XtalOpt Installation Guide

Release 9.0

Generated by Doxygen 1.8.9.1

Contents

1 Installation for Linux

1.1 Dependencies

The following dependencies can be installed from the package manager of most linux distributions:

- `cmake` (and optionally the ncurses GUI, ccmake) $>= 2.6$

- `Qt4` $>= 4.6.0$

- `Eigen` $>= 2$

- `git`, any version

If you wish to enable SSH (default), you will also need:

- `openssh`, any version

- `libssh`, any version

Using the package manager for your linux distribution, install the dependencies listed above. For example, on Arch Linux, one can use the command

```
pacman -S cmake git eigen glu qt4 libssh openssh
```

On Ubuntu, one can use the command

```
sudo apt-get cmake qt4-default qt4-dev-tools libeigen-3-dev git libssh-dev zlib1g-dev
```

1.2 Source Installations

Remember to uninstall any non-development installations of OpenBabel and Avogadro before installing the development versions.

1.2.1 OpenBabel

First, the development version of OpenBabel must be installed from source. These instructions will build and install the packages in your user's $HOME directory.

Change to your users home directory:

```
cd ~
```

Make a directory to hold the source code and then enter it:

```
mkdir src
cd src
```

Check out the OpenBabel trunk sources:

```
git clone git://github.com/openbabel/openbabel.git
```

Once the above command completes, make a build subdirectory and enter it:

```
mkdir openbabel/build
cd openbabel/build
```

Configure OpenBabel:

```
cmake .. -DCMAKE_INSTALL_PREFIX=$HOME
```

Compile and install:

```
make -j3
make install
```

OpenBabel should now be installed.

1.2.2 Avogadro

Next, Avogadro must be installed.

First, change to the source directory created earlier:

```
cd $HOME/src
```

Check out the Avogadro branch from GitHub:

```
git clone git://github.com/cryos/avogadro.git
```

Just like with OpenBabel, make a build directory and enter it:

```
mkdir avogadro/build
cd avogadro/build
```

Configure, build, and install Avogadro:

```
cmake .. -DOPENBABEL2_INCLUDE_DIR=$HOME/include/openbabel-2.0 -DOPENBABEL2_LIBRARIES=$HOME/lib/libopenbabel
    .so -DOPENBABEL2_VERSION_MET=true -DOPENBABEL_IS_NEWER_THAN_2_2_99=true -DENABLE_PYTHON=false -
    DCMAKE_INSTALL_PREFIX=$HOME
make -j3
make install
```

Avogadro should now be installed.

1.2.3   XtalOpt

Installing XtalOpt from source is very similar to installing OpenBabel and Avogadro. Once again, change to your source directory:

```
cd $HOME/src
```

Check out the stable branch of the XtalOpt sources:

```
git clone -b stable git://github.com/xtalopt/XtalOpt.git xtalopt
```

Make a build directory and enter it:

```
mkdir xtalopt/build
cd xtalopt/build
```

Configure, build, and install:

```
cmake .. -DOPENBABEL2_INCLUDE_DIR=$HOME/include/openbabel-2.0 -DOPENBABEL2_LIBRARIES=$HOME/lib/libopenbabel
    .so -DOPENBABEL2_VERSION_MET=true -DOPENBABEL_IS_NEWER_THAN_2_2_99=true -DCMAKE_INSTALL_PREFIX=$HOME
make -j3
make install
```

Note: if you would like to install RandomDock, simply add -DENABLE_RANDOMDOCK=1 to the cmake command.

Note: if you see errors like

```
/usr/bin/ld: cannot find -lbsdyengine
/usr/bin/ld: cannot find -lnavigatetool
/usr/bin/ld: cannot find -lelementcolor
```

during the compilation, follow the instructions here.

Note: if you need to use Kerberos authentication to establish a SSH connection to the remote server, the libssh library used by XtalOpt will not work. There is a workaround for Linux (and possibly Mac) users, which will call the command line ssh/scp commands to communicate with the remote cluster. This can be enabled by adding -DUSE_CLI_SSH=true to the cmake command above. This ssh backend will not prompt for a password, and expects the ssh commands to "just work". Passwordless ssh logins can be enabled using the ssh-copy-id command.

XtalOpt is now installed.

1.3   Test the installation

To use XtalOpt, you need to run the avogadro executable installed above. There are two ways to do this:

- Run $HOME/bin/avogadro from a terminal, or

- Add $HOME/bin to your $PATH environment variable and then just run avogadro.

Once Avogadro is running, check for "XtalOpt" in the "Extensions" menu. If you see it, the installation completed successfully.

2   Installation for Mac OS X

2.1   Dependencies

First, and foremost, Mac OS X users must install Xcode to begin compiling the following programs.

The following dependencies can be installed from the package manager <a href="https://www.macports.org">Ma

- `cmake` (and optionally the ncurses GUI, ccmake) $>=$ 2.6

- `Qt` $>=$ 4.6.0

- `Eigen` $>=$ 2

- `git`, any version

If you wish to enable SSH (default), you will also need:

- `libssh`, any version

Using the package manager for your mac distribution, install the dependencies listed above. For example, using MacPorts,

```
port install cmake git eigen qt4-mac cairo libssh
```

or using Homebrew,

```
brew install cmake git eigen qt cairo libssh
```

2.2 Source Installations

Remember to uninstall any non-development installations of OpenBabel and Avogadro before installing the development versions.

2.2.1 OpenBabel

First, the development version of OpenBabel must be installed from source. These instructions will build and install the packages in your user's $HOME directory.

Change to your users home directory:

```
cd ~
```

Make a directory to hold the source code and then enter it:

```
mkdir src
cd src
```

Check out the OpenBabel trunk sources:

```
git clone git://github.com/openbabel/openbabel.git
```

Once the above command completes, make a build subdirectory and enter it:

```
mkdir openbabel/build
cd openbabel/build
```

Configure OpenBabel:

```
cmake .. -DCMAKE_CXX_FLAGS=-stdlib=libstdc++ -DCMAKE_INSTALL_PREFIX=$HOME -DBUILD_GUI=FALSE
```

Compile and install:

```
make -j3
make install
```

OpenBabel should now be installed.

2.2.2 Avogadro

Next, Avogadro must be installed.

First, change to the source directory created earlier:

```
cd $HOME/src
```

Check out Avogadro from GitHub:

```
git clone git://github.com/cryos/avogadro.git
```

Just like with OpenBabel, make a build directory and enter it:

```
mkdir avogadro/build
cd avogadro/build
```

Configure, build, and install Avogadro:

```
cmake .. -DCMAKE_CXX_FLAGS=-stdlib=libstdc++ -DOPENBABEL2_INCLUDE_DIR=$HOME/include/openbabel-2.0 -
    DOPENBABEL2_LIBRARIES=$HOME/lib/libopenbabel.4.0.0.dylib -DOPENBABEL2_VERSION_MET=true -
    DOPENBABEL_IS_NEWER_THAN_2_2_99=true -DENABLE_PYTHON=false -DCMAKE_INSTALL_PREFIX=$HOME
make -j3
make install
```

Avogadro should now be installed.

2.3 XtalOpt

Installing XtalOpt from source is very similar to installing OpenBabel and Avogadro. Once again, change to your source directory:

```
cd $HOME/src
```

Check out the stable branch of the XtalOpt sources:

```
git clone -b stable git://github.com/dlonie/XtalOpt.git xtalopt
```

Make a build directory and enter it:

```
mkdir xtalopt/build
cd xtalopt/build
```

Configure, build, and install:

```
cmake .. -DCMAKE_CXX_FLAGS=-stdlib=libstdc++ -DOPENBABEL2_INCLUDE_DIR=$HOME/include/openbabel-2.0 -
    DOPENBABEL2_LIBRARIES=$HOME/lib/libopenbabel.4.0.0.dylib -DOPENBABEL2_VERSION_MET=true -
    DOPENBABEL_IS_NEWER_THAN_2_2_99=true -DCMAKE_INSTALL_PREFIX=$HOME
make -j3
make install
```

Note: if you would like to install RandomDock, simply add -DENABLE_RANDOMDOCK=1 to the cmake command.

Note: if you see errors like

```
/usr/bin/ld: cannot find -lbsdyengine
/usr/bin/ld: cannot find -lnavigatetool
/usr/bin/ld: cannot find -lelementcolor
```

during the compilation, follow the instructions here.

Note: if you need to use Kerberos authentication to establish a SSH connection to the remote server, the `libssh` library used by XtalOpt will not work. There is a workaround for Linux (and possibly Mac) users, which will call the command line `ssh/scp` commands to communicate with the remote cluster. This can be enabled by adding `-DUSE_CLI_SSH=true` to the cmake command above. This `ssh` backend will not prompt for a password, and expects the `ssh` commands to "just work". Passwordless `ssh` logins can be enabled using the `ssh-copy-id` command.

XtalOpt is now installed.

2.4 Test the installation

To use XtalOpt, you need to run the avogadro executable installed above. There are two ways to do this:

- Run `/Applications/Avogadro.app/Contents/MacOS/Avogadro` from a terminal, or

- Open Finder and run Avogadro in `/Applications`.

Once Avogadro is running, check for "XtalOpt" in the "Extensions" menu. If you see it, the installation completed successfully.

3 Installation for Windows

3.1 Instructions

1. Download the Windows .exe installer here.

2. Follow the instructions to install Avogadro with the XtalOpt extension.

3. Run the program.