

# Additional Information for TOUGH3 Installation

## 1. Introduction

TOUGH3 installation uses cmake scripts to perform the compilation of the source codes, which involves download of the dependent libraries, compilations of libraries and TOUGH3 source codes, linking with the libraries, and installation of the software. The dependent libraries include PETSC, AZTEC, Metis, parMetis, BLAS, and LAPACK. Users may face challenging in TOUGH3 installation as it is difficult to get the whole procedures performed successfully. After analyzing the installation cmake scripts and examining the installation problems raised by the users, I realize that the most popular reasons caused installation failure are the installation PETSC, and the configure for linking of dependent libraries. In order to make the TOUGH3 installation more reliable, the following actions have been taken:

- (1) Avoid download of any library package during installation procedure. All required library packages will be provided with the TOUGH3 software package.
- (2) Separate the PETSC installation from the TOUGH3 installation. PETSC must be installed before starting of TOUGH3 installation.
- (3) Remove unnecessary library installations and link.
- (4) Debug the cmake scripts, fix the potential bugs.

The new TOUGH3 package is expected to be more easy to install.

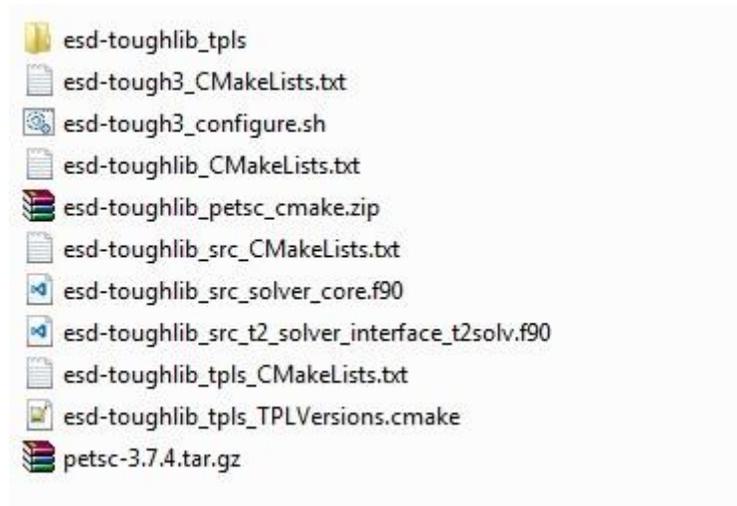
## 2. Preparation of the installation files (only required for using original installation package)

The original TOUGH3 Ver 1.0 installation package has following directory structure:

```
1 TOUGH3-Codes
  2.1 esd-tough3
    2.1.1 cmake
    2.1.2 manuals
    2.1.3 samples
    2.1.4 scripts
    2.1.5 src
      2.5.1 aztec_interface
      .....
      2.5.6 t2-solver_interface
    2.1.6 tpls
  2.2 esd-toughlib
    2.2.1 cmake
    2.2.2 src
    2.2.3 tests
    2.2.4 tpls
```

Figure 1. TOUGH3 file directory structure

Many files in the installation package must be replaced and several additional files must be included. Following is the list of files needed for new installation:



**Figure 2. list of the new installation files**

These files must be copied into or replace the files in original installation packages:

- (1) Replace the TOUGH3-Codes/esd-tough3/CMakeLists.txt by esd-tough3\_CMakeLists.txt
- (2) Replace the TOUGH3-Codes/esd-tough3/configure.sh by esd-tough3\_configure.sh
- (3) Replace the TOUGH3-Codes/esd-toughlib/CMakeLists.txt by esd-toughlib\_CMakeLists.txt
- (4) Unzip file esd-toughlib\_petsc\_cmake.zip in TOUGH3-Codes/esd-toughlib (2.2, see Figure 1)
- (5) Copy the files under folder /esd-toughlib\_tpls/ to TOUGH3-Codes/esd-toughlib/tpls (2.2.4, see Figure 1)
- (6) Replace the TOUGH3-Codes/esd-toughlib/tpls/CMakeLists.txt by esd-toughlib\_tpls\_CMakeLists.txt
- (7) Replace the TOUGH3-Codes/esd-toughlib/TPLVersions.cmake by esd-toughlib\_tpls\_TPLVersions.cmake
- (8) Replace the TOUGH3-Codes/esd-toughlib/src/CMakeLists.txt by esd-toughlib\_src\_CMakeLists.txt
- (9) Replace the TOUGH3-Codes/esd-toughlib/src/ solver\_core.f90 by esd-toughlib\_src\_solver\_core.f90
- (10) Replace the TOUGH3-Codes/esd-toughlib/src/ t2\_solver\_interface/t2solv.f90 by esd-toughlib\_src\_t2\_solver\_interface\_t2solv.f90

The above file replacements are done by renaming the provided source file to the same name as the target file and then copying into the target folder. If you are using the updated installation package, you can skip the steps discussed in this section.

### 3. Installation of PETSC

It seems the newer version of PETSC does not work for TOUGH3. Original readme file suggests using version 3.7.x. I have included v3.7.4 in the file package. If you like to try different versions, you can download them online. PETSC has a large user community. There is a lot information regarding PETSC installation online. PETSC can be installed at anywhere. I would suggest installing at your home directory, ~/petsc. Following several options for configuring the PETSC installation may be helpful for late TOUGH3 installation:

--with-debugging=0, optimized library for better performance.

--download-mpich, if no MPI installed in your computer.

---download-fblaslapack, if no BLAS and LAPACK installed in your computer

--with-shared-libraries=0, will build static library.

--PETSC\_ARCH=arch-t3, TOUGH3 default arch. If you use it, you do not need to specify the PETSC\_ARCH when configuring TOUGH3 installation.

Following is the steps for PETSC installation:

(1) Copy file petsc-3.7.4.tar.gz to you home directory:

```
cp ./petsc-3.7.4.tar.gz ~
```

(2) Unzip and untar the compressed file:

```
cd ~
```

```
tar -xf ./petsc-3.7.4.tar.gz
```

(3) Configure and build PETSC:

```
cd petsc-3.7.4
```

```
./configure --with-debugging=0 --with-shared-libraries=0 --PETSC_ARCH=arch-t3
```

```
make
```

You need to find out the PETSC directory (*PETSC\_DIR*, can be found by typing *pwd* in ~/petsc-3.7.4) and name of build directory (*PETSC\_ARCH*), which is needed in TOUGH3 installation.

If you have difficulty to install PETSC, do not worry. We still have AZTEC which can also perform parallel solving linear equations for TOUGH3.

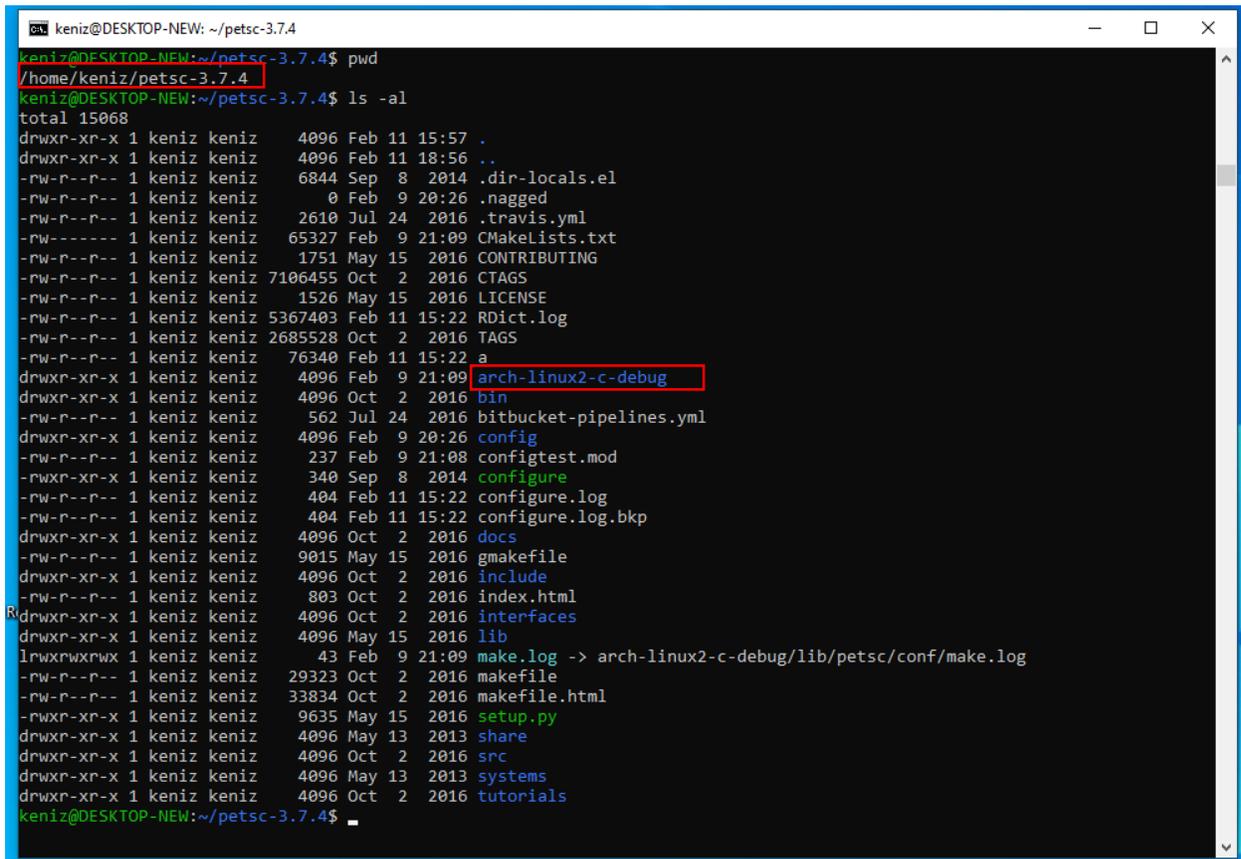
### 4. Installation of TOUGH3

Once you successfully install PETSC, compilation of TOUGH3 should be easy. You may follow the procedure in the readme file provided in original TOUGH3 package to setup basic installation requirements. With the new installation files, the download of third-party libraries is avoided. All library packages have been included in the installation package at directory 2.2.4 (see Figure 1). If you want to use different version of the software, you can save new file at directory 2.2.4 and edit “TPLVersions.cmake” for using corresponding version of the library. In

addition, with the new installation files, you can avoid installation of unnecessary libraries, for example:

- (1) Compilation for series version, no any other third-party library required.
- (2) Compilation for parallel version with AZTEC solver only, PETSC compilation can be avoided.

Compilation and installation can be done by running the `configure.sh` script in the same way as described in original readme file, except two additional parameters, `petsc-dir` and `petsc-arch` must be provided. The parameter `petsc-dir` specifies the installed PETSC directory and `petsc-arch` gives the build name. The build name is the name of PETSC build directory. The default PETSC build directory can be found in the PETSC installation directory.



```
keniz@DESKTOP-NEW: ~/petsc-3.7.4
keniz@DESKTOP-NEW:~/petsc-3.7.4$ pwd
/home/keniz/petsc-3.7.4
keniz@DESKTOP-NEW:~/petsc-3.7.4$ ls -al
total 15068
drwxr-xr-x 1 keniz keniz 4096 Feb 11 15:57 .
drwxr-xr-x 1 keniz keniz 4096 Feb 11 18:56 ..
-rw-r--r-- 1 keniz keniz 6844 Sep 8 2014 .dir-locals.el
-rw-r--r-- 1 keniz keniz 0 Feb 9 20:26 .nagged
-rw-r--r-- 1 keniz keniz 2610 Jul 24 2016 .travis.yml
-rw-r--r-- 1 keniz keniz 65327 Feb 9 21:09 CMakeLists.txt
-rw-r--r-- 1 keniz keniz 1751 May 15 2016 CONTRIBUTING
-rw-r--r-- 1 keniz keniz 7106455 Oct 2 2016 CTAGS
-rw-r--r-- 1 keniz keniz 1526 May 15 2016 LICENSE
-rw-r--r-- 1 keniz keniz 5367403 Feb 11 15:22 RDict.log
-rw-r--r-- 1 keniz keniz 2685528 Oct 2 2016 TAGS
-rw-r--r-- 1 keniz keniz 76340 Feb 11 15:22 a
drwxr-xr-x 1 keniz keniz 4096 Feb 9 21:09 arch-linux2-c-debug
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 bin
-rw-r--r-- 1 keniz keniz 562 Jul 24 2016 bitbucket-pipelines.yml
drwxr-xr-x 1 keniz keniz 4096 Feb 9 20:26 config
-rw-r--r-- 1 keniz keniz 237 Feb 9 21:08 configtest.mod
-rwxr-xr-x 1 keniz keniz 340 Sep 8 2014 configure
-rw-r--r-- 1 keniz keniz 404 Feb 11 15:22 configure.log
-rw-r--r-- 1 keniz keniz 404 Feb 11 15:22 configure.log.bkp
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 docs
-rw-r--r-- 1 keniz keniz 9015 May 15 2016 gmakefile
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 include
-rw-r--r-- 1 keniz keniz 803 Oct 2 2016 index.html
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 interfaces
drwxr-xr-x 1 keniz keniz 4096 May 15 2016 lib
lrwxrwxrwx 1 keniz keniz 43 Feb 9 21:09 make.log -> arch-linux2-c-debug/lib/petsc/conf/make.log
-rw-r--r-- 1 keniz keniz 29323 Oct 2 2016 makefile
-rw-r--r-- 1 keniz keniz 33834 Oct 2 2016 makefile.html
-rwxr-xr-x 1 keniz keniz 9635 May 15 2016 setup.py
drwxr-xr-x 1 keniz keniz 4096 May 13 2013 share
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 src
drwxr-xr-x 1 keniz keniz 4096 May 13 2013 systems
drwxr-xr-x 1 keniz keniz 4096 Oct 2 2016 tutorials
keniz@DESKTOP-NEW:~/petsc-3.7.4$
```

Figure 3. PETSC installation directory and arch

Figure 3 show an example of PETSC installation, which has `--petsc-dir= /home/keniz/petsc-3.7.4` and `--petsc-arch=arch-linux2-c-debug`. Following gives the examples of different installation options:

- (1) For parallel version install with PETSC and AZTEC linear solvers

```
./configure.sh --build-type=RELEASE --eos=$EOS_NUM --no-x11 --petsc-dir=$PETSC-DIR
--petsc-arch=$PETSC-ARCH.
```

For example, installation of ECO2N with the PETSC installed as Figure 3, the command will be:

```
./configure.sh --build-type=RELEASE --eos=eco2n --no-x11 --petsc-dir=/home/keniz/petsc-3.7.4  
--petsc-arch=arch-linux2-c-debug
```

If you use *arch-t3* as the build name during installation of PETSC, you do not need specifying *--petsc-arch* parameter for the configure.

(2) For parallel version install with AZTEC linear solver only

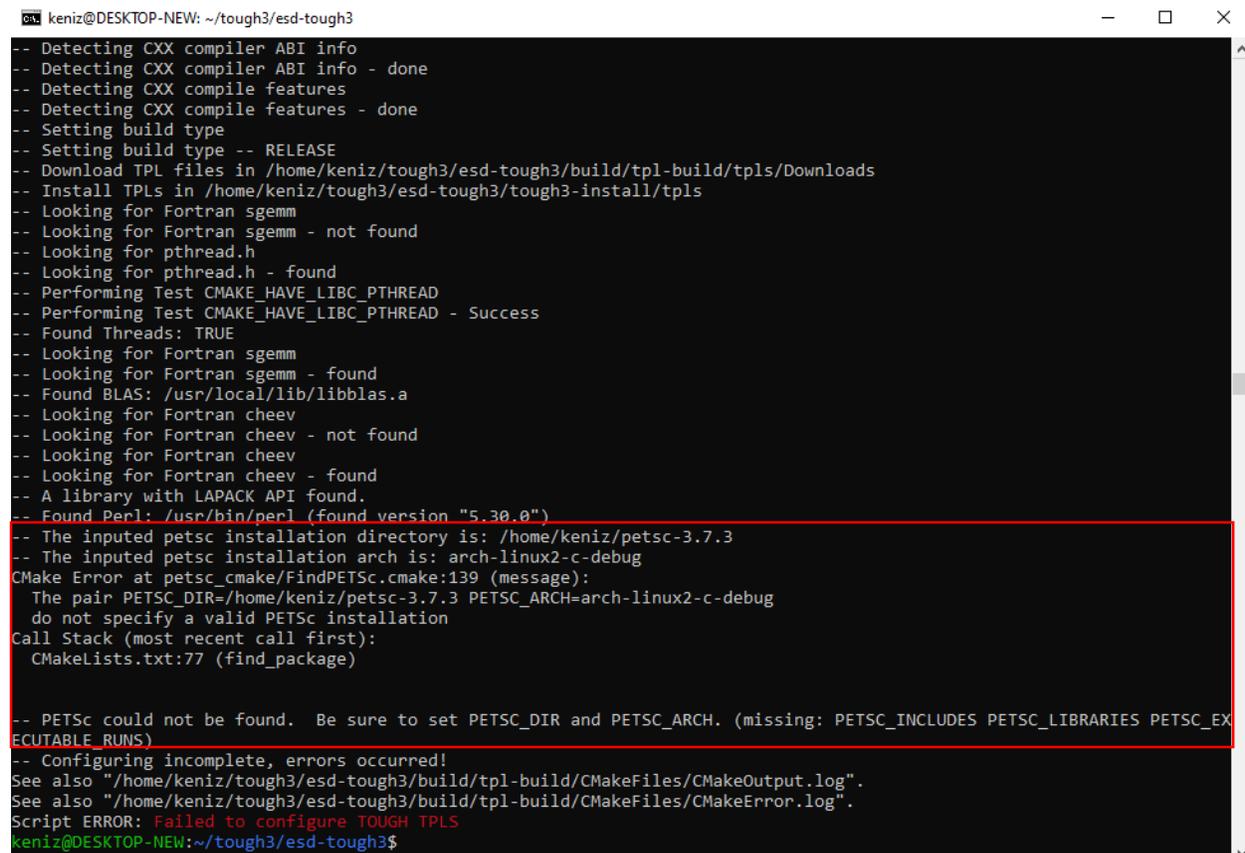
If installation of PETSC was fail and you give up, you are still able to run the parallel simulations with AZTEC solvers. The *use-petsc* parameter must be specified with 0 in order to avoid usage of PETSC.

```
./configure.sh --build-type=RELEASE --eos=$EOS_NUM --no-x11 --use-petsc=0
```

(3) For series version installation

```
./configure.sh --build-type=RELEASE --eos=$EOS_NUM --no-x11 --use-mpi=0
```

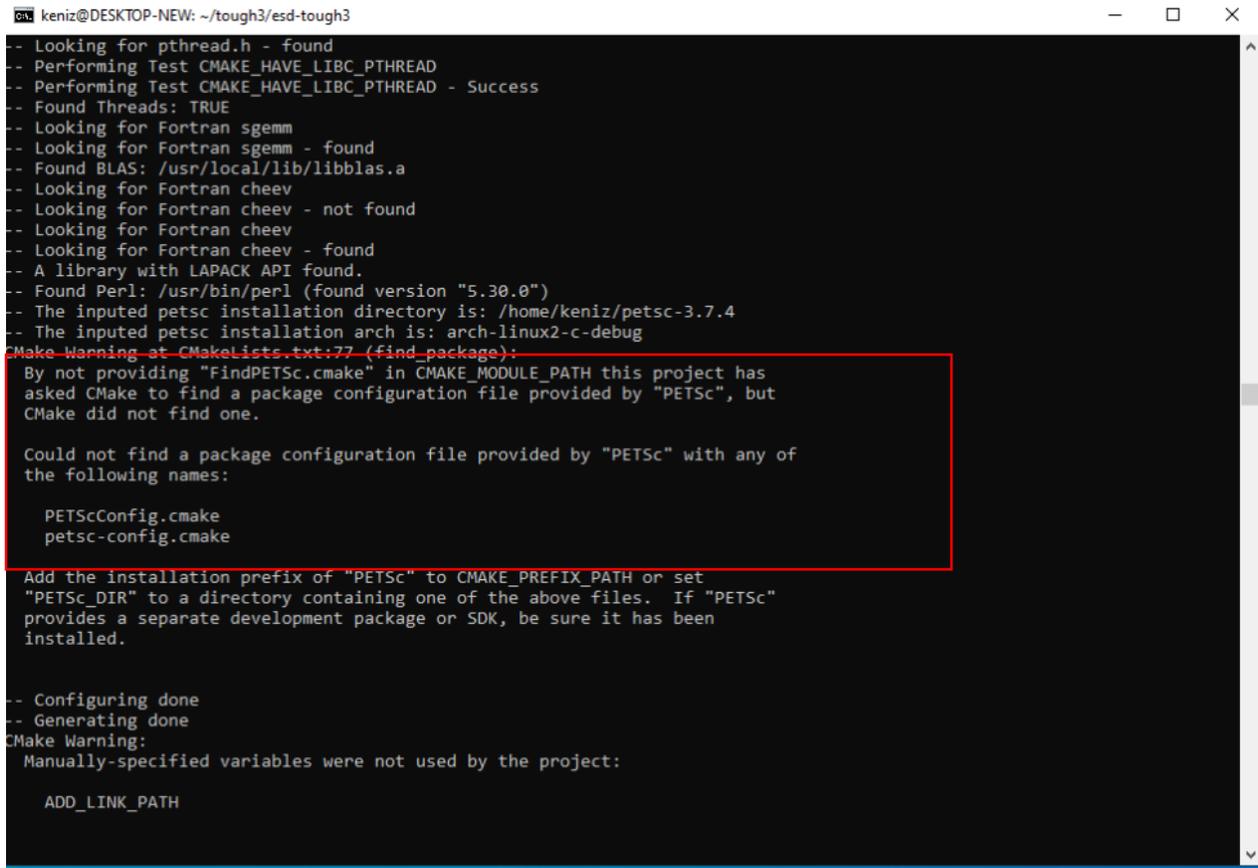
The most popular failure reason for unsuccessful installation is the mistakes in specifying the *--petsc-dir* and *--petsc-arch*. If you see following messages (Figure 4) during installation, it means that the two parameters or one of them are wrong.

A terminal window screenshot showing the output of a configure script. The window title is 'keniz@DESKTOP-NEW: ~/tough3/esd-tough3'. The output shows various compiler and library detection steps. A red box highlights the error message: 'CMake Error at petsc\_cmake/FindPETSc.cmake:139 (message): The pair PETSC\_DIR=/home/keniz/petsc-3.7.3 PETSC\_ARCH=arch-linux2-c-debug do not specify a valid PETSc installation'. Below this, it shows the call stack and the final error: '-- PETSc could not be found. Be sure to set PETSC\_DIR and PETSC\_ARCH. (missing: PETSC\_INCLUDES PETSC\_LIBRARIES PETSC\_EXECUTABLE\_RUNS)'. The prompt at the bottom is 'keniz@DESKTOP-NEW:~/tough3/esd-tough3\$'.

```
keniz@DESKTOP-NEW: ~/tough3/esd-tough3  
-- Detecting CXX compiler ABI info  
-- Detecting CXX compiler ABI info - done  
-- Detecting CXX compile features  
-- Detecting CXX compile features - done  
-- Setting build type  
-- Setting build type -- RELEASE  
-- Download TPL files in /home/keniz/tough3/esd-tough3/build/tpl-build/tpls/Downloads  
-- Install TPLs in /home/keniz/tough3/esd-tough3/tough3-install/tpls  
-- Looking for Fortran sgemm  
-- Looking for Fortran sgemm - not found  
-- Looking for pthread.h  
-- Looking for pthread.h - found  
-- Performing Test CMAKE_HAVE_LIBC_PTHREAD  
-- Performing Test CMAKE_HAVE_LIBC_PTHREAD - Success  
-- Found Threads: TRUE  
-- Looking for Fortran sgemm  
-- Looking for Fortran sgemm - found  
-- Found BLAS: /usr/local/lib/libblas.a  
-- Looking for Fortran cheev  
-- Looking for Fortran cheev - not found  
-- Looking for Fortran cheev  
-- Looking for Fortran cheev - found  
-- A library with LAPACK API found.  
-- Found Perl: /usr/bin/perl (found version "5.30.0")  
-- The inputed petsc installation directory is: /home/keniz/petsc-3.7.3  
-- The inputed petsc installation arch is: arch-linux2-c-debug  
CMake Error at petsc_cmake/FindPETSc.cmake:139 (message):  
  The pair PETSC_DIR=/home/keniz/petsc-3.7.3 PETSC_ARCH=arch-linux2-c-debug  
  do not specify a valid PETSc installation  
Call Stack (most recent call first):  
  CMakeLists.txt:77 (find_package)  
  
-- PETSc could not be found. Be sure to set PETSC_DIR and PETSC_ARCH. (missing: PETSC_INCLUDES PETSC_LIBRARIES PETSC_EX  
ECUTABLE_RUNS)  
-- Configuring incomplete, errors occurred!  
See also "/home/keniz/tough3/esd-tough3/build/tpl-build/CMakeFiles/CMakeOutput.log".  
See also "/home/keniz/tough3/esd-tough3/build/tpl-build/CMakeFiles/CMakeError.log".  
Script ERROR: Failed to configure TOUGH TPLS  
keniz@DESKTOP-NEW:~/tough3/esd-tough3$
```

#### Figure 4. Messages for wrong input of `--petsc-dir` and `--petsc-arch`

Another PETSC related reason causes failure of the installation is that you did not correctly unzip the file `esd-toughlib_petsc_cmake.zip` into `TOUGH3-Codes/esd-toughlib`. If you do it correctly, you should be able to see a folder with name `petsc-cmake` under the directory `TOUGH3-Codes/esd-toughlib`. The error message for this problem is as Figure 5.



```
keniz@DESKTOP-NEW: ~/tough3/esd-tough3
-- Looking for pthread.h - found
-- Performing Test CMAKE_HAVE_LIBC_PTHREAD
-- Performing Test CMAKE_HAVE_LIBC_PTHREAD - Success
-- Found Threads: TRUE
-- Looking for Fortran sgemm
-- Looking for Fortran sgemm - found
-- Found BLAS: /usr/local/lib/libblas.a
-- Looking for Fortran cheev
-- Looking for Fortran cheev - not found
-- Looking for Fortran cheev
-- Looking for Fortran cheev - found
-- A library with LAPACK API found.
-- Found Perl: /usr/bin/perl (found version "5.30.0")
-- The inputted petsc installation directory is: /home/keniz/petsc-3.7.4
-- The inputted petsc installation arch is: arch-linux2-c-debug
CMake Warning at CMakeLists.txt:77 (find_package):
By not providing "FindPETSc.cmake" in CMAKE_MODULE_PATH this project has
asked CMake to find a package configuration file provided by "PETSc", but
CMake did not find one.

Could not find a package configuration file provided by "PETSc" with any of
the following names:

  PETScConfig.cmake
  petsc-config.cmake

Add the installation prefix of "PETSc" to CMAKE_PREFIX_PATH or set
"PETSc_DIR" to a directory containing one of the above files.  If "PETSc"
provides a separate development package or SDK, be sure it has been
installed.

-- Configuring done
-- Generating done
CMake Warning:
  Manually-specified variables were not used by the project:

  ADD_LINK_PATH
```

Figure 5. Message for missing `petsc-cmake`

The installation procedures discussed in this document are supposed to be correct for all linux-like system, including Cygwin.

For more information, contact Kenny at [KZhang@lbl.gov](mailto:KZhang@lbl.gov)