Installing and compiling Albany/LCM and Trilinos on Fedora or SEMS/CEE

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1 Introduction

This document describes the necessary steps to install Albany/LCM and Trilinos on a machine with Fedora Linux or the Linux CEE/SEMS environment. If you want a shortcut, obtain the script install_albany.sh (stored in Albany/doc/LCM/install) and then try

```
./install_albany
```

This will install and build TRILINOS and ALBANY in the current directory. If the script does not complete it will tell you why and with help from this document you will be able to complete the install.

2 Required Packages

The following packages should be installed using the dnf command

blas blas-devel boost boost-devel boost-openmpi boost-openmpi-devel boost-static cmake hdf5 hdf5-devel hdf5-openmpi hdf5-openmpi-devel hdf5-static lapack lapack-devel matio matio-devel netcdf netcdf-devel netcdf-openmpi netcdf-openmpi-devel netcdf-static openmpi openmpi-devel

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```
yaml-cpp
yaml-cpp-devel
environment-modules
gcc-c++
git
```

For example, to install the first package you should type

```
sudo dnf install blas
```

Make sure that all these packages are installed, specially if you create a script to do so. If a package is not installed because of a typo then the compilation will fail.

It may be necessary to logout and login for the module alias from the environment-modules package to become active.

Optional but strongly recommended packages:

```
clang
clang-devel
gitk
```

3 Repository Setup with GitHub

In a web browser go to www.github.com, create an account and set up ssh public keys. If you require push privilges for Albany, email Glen Hansen at gahanse@sandia.gov and let him know that. On the other hand, if you require push privileges for Trilinos, it is best if you contact the Trilinos developers directly. Go to www.trilinos.org for more information.

It is strongly recommended that you join the AlbanyLCM Google group to receive commit notices. Go to groups.google.com/forum/#!forum/albanylcm and join the group. You can also browse the source code at github.com/gahansen/Albany.

4 Directory Structure

In your home directory, create a directory with the name LCM:

```
mkdir LCM
```

Change directory to the newly created one:

cd LCM

Check out the latest version of Trillinos, which is hosted now on GitHub:

```
git clone git@github.com:trilinos/Trilinos.git Trilinos
```

Finally, check out the latest version of Albany:

```
git clone git@github.com:gahansen/Albany.git Albany
```

At this point, the directory structure should look like this:

LCM

- |- Albany
- |- Trilinos

5 Environment Variables

In ~/.bashrc, the following variables are needed:

```
export LCM_DIR=~/LCM
export MODULEPATH=$LCM_DIR/Albany/doc/LCM/modulefiles
```

The LCM_DIR variable should contain the location of the top-level LCM directory.

6 Build Script

Create a symbolic link to the build script LCM/Albany/doc/LCM/build/build.sh to the top-level LCM directory. Make sure that the build script is executable and read only:

```
cd ~/LCM
chmod 0555 build.sh
```

The build.sh script performs different actions according to the name with which it is invoked. This is accomplshed by creating symlinks to build.sh and using them to run it. For example:

- clean.sh will delete all traces of the corresponding build and will create a new configuration script based on the corresponding template.
- config.sh will attempt to configure the build.
- build.sh (original name) will build using cmake.
- test.sh will run the cmake tests.
- update.sh will execute git pull in the package repository, and if combined with dash below, it will send a report of changed files to CDash.
- dash.sh will post the results of ctest to configured CDash site.
- symlinks with combinations of the above (e.g. clean-config-build.sh) will perform the specified actions in sequence. See build.sh for valid sequences.

For example, the following symbolic links will create separate commands for clean up, configuring and testing:

```
ln -s build.sh clean.sh
ln -s build.sh config.sh
ln -s build.sh test.sh
```

They could also be combined for convenience:

```
ln -s build.sh clean-config.sh
ln -s build.sh clean-config-build.sh
ln -s build.sh clean-config-build-test.sh
ln -s build.sh config-build.sh
ln -s build.sh config-build-test.sh
```

There is also a script LCM/Albany/doc/LCM/install/albany-lcm-symlinks.sh that will create the appropriate symbolic links.

7 Parallel Schwarz and DTK

This section applies only if using the Schwarz alternating method in parallel by means of the Data Transfer Kit (DTK). Otherwise it can be safely ignored.

The current parallel implementation of the Schwarz method requires DTK, which is tightly integrated to Trilinos, specifically STK. Go to the the top-level LCM directory and create a symbolic link to the DTK CMake fragment that resides in LCM/Albany/doc/LCM/build, then download the DTK package from:

https://github.com/ORNL-CEES/DataTransferKit/archive/2.0.0.tar.gz. Expand the package inside the TRILINOS directory and rename it:

```
cd ~/LCM
ln -s Albany/doc/LCM/build/dtk-frag.sh .
cd Trilinos
curl -L https://github.com/ORNL-CEES/DataTransferKit/archive/2.0.0.tar.gz -0
tar zxf 2.0.0.tar.gz
mv DataTransferKit-2.0.0 DataTransferKit
```

The configuration scripts will detect the presence of DTK and configure it appropriately. Also, parallel Schwarz will be enabled when compiling Albany.

8 Modules

Modules are used to create different environments for the configuration and compilation of both Albany and Trilinos. To see the available modules that correspond to different thread models, compilers and build types:

module avail

This results in something like:

```
-----/home/amota/LCM/Albany/doc/LCM/modulefiles
                     lcm/sems
                                          pthreads-gcc-small
cuda-gcc-debug
cuda-gcc-mixed
                     lcm/serial
                                          release
cuda-gcc-profile
                     lcm/small
                                          serial-clang-debug
                     lcm/tpls
                                          serial-clang-mixed
cuda-gcc-release
                     mixed
cuda-gcc-small
                                          serial-clang-profile
                     openmp-gcc-debug
debug
                                          serial-clang-release
lcm/cee
                     openmp-gcc-mixed
                                          serial-clang-small
1cm/clang
                     openmp-gcc-profile
                                          serial-gcc-debug
1cm/common
                                          serial-gcc-mixed
                     openmp-gcc-release
1cm/cuda
                     openmp-gcc-small
                                          serial-gcc-profile
lcm/debug
                     openmp-intel-debug
                                          serial-gcc-release
1cm/fedora
                     openmp-intel-mixed
                                          serial-gcc-small
lcm/finalize
                     openmp-intel-profile serial-intel-debug
lcm/gcc
                     openmp-intel-release serial-intel-mixed
lcm/intel
                     openmp-intel-small
                                          serial-intel-profile
lcm/mixed
                     profile
                                          serial-intel-release
1cm/openmp
                     pthreads-gcc-debug
                                          serial-intel-small
lcm/profile
                     pthreads-gcc-mixed
                                          small
lcm/pthreads
                     pthreads-gcc-profile
                     pthreads-gcc-release
lcm/release
```

The naming convention for the *-*-* modules follows the pattern

```
[thread model]-[toolchain]-[build type]
```

The [thread model] option refers to the thread parallelism model that the code will use by means of the KOKKOS package in TRILINOS. Currently the sopported models are: serial that works for all supported compilers, openmp that works with the GCC and Intel toolchains, pthreads that works for all supported compilers, and cuda that is only supported for the GCC toolchain. The installation and configuration of the Cuda framework is complex. Much more detailed information can be found at http://developer.nvidia.com/cuda.

Currently the options for [toolchain] are gcc, clang and intel if the Intel compilers are installed, and for [build type] are debug (includes symbolic information), release (optimization enabled), profile (symbolic information and optimization enabled for profiling), small (minimizes size of executables) and mixed (TRILINOS compiled in release mode and ALBANY compiled in debug mode). The clang toolchain requires installation of the clang and clang-devel packages. The debug, release, profile, small and mixed modules are convenience aliases for

serial-gcc-debug, serial-gcc-release, serial-gcc-profile, serial-gcc-small and serial-gcc-mixed modules, respectively.

Build directories are created within the LCM top-level directory and named according to the loaded module and package specified to the build.sh script, e.g.:

```
albany-build-gcc-release
```

In addition, for Trilinos an install directory similarly named is created at the LCM top-level directory.

9 Configuring and compiling

Assuming that we want to compile with a serial thread model using the gcc tool chain in debug mode, load the appropriate module:

```
module load lcm/fedora
module load serial-gcc-debug
```

For the SEMS/CEE environment, this would be:

```
module load lcm/sems
module load serial-gcc-debug
```

Now first configure and compile Trillinos. Within the top-level LCM directory type:

```
./config-build.sh trilinos [# processors]
```

For example, if you want to build using 16 processors, type:

```
./config-build.sh trilinos 16
```

Finally, repeat the procedure for ALBANY:

```
./config-build.sh albany [# processors]
```

For example, if you want to build a version of the code using 16 processors, type:

```
./config-build.sh albany 16
```

Note that to compile a version of Albany with a specific thread model, toolchain and build type, the corresponding version of Trilinos must exist.

10 After Initial Setup

The procedure described above configures and compiles the code. From now on, configuration is no longer required so you can rebuild the code after any modification by simply using the build.sh script. For example:

```
./build.sh albany 16
```

There are times when it is necessary to reconfigure, for example when adding or deleting files under the LCM/Albany/src/LCM directory. This is generally anounced in the commit notices.

Also, note that both Trilinos and Albany are heavily templetized C++ codes. Building the debug version of Albany requires large amounts of memory because of the huge size of the symbolic information required for debugging. Thus, if the compiling procedure stalls, try reducing the number of processors.

11 Running and Debugging LCM

After building Albany, you might want to run and/or debug the code. Tools were built in Trilinos (decomp, epu, etc.) that are necessary for parallel execution. The environment created by loading the appropriate module

sets the proper paths so that the executables that correspond to the type of build are accessible.

12 Committing Changes and Code Style

ALBANY is a simulation code for researchers by researchers. As such, vibrant development of new and exciting capabilities is strongly encouraged. For these reasons, don't be afraid to commit changes to the master git repository. We only ask that you don't break compilation or testing. So please make sure that the tests pass before you commit changes. Also, follow the development discussion here:

https://github.com/gahansen/Albany/issues

In addition, within LCM we strongly encourage you to follow the C++ Google style guide that can be found at http://google-styleguide.googlecode.com/svn/trunk/cppguide.html. This style is somewhat different to what is currently used in the rest of Albany, but we believe that the Google style is better in that it advocates more style differentiation between the different syntactic elements of C++. This in turn makes reading code easier and helps to avoid coding errors.

The clang-format tool can be used for this. There is a .clang-format file in the Albany/src/LCM directory that conforms to the C++ Google conding standard. Thus, all that is needed to reformat a source file in place is the command:

clang-format -i [source file name]