MOMAP

Installation Guide

Version 2024A

Molecular Material Property Prediction Package

Version 2024A

October 1, 2024

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Version 2024A edited by:

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The information in this document applies to MOMAP version 2024A

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Chapter 1. Installation

Introduction

Here we will describe how to install MOMAP 2024A 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 Co. Ltd for 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, by simply clicking the related link or DOWNLOAD button 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-2024A-linux-el7-openmpi.run.gz
```

Unzip the file and add executable attribute to the file, and install MOMAP by running:

```
$ gunzip momap-2024A-linux-el7-openmpi.run.gz
$ chmod a+x momap-2024A-linux-el-openmpi.run
$ ./momap-2024A-linux-el7-openmpi.run
```

Or more generally, install MOMAP by running:

```
$ sh momap-2024A-linux-el7-openmpi.run
```

The default installation folder is `$HOME/MOMAP-2024A`, however, one can change the target installation folder in the installation process.

Before using MOMAP, one should first set up the running environment by adding the following line to `~/.bashrc` if Bash is used:

```
. <installed_momap_folder>/env.sh
```

Log out and log back in again for it to take effect, then we can proceed to run MOMAP.

If the `Environment Modules` is installed, one can use the command `module` to manage the MOMAP running environment. Suppose the `Environment Modules` is installed to `/opt/Modules`, and the module files are put under `/opt/Modules/modulefiles`, one can create a directory, e.g., `momap`:

```
$ mkdir -p /opt/Modules/modulefiles/momap
```

Then, copy `<installed_momap_folder>/modulefile/2024A-openmpi` to that newly created directory.

However, if the user doesn't have the right to put the module file in the global `modulefiles` directory, one can do it in one's own `$HOME` directory, similarly, one first creates a directory, e.g., `momap`:

```
$ mkdir -p ~/.modulefiles/momap
```

Copy the `<installed_momap_folder>/modulefile/2024A-openmpi` to the newly created directory. Next, make it available to `Environment Modules` by using the following command:

```
$ module use ~/.modulefiles
```

Now one can use the module files as usual. For example, we can load the MOMAP environment by simply running the command:

```
$ module load momap/2024A-openmpi
```

More information on how to use the `Environment Modules`, please refer to the website at http://modules.sourceforge.net/.

In some supercomputing centers, the SSH port may not be the default 22, in that case, we need to setup the SSH environment variable, for example:

```
export MOMAP_SSH_PORT=5577
```

As to the specific port used, please contact the supercomputing center's system administrator for information.

If MOMAP is to be run under the Ubuntu Linux system, before we start to install MOMAP, we need first to promote the user rights and make the user to be an administrator. Here, we will show you how to make a user an administrator in Ubuntu through the command line:

```
$ sudo usermod -aG sudo sampleuser
```

You can verify that the user is now in the "sudo" group by checking the groups a user belongs to, through the following command:

```
$ groups sampleuser
```

Log out and log back in again for it to take effect, then we can proceed to have a normal MOMAP installation.

In addition, more environment variables can be added to one's `~/.bashrc` as described in the User Guide.

If you encounter messages like the following:

```
[/home/…/MOMAP-2024A] >>>
Install MOMAP to /home/qkli/MOMAP-2024A...
./install.sh: 109: source: not found
<…>/bin/get_LicenseNumber.exe: error while loading shared libraries:
libILasMatInterface.so: cannot open shared object file: No such file
or directory
```

Or

```
<…>/bin/openmpi/bin/mpiexec: Error: unknown option "-machinefile"
Terminated with ERROR for spec ft calculation
STOP
```
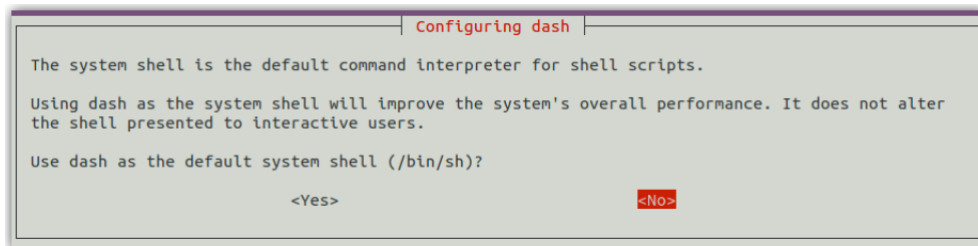
Then, run the command:

```
$ ls -l /bin/sh
… /bin/sh -> dash
```

It shows that /bin/sh is linked to dash, run the following command:

```
$ sudo dpkg-reconfigure dash
```

And select "No" as follows:

```
┤ Configuring dash ├
The system shell is the default command interpreter for shell scripts.

Using dash as the system shell will improve the system's overall performance. It does not alter
the shell presented to interactive users.

Use dash as the default system shell (/bin/sh)?

            <Yes>                                    <No>
```

If you encounter messages like the following:

```
... ifconfig: command not found
... /sbin/udevadm: No such file or directory
```

The missing ifconfig can be solved by installing the net-tools:

```
$ sudo apt install net-tools
```

The missing /sbin/udevadm can be solved by making a soft link:

```
$ sudo ln -s /usr/bin/udevadm /sbin/udevadm
```

Finally, run the MOMAP installation file again.

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:

1. Install Homebrew if not installed already

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

2. Install GCC, Open-mpi, FFTW3 and Lapack

```
$ brew install gcc@12
$ brew install open-mpi
$ 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 MSYS2 as detailed below.

Download MSYS2 at the link: https://www.msys2.org, and install MSYS2 to location `C:\msys64`.

Once the installation finishes, launch MSYS2. We need to install Python and MSMPI.

First, update the package database and core system package with:

```
$ pacman -Syu
```

Press ENTER to proceed the installation.

Now we use `pacman` to install `Python` and `vim` *etc.*:

```
$ pacman -S python
$ pacman -S vim
$ pacman -S openssh
```

Download MSMPI at the link: https://docs.microsoft.com/en-us/message-passing-interface/microsoft-mpi, and install to `C:\msys64\msmpi`.

Once the above MOMAP running environment settings are done, we can continue to

install the MOMAP for Windows. For example, put the downloaded file to `D:\`, and extract the archived files to the directory `D:\MOMAP-2024A`. Check the file `env-mingw.sh` to see if the environment variable MOMAP_ROOT points to the installed directory.

Edit `~/.bashrc` and add the following line:

```
. /d/MOMAP-2024A/env-mingw.sh
```

If Gaussian `g16` is used as the QC program and installed to directory `C:\g16w`, we need also add the path to the environment variable `PATH` as follows:

```
export PATH = $PATH:/c/g16w
export GAUSS_EXEDIR = /c/g16w
```

The users may add other necessary settings to `~/.bashrc` as needed.

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

For example, we would like to do some tests, first go to the directory `D:/MOMAP-2024A/tests`:

```
$ cd /d/MOMAP-2024A/
```

Then we do the various test runs 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 four license options, that is, `Trial PC version`, `All-in-one PC version`, `Intranet cluster version` and `Super HPC cluster version`.

- Trial PC version: Choose this option if you'd like to try the software with a desktop/laptop PC.
- All-in-one PC version: Choose this option if you plan to use the software in a workstation.
- Intranet cluster version: Choose this option if you plan to use the software in a small group-wise intranet computing cluster.
- Super HPC cluster version: Choose this option if you plan to use the software in the public domain super HPC cluster.

The program to collect the license data is `get_LicenseNumber.exe`, the program is called automatically at the end of MOMAP installation.

For the MOMAP for Windows case, we need to run `get_LicenseNumber.exe`, that is,

```
$ $MOMAP_ROOT/bin/get_LicenseNumber.exe
```

The generated license data file is located at directory `$MOMAP_ROOT/license/`, named as `LicenseNumber.txt`. One should send this file to HZW Co. Ltd.

Later on, a MOMAP license file, `hzwtech.lic`, will be sent to you by a sales representative from HZW Co. Ltd., you can simply copy the license file to `$MOMAP_ROOT/license` directory.

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 Co. Ltd. for support.