Setting Up THAMES v2.5 Input

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Contents

This document provides guidance on how to build THAMES on an Apple computer running Mac OS. Very similar instructions should apply to Windows and especially to Linux computers. The build process from scratch is somewhat complicated due to the need to build and install the GEMS3K standalone library and the GEM-Selektor software.

1 Software Requirements

The following software must be installed and running properly on your computer to build and install all the components:

- Git software versioning system.
- Cmake version 3.0 or later.
- A C++11 compiler. This document will assume the Gnu C/C++ compiler suite with full support for C++11.

[1]Special thanks to Dr. Dmitrii Kulik who provided invaluable guidance for building GEMS3K and GEM-Selektor.

- Doxygen version 1.18.13 or later. This is needed only for generating the documentation.
- (Optional) LaTeXtypesetting software. This is needed only for building the PDF versions of the documentation. A recent installation of TeXLive will suffice.
- (For Linux) The packages build-essentials, libx11-xcb-dev, and libglu1-mesa-dev. These can be installed on Linux using a command like `sudo apt-get install build-essentials`. On Mac OS, the first two should not need to be installed, but mesa can be installed using Macports or Homebrew, for example `sudo port install mesa` when using Macports.

This document will assume that all of these packages have been installed already.

2 Downloading the Software

Create a working directory somewhere in your home path. For this document, the working directory will be called `$WORKDIR`. You should substitute to the path to your working directory everywhere you see that.

The remainder of these instructions require that you enter commands on the command line (the Terminal app on Mac OS, for example). These commands will be typeset in monospace font to distinguish them from other instructions.

2.1 GEMS3K Standalone Library

1. `cd $WORKDIR`
2. `mkdir gitGEMS`
3. `cd gitGEMS`
4. `mkdir standalone`
5. `cd standalone`
6. `git clone https://bitbucket.org/gems4/gems3k.git .`

2.2 GEM-Selektor

1. `cd $WORKDIR/gitGEMS`
2. `mkdir GEMS3GUI`
3. `cd GEMS3GUI`
4. `git clone https://bitbucket.org/gems4/gems3gui.git .`

2.3 THAMES 2.5

If you already have THAMES installed from github and you want to keep any local changes you have made, then go to the directory where you installed it and execute these commands:

1. git stash
2. git pull

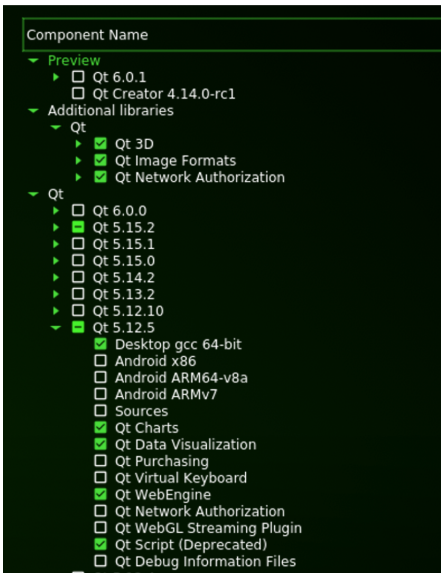
The first command stashes away your local changes so they won't be lost. The second command pulls all the updates from the remote repository. Later, if you want to put your local changes back into the updated version, you can run the command `git stash pop`

On the other hand, if you have never installed THAMES on your computer, then follow these steps:

1. `cd $WORKDIR`
2. `mkdir THAMES`
3. `cd THAMES`
4. `git clone https://github.tamu.edu/jwbullard/THAMES.git .`

2.4 Qt

1. `cd $WORKDIR`
2. `mkdir Qt`
3. Download the Qt software version 5.12.5 (community) for Gnu C++ from https://qt.io into the Qt directory you just made. Use the settings shown in the figure.



3 Build and Install GEMS3K Standalone Library

First, there is one tweak that must be made to the downloaded version of GEMS3K so that longer phase nammes can be used (this is needed when working with the cemdata18 database). You can apply that tweak with the following command:

1. `/bin/cp $WORKDIR/THAMES/src/GEMS3K-mods/*.h $WORKDIR/gitGEMS/standalone/GEMS3K/.`

If you have administrator privileges on your computer (Mac or Linux), then these commands will install the library:

1. `cd $WORKDIR/gitGEMS/standalone`
2. `sudo ./install.sh`

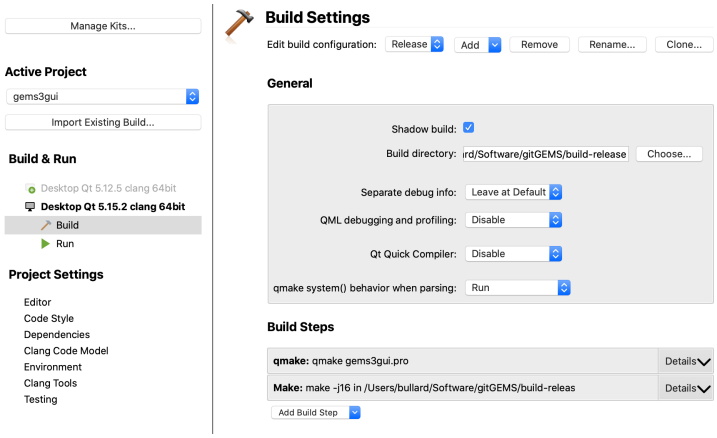
If you do not have administrator privileges, then you will need to work with your IT help desk to get this installed.

4 Build and Install GEM-Selektor

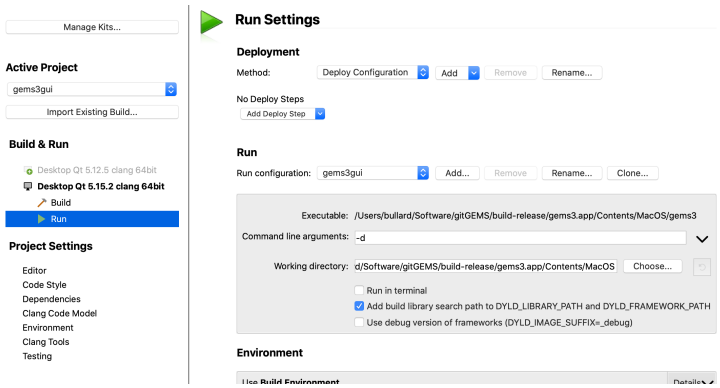
Start up Qt. On Linux, the Qt executable is in `$WORKDIR/Qt/Tools/QtCreator/bin/` On a Mac, it is easiest to just use the Finder, navigate to `$WORKDIR/Qt`, and then double-click on the "Qt Creator" app.

From within the QtCreator Software, open the project `$WORKDIR/gitGEMS/GEMS3GUI/gems3gui.pro`. This step may take some time to complete. The progress will be shown in a small window. Wait until it is finished.

Click on the Build item in the sidebar to set the Build settings as shown in the figure:



Next, click on the Run item in the sidebar to set the Runtime settings as shown in the figure:



Next, build the GEM-Selektor from within Qt by clicking on the Build icon (looks like a hammer). This could take a while to build. When it is finished, check the output log to make sure there are no fatal errors. Multiple warnings are okay, though. If you configured the build settings correctly, this build step will create a new directory, `$WORKDIR/gitGEMS/build-release`

4.1 One Extra Step for a Mac

On a Mac, you now need to go to the command line and run this command:

```
/bin/cp -R $WORKDIR/gitGEMS/GEMS3GUI/Resources \\
    $WORKDIR/gitGEMS/build-release/Contents/gems3.app/Contents/.
```

4.2 Install Third-Party Data Repositories

Make sure that GEM-Selektor is not running for this step. Any third-party thermodynamic databases, such as Cemdata18 or Mines, should be copied into their new

location, which is

`$WORKDIR/gitGEMS/build-release/gems3.app/Contents/Resources/DB.default`

If you have a previous version of GEM-Selektor installed on your computer with the third-party libraries already there, you can just copy the contents of your old DB.default directory to this new location.

4.3 Test GEM-Selektor

You should now be able to run GEM-Selektor from within Qt by clicking on the Run icon (looks like a green triangle pointing to the right).

5 Build and Install THAMES

If all the previous steps have been executed successfully, installing THAMES should be pretty straightforward.

1. `cd $WORKDIR/THAMES/build`
2. `cmake ..`
3. `make`
4. `make install`

The last step will put the thames and vcctl2thames executables into the directory

`$WORKDIR/THAMES/bin`