr. Qikai Li

CONTENTS

Chapter 1. Installation

Introduction

Here we will describe how to install MOMAP 2019B Package.

We assume that you have the basic knowledge on how to install programs and manage your operating system. If this is not the case, please consult your local system administrator or consult HZW support.

Installing MOMAP – Basic Procedure

Installing MOMAP and configuring the license can be done in a few steps, that is,

1. Install MOMAP package
2. Obtain and install MOMAP license

Installing MOMAP – In Details

MOMAP is mainly targeted to be running in a UNIX-like environment, however, it can also be used on Windows or MacOS environment.

Install MOMAP

First download the MOMAP package from website: http://www.momap.net.cn/index.php/download, that is, right click and use the Save Link As option to download the file.

a) Install MOMAP for Linux

The MOMAP package for Linux is downloaded as a single zipped installable run file, e.g.,

```
momap-2019B-linux-mpich2.run.gz
```

When the download finishes, for example, in a Linux environment, use `gunzip` command to decompress the downloaded file:

```
$ gunzip momap-2019B-linux-mpich2.run.gz
```

Depending the downloaded file attribute, that is, if it retains the executable attribute, we can simply install MOMAP package by running:

```
$ ./momap-2019B-linux-mpich2.run
```

Or more generally, install MOMAP package by running:

```
$ sh momap-2019B-linux-mpich2.run
```

Before using the MOMAP software, users should first have a read of the files `README` and `INSTALL`, and add `env.sh` to `~/.bashrc`:

```
. <MOMAP_installed_dir>/env.sh
```

In addition, more environment variables can be added to `env.sh` as will be described in the User Guide.

If users would like to use the MOMAP with the Openmpi parallel environment (that is, by downloading file `momap-2019B-linux-openmpi314.run.gz`), then the users have to install the Openmpi 3.1.4 (with GCC 5.4.0, other versions may also work) before using the MOMAP package. However, we recommend users to use the MOMAP for Linux mpich2 version, as no installations with mpich2 1.5 and GCC 5.4.0 are needed.

b) Install MOMAP for macOS

For the macOS case, the installation process is similar to that in the Linux case, however, we need to install the necessary libraries used in the MOMAP package, and here the Homebrew package manager for macOS is used. The installation procedure is as follows:

a) Install Homebrew if not installed already

```
$ /usr/bin/ruby -e "$(curl -fsSL
https://raw.githubusercontent.com/Homebrew/install/master
/install)"
```

b) Install GCC 9, MPICH 3.3, FFTW3 and Lapack 3.8

```
$ brew install gcc@9
```

```
$ brew install mpich
$ brew install fftw
$ brew install lapack
```

Other settings are similar to those in the Linux situation. Once the above installations are finished, we can use the MOMAP for macOS as in the Linux's case.

c) Install MOMAP for Windows

To install MOMAP for Windows, we need first to install minGW64, Git Bash, Python, and MSMPI as detailed below.

Download minGW64 at the link: https://sourceforge.net/projects/mingw-w64/, and install minGW64 to location `C:\mingw-w64`.
Note: Remember to change the Architecture to `x86_64`.

Download Git for Windows at the link: https://gitforwindows.org/, and install to `C:\mingw-w64\Git`.

Download Python for Windows at the link: https://www.python.org/downloads/, and install to `C:\mingw-w64\Python37` (version may not be the same).

Download MSMPI at the link: https://docs.microsoft.com/en-us/message-passing-interface/microsoft-mpi, and install to `C:\mingw-w64\msmpi`.

Next, we need to modify the environment variable PATH in order to let the MOMAP run properly.

In both Windows 7 and Windows 10, open the Explorer, Right click on **This PC (My Computer)**, then Left Click **Properties**, and further Left Click **Advanced system settings**. In the pop-up window, Click the **Advanced** tab, and Left Click **Environment Variables**, then you can add or edit the various environment variables. In our case, we add the following lines to the PATH variable:

```
C:\mingw-w64\mingw64\bin
C:\mingw-w64\msmpi\bin
C:\mingw-w64\Python37
```

The current Git Bash has problem with python, before running python, we need first to add an alias for python:

Open Git Bash, edit `~/.bashrc` and add the following line:

```
alias python='winpty python.exe'
```

Also make a symbolic link to <installed-dir>/python.exe:

```
$ ln -s <installed-dir>/python.exe /usr/bin/python
```

Exit and reopen Git Bash, issue command `python` should be okay now.

Once the above MOMAP running environment settings are done, we can further install the MOMAP for Windows. For example, put the downloaded file to D:\, extract the archived files to the directory D:\MOMAP-2019B. Check the file `env-mingw.sh` to see if the environment variable MOMAP_ROOT points to the installed directory.

Again open Git Bash, edit `~/.bashrc` and add the following line:

```
source /d/MOMAP-2019B/env-mingw.sh
```

Exit and reopen Git Bash, then we can use MOMAP now.

For example, we would like to do some tests, then go to the directory D:/MOMAP/tests by issuing:

```
$ cd /d/MOMAP-2019B/tests
$ ls
$ cd azulene
```

Then we can do our work just as we do in the Linux situation.

Chapter 2. Licensing

Generate MOMAP license data

Before we can use MOMAP package, we need a license. There exist three license options, that is, `Network`, `Single`, and `MacFree`.

- Network: Choose this option if you will be using a floating license server.
- Single: Choose this option if you will be using node-locked license.
- MacFree: Choose this option if you will be using a trial license.

The program to collect license data is `get_license_data.exe`, users can use `--help` option to run the program to get the help message like the following:

```
$ get_license_data.exe --help
MOMAP license data collection utility, version 2019B (2.1.2)

Usage: get_license_data.exe [opts]
  -outfile license.dat              : set output filename, default to 'license.dat'
  -type [Network | Single | MacFree]      : set license type, default to 'Network'
  -cat [Purchased | Free]           : set license category, default to 'Purchased'
  -hosts machinefile                : set machine list file, default to rhosts
  -year_inc yy                      : set year increment for purchased license, default to 3
  -month_inc mm                     : set month increment for free license, default to 1
  -version x.y.z                    : set version number, default to 2.1.2

e.g.:
  get_license_data.exe
  get_license_data.exe -outfile license.dat
  get_license_data.exe -version 2.1.2
  get_license_data.exe -type MacFree -version 2.1.2
  get_license_data.exe -type Network -version 2.1.2
  get_license_data.exe -type Single -hosts hosts -version 2.1.2
```

If the program is run without any option, it will generate the `license.dat` file for the current node (assumed to be master node) as `Network` type licensing, the MAC information will be automatically filled in as follows:

```
$ cat license.dat
sales_name = 'HONGZHIWEI TECHNOLOGY(SHANGHAI) CO,.LTD';
sales_webSite = 'www.hzwtech.com';
sales_email = 'sales@hzwtech.com';


licenseInput.user_name = 'Change here';
licenseInput.user_researchGroup = 'Change here';
licenseInput.user_institution = 'Change here';
licenseInput.user_email = 'Change here';
licenseInput.user_address = 'Change here';


licenseInput.user_type = 'Group';


licenseInput.product_name = 'MOMAP';
licenseInput.product_moduleName = 'dushin, transport';
licenseInput.product_version = '2.1.2';


licenseInput.license_type = 'Network';
licenseInput.license_releaseDate = '20191211';
licenseInput.license_maintenanceDate = '20221211';
licenseInput.license_expireDate = '20221211';
licenseInput.license_category = 'Purchased';


licenseInput.computer_MAC = {
'94-57-A5-57-D4-00',
'94-57-A5-57-D4-01',
'94-57-A5-57-D4-02',
'94-57-A5-57-D4-03'
};
```

Users need to fill the user information marked with "*Change here*" with your actual name, group, institution *etc.* as required, and send this `license.dat` file to the email address as shown in `license.dat`.

Later on, a MOMAP license file, for example, `license.lic`, will be sent to you by a sales representative, you simply copy the license file to $MOMAP_ROOT, modify `~/.bashrc` and let the environment variable `MOMAP_LICENSE` point to this file if you have not done so:

```
$ export MOMAP_LICENSE=$MOMAP_ROOT/license.lic
```

Testing the installation

To verify that the MOMAP package has been properly installed, and the license is correctly configured and installed, users can run a short test to verify the installation.

Troubleshooting installation problems

If you encounter any problems during the installation, please contact the HZW for support.