Setting Up THAMES v2.5 Input

Jeffrey W. Bullard[1]

2024-03-13 14:46:02-05:00

Contents

This document provides guidance on how to build THAMES on various operating systems 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. Separate sections are given for Mac OS, Linux and Windows.

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

1 Mac OS

1.1 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.
- 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.

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

1.2 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 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 or iTerm2). These commands will be typeset in monospace font to distinguish them from other instructions.

1.2.1 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. `git clone https://github.tamu.edu/jwbullard/THAMES.git`

Please contact the developer if you discover that GitHub prevents you from cloning the repository. You may need to be added as a collaborator.

1.2.2 GEM-Selektor

GEM-Selektor is only needed to create basic thermodynamic input files for THAMES. The downloadable binaries for GEM-Selektor can be found at https://gems.web.psi.ch/GEMS3/downloads/index.html.

The installer is simple to use. Double-clicking on it will open a window from which you can just drag the gems3k application to where you want it to reside. For convenience, it is helpful to put it somewhere within your own home folder and to make sure that the folder is also in your 'PATH'. For these instructions, we will call this folder `PathToGems`. You should substitute the actual path to this folder on your computer in these instructions.

1.2.3 Install GEM-Selektor Third-Party Thermodynamic Databases

You will need *at a minimum* the Cemdata18 database, which is already a part of the THAMES git repository.

Next, ensure that GEM-Selektor is not running. Navigate to the GEM-Selektor DB.default folder using either the command line or the Finder:

From the command line:

```
cp $WORKDIR/THAMES/src/Cemdata18.01/*
↪  PathToGEMS/gems3.app/Contents/Resources/DB.default/.
```

Using the Finder:

1. Navigate to the folder `PathToGems`
2. Right-click on `gems3` icon, and select "Show Package Contents".
3. Continue navigating within the package contents to `Contents/Resources/DB.default`
4. In a separate Finder window, navigate into to the folder `WORKDIR/THAMES/src/Cemdata18.01/` and drag all the contents of that folder into the `DB.default` folder of the gems3 app from step 3 above.

1.3 Build and Install GEMS3K Standalone Library

These commands will install the library:

1. `cd $WORKDIR/THAMES/src/GEMS3K-standalone`
2. `./install.sh`

1.4 Test GEM-Selektor

You should now be able to run GEM-Selektor by double-clicking on the "GEMSelektor" icon wherever you installed it.

1.5 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`

2 Linux

Installation and use of THAMES has not been thoroughly tested on Linux computers. Please alert the developer of any changes to the instructions that you discovered to enable successful installation.

2.1 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.
- 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.
- 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`.

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

2.2 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 the path to your working directory everywhere you see that.

The remainder of these instructions require that you enter commands on the command line. These commands will be typeset in monospace font to distinguish them from other instructions.

2.2.1 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. `git clone https://github.tamu.edu/jwbullard/THAMES.git`

Please contact the developer if you discover that GitHub prevents you from cloning the repository. You may need to be added as a collaborator.

2.2.2 GEM-Selektor

GEM-Selektor is only needed to create basic thermodynamic input files for THAMES. The downloadable binaries for GEM-Selektor can be found at https://gems.web.psi.ch/GEMS3/downloads/index.html. Follow the installation instructions.

2.2.3 Install Third-Party Data Repositories

You will need *at a minimum* the Cemdata18 database, which is already a part of the THAMES git repository.

Next, ensure that GEM-Selektor is not running. Navigate to the GEM-Selektor DB.default folder using the command line:

```
cp $WORKDIR/THAMES/src/Cemdata18.01/*
↪  PathToGEMS/gems3.app/Contents/Resources/DB.default/.
```

2.3 Build and Install GEMS3K Standalone Library

These commands will install the library:

1. `cd $WORKDIR/THAMES/src/GEMS3K-standalone`
2. `sudo ./install.sh`

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

2.4 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`

3 Windows

3.1 MSYS installation

1. Direct link to the installer is https://github.com/msys2/msys2-installer/releases/download/2022-06-03/msys2-x86_64-20220603.exe
2. Use default installation folder
3. Start MSYS2 MinGW x64 from the Start menu, then execute the command `pacman -Syu`
4. The MSYS window will close automatically after that command.
5. Start MSYS2 MSYS from the Start menu, then execute the following commands:
   (a) `pacman -Syu`
   (b) `pacman -S --needed base-devel mingw-w64-x86_64-toolchain`
   (c) `pacman -S mingw-w64-x86_64-cmake`
   (d) `pacman -S mingw-w64-x86_64-make`
   (e) `pacman -S git`
6. Close the MSYS window

3.2 Download THAMES source code

Start MSYS2 MinGW x64 from the Start menu and execute the command

```
git clone https://github.com/jwbullard/THAMES.git
```

You will need a username and password for GitHub. Contact the developer if you are unable to to clone the repository once you have established your GitHub credentials. You may need to be added to the project as a collaborator.

3.3 GEM-Selektor Installation

GEM-Selektor is only needed to create basic thermodynamic input files for THAMES. The downloadable binaries for GEM-Selektor can be found at https://gems.web.psi.ch/GEMS3/downloads/index.html. Follow the installation instructions.

3.3.1 Install Third-Party Data Repositories

You will need *at a minimum* the Cemdata18 database, which is already a part of the THAMES git repository.

Next, ensure that GEM-Selektor is not running. In one Windows File Explorer window, navigate to the GEM-Selektor DB.default folder. It should be found at

```
C:\Users\"your name"\GEMS39\Gems3-app\Resources\DB.default
```

In another Windows File explorer window, navigate to

```
WORKDIR/THAMES/src/Cemdata18.01
```

Select all the files of this folder and drag them to the DB.default folder in the other File Explorer window above.

3.4 Build GEMS3K-Standalone

Start MSYS MinGW x64 from the Start menu if it is not already open. Within the MSYS window execute the following commands:

1. `cd THAMES/src/GEMS3K-Standalone`
2. `mkdir build`
3. `cd build`
4.
```
cmake .. -G "MinGW Makefiles" -DCMAKE_CXX_FLAGS=-fPIC
↪ -DCMAKE_BUILD_TYPE=Release
↪ -DCMAKE_INSTALL_PREFIX=../Resources
```
5. `/mingw64/bin/mingw32-make.exe`
6. `/mingw64/bin/mingw32-make.exe install`

3.5 Build THAMES

1. `cd ../../../build`
2. ```
   cmake .. -G "MinGW Makefiles" -DCMAKE_BUILD_TYPE=Release
   ↪ -DCMAKE_INSTALL_PREFIX=../bin
   ```
3. `/mingw64/bin/mingw32-make.exe`
4. `/mingw64/bin/mingw32-make.exe install`

3.6 Edit Windows Path

1. Start Edit the System Variables form the Start menu
2. Click "Environment Variables" button
3. Under "System Variables", scroll down until you see Path
4. Select that line, and press "Edit"
5. Edit Environment variable window will come up
6. Press "New"
7. Add `C:\msys64\mingw64\bin` to the bottom
8. OK ⟶ OK ⟶ OK

At this point, the THAMES executable, `thames.exe`, should be under

`C:\msys64\home\<username>\THAMES\bin`
   ```