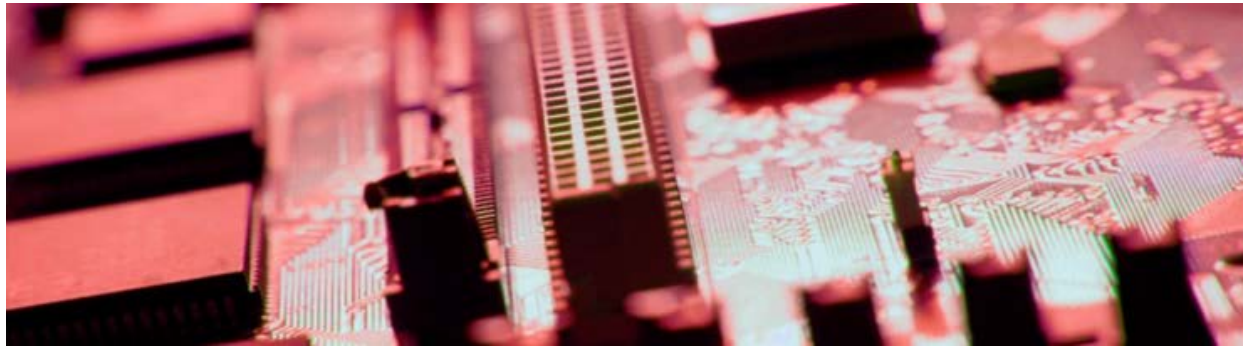

LCI workshop
on high performance clustered computing

Linux Cluster Institute:

Lmod, A Modern Environment Module System

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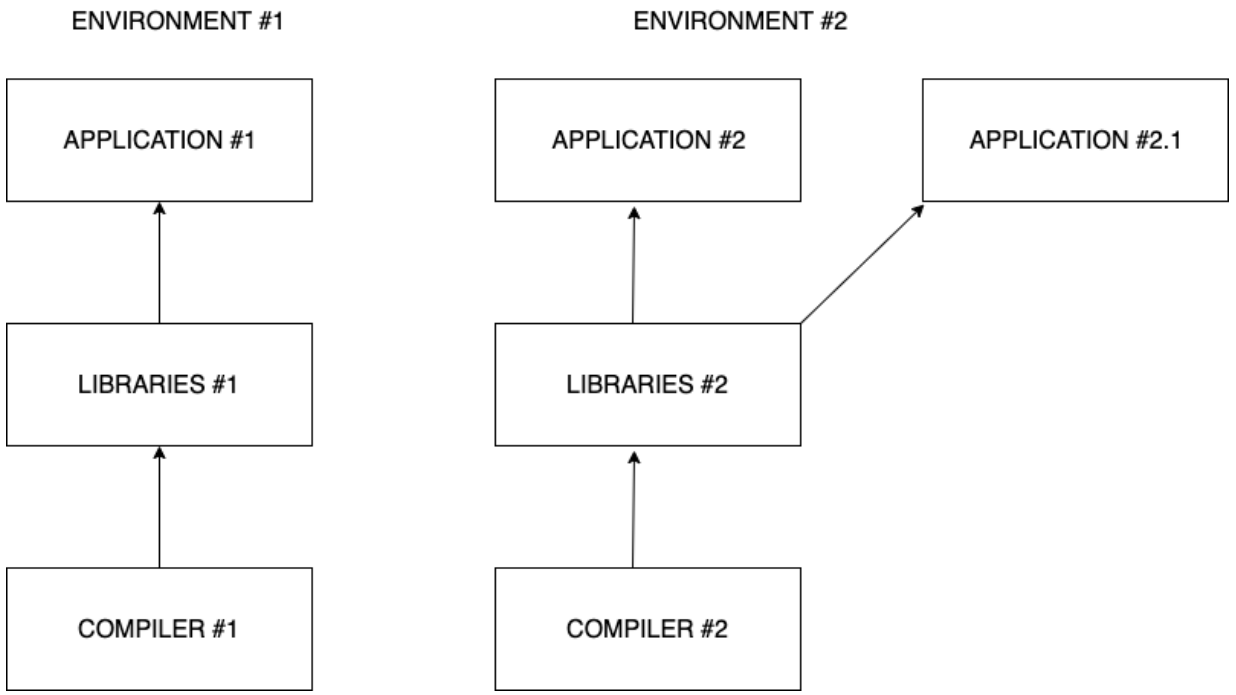
Outline of the presentation

- User environments in the Unix/Linux shell.
- Tcl/C module examples and motivation for the Lua based Lmod modules.
- Setup Lmod for the lab exercises.
- MODULEPATH and explanation how LMOD works
- Practice with basic module commands and examples.
- Module lua file structure.
- Useful features of LMOD
- LMOD usage tracking through syslog

Why to use environment modules

Reason:	Environment variables affected:
Different Compilers: gcc 8.5.0, gcc 12.0.0, Intel 2020, etc	PATH, CPATH, LIBRARY_PATH
Different apps: shared object libs (*.so), MPI, Java, Licenses, etc	LD_LIBRARY_PATH, MPI_HOME, JAVA_HOME, LM_LICENSE_FILE

Environment modules allow switching seamlessly between the user environments without need for modifying `/etc/profile` or `.bashrc` files.


ENVIRONMENT #1
APPLICATION #1
LIBRARIES #1
COMPILER #1
ENVIRONMENT #2
APPLICATION #2
APPLICATION #2.1
LIBRARIES #2
COMPILER #2

Classical TCL/C Environment Modules

- To overcome the difficulty of setting and changing the Environment variables, the TCL/C Modules were introduced over 2 decades ago.
- They were written in C and used TCL language for environment configuration.
- Very robust and easy to use, for example, to load Intel 2018 compiler:

```
module load intel/2018
```

- Check what the modules are loaded:

```
module list
```

- See what the modules are available to load:

```
module avail
```

- Unload the module:

```
module unload intel/2018
```

TCL/C modules drawback and motivation for migration to Lmod

- The classical TCL/C modules allow conflicting environment modules to be loaded at the same time. For example:

```
module switch intel/2018 intel/2013
module list
```

  shows: `intel/2013 openmpi/2.1.2-intel2018`
- Users should watch what modules are loaded before performing compilation and running their codes.
- The rule of thumb is, first, to unload all the modules with command

```
module purge
```

- Then load specifically what is needed, for example:

```
module load intel/2018
module load openmpi/2.1.2-intel2018
```

- Better approach is switching to Lmod.
- The Lmod configuration can protect users from loading incompatible environment settings.

Lmod (“L” stands for Lua) vs TCL/C modules

- Lmod is an environment modules implementation that provides all of the functionality of TCL/C Environment Modules plus more features.
- Lmod can read modules written in TCL and in lua.
- Support for hierarchical module file structure.
- MODULEPATH is dynamically updated when modules are loaded.
- Makes loaded modules inactive and active to provide sane environment.
- User module collections.
- Hidden modules.
- Optional usage tracking.
- Many useful functions in Lua module configuration files, such as family(“compiler”), property(“gpu”), etc

LMOD installation steps

- Install Lua
- Install LMOD
- Setup the environment configuration in .lua files.

- Initialize MODULEPATH and MODULEPATH_ROOT entries in .bashrc

- Details are here: Installing Lua and Lmod

LMOD setup on your lab cluster

SSH to to the cluster.

Copy folder Ansible-lmod from git repository into the home directory:

```
cp -a lci-scripts/introductory/lmod/Ansible-lmod .
```

Step into directory Ansible-lmod and install Lmod:

```
cd Ansible-lmod
ansible-playbook install_lmod.yml
```

In `.bashrc` file of user `mpiuser`, remove the settings for openmpi, and add the following block at the bottom:

```
if [ -z "$BASHRC_READ" ]
then
  export BASHRC_READ=1
  . /usr/share/lmod/lmod/init/profile
  export MODULEPATH_ROOT=/usr/share/lmod/lmod/modulefiles
  export MODULEPATH=$MODULEPATH_ROOT/Core
  export LMOD_PACKAGE_PATH=/usr/share/lmod/lmod/libexec
fi
```

Alternatively you can overwrite his .bashrc file as follows:

```
cp Modules/bashrc-lmod ~mpiuser/.bashrc
```

Become mpiuser and run command module:

```
sudo su - mpiuser
module avail
```

LMOD demo with loading and unloading the modules.

- Check available modules:

  ```
  module available
  ```

- Shortcut:

  ```
  ml av
  ```

- See all modules via spider:

  ```
  module spider
  ```

- Shortcut:

  ```
  ml spider
  ```

- Load module gcc/8.5.0

  ```
  module load gcc/8.5.0
  ```

- Shortcut

  ```
  ml gcc/8.5.0
  ```

- List loaded modules:

  ```
  module list
  ```

- Shortcut:

  ```
  ml
  ```

- See what modules need to be loaded for application lammps:

  ```
  module spider lammps
  ```

  If it doesn't show up because it is `hidden`

- Try the following:

  ```
  module --show-hidden spider
  ```

- Load the prereq modules:

```
module load openmpi/5.0.1
```

- See what modules are available now:

```
ml av
```

- See the hidden modules:

```
ml --show-hidden av
```

- Load `lammps`:

```
ml lammps
```

- Unloading the base module, gcc/8.5.0, will deactivate the others, openmpi/4.1.4 and lammps:

```
module unload gcc/8.5.0
```

- The dependent modules will also get deactivated if the different compiler is loaded, for example:

```
module load intel/2018
```

- To unload all the modules:

```
module purge
```

How the things work

- File .bashrc references the Lua modules and initialize MODULEPATH_ROOT and MODULEPATH environment variables:

```
if [ -z "$BASHRC_READ" ]
then
  export BASHRC_READ=1
  . /usr/share/lmod/lmod/init/profile
  export MODULEPATH_ROOT=/usr/share/lmod/lmod/modulefiles
  export MODULEPATH=$MODULEPATH_ROOT/Core

fi
```

- The initial MODULEPATH=modulefiles/Core
- After command `module load gcc/8.5.0`, the MODULEPATH gets updated: `MODULEPATH=modulefiles/Compiler/gcc/8.5.0:modulefiles/Core`
- After adding another module, `module load openmpi/5.0.1`, the MODULEPATH contains the directory with file `lammps.lua`

```
modulefiles/
|-- Compiler
|   |-- gcc
|   |    \-- 8.5.0
|   |         \-- openmpi
|   |              \-- 5.0.1.lua <-- 2 updates:
|    \-- intel      "MODULEPATH=modulefiles/MPI/gcc/8.5.0/5.0.1:$MODULEPATH"
|       |-- 2013
|       |    \-- openmpi
|       |       |-- 1.6.5.lua
|       |        \-- 1.8.8.lua
|        \-- 2018
|            -- openmpi
|               |-- 1.8.8.lua
|               |-- 2.1.1.lua
|               \-- 2.1.2.lua
|-- Core
|   |-- gcc
|   |    \-- 8.5.0.lua <--- 1 updates:
|    \-- intel     "MODULEPATH=modulefiles/Compiler/gcc/8.5.0:modulefiles/Core"
|       |-- 2013.lua
|        \-- 2018.lua
 \-- MPI
    |-- gcc
    |    \-- 8.5.0
    |         \-- 5.0.1
    |              \-- lammps.lua  <-- 3 is in the updated MODULEPATH
     \-- intel
          \-- 2018
              \-- 2.1.2
                  \-- vasp.lua
```

Module file example: `8.5.0.lua`

```
-- -*- lua -*-

help([[ This is a gcc 8.5.0 compiler, came with Red Hat 8.6 packages]])

-- Local variables
local version = "8.5.0"

-- Whatis description
whatis("Description: GCC compiler")

-- Setup Modulepath for packages built by this compiler
local mroot = os.getenv("MODULEPATH_ROOT")
local mdir = pathJoin(mroot,"Compiler/gcc", version)
prepend_path("MODULEPATH", mdir)


-- Set family for this module
family("compiler")
```

Helpful LMOD functionalities.

- Module tags, for example:

```
add_property("state","testing")
add_property("arch","gpu")
```

- Hide modules when software is updated or decommissioned. Place file `.modulerc.lua` in the same directory with the module, for example, in directory `modulefiles/MPI/gcc/8.5.0/5.0.1`:

```
hide_version("lammps")
```

- User module collections can be saved and restored by a user, for example:

```
module load gcc/8.5.0
module load openmpi/5.0.1
module save gcc-openmpi
```

  It saves the environment configuration into `~/.lmod.d/gcc-openmpi` Lua file.

To restore the environment:

```
module restore gcc-openmpi
```

Lmod configuration for module usage.

- Add new path, `/usr/share/lmod/lmod/libexec_log`, to LMOD_PACKAGE_PATH into file .bashrc for mpiuser:

```
export LMOD_PACKAGE_PATH=/usr/share/lmod/lmod/libexec:/usr/share/lmod/lmod/libexec_log
```

- Create directory `/usr/share/lmod/lmod/libexec_log`:

```
sudo mkdir /usr/share/lmod/lmod/libexec_log
```

- Copy file `SitePackage_LOGS.lua` into `SitePackage.lua` in the new directory:

```
sudo cp /usr/share/lmod/lmod/libexec/SitePackage_LOGS.lua /usr/share/lmod/lmod/libexec_log/SitePackage.lua
```

- Login to `mpiuser`.

```
sudo su - mpiuser
```

- Make sure the updated LMOD_PACKAGE_PATH environment variable is in the user environment.

```
echo $LMOD_PACKAGE_PATH
```

- Start loading modules as `mpiuser`, for example:

```
module load gcc/8.5 openmpi/5.0.1
```

- Check the log updates with ModuleUsageTracking tag in /var/log/messages

```
grep ModuleUsageTracking /var/log/messages
```

References

Jeff Layton’s article in admin magazine with excellent explanation on how Lmod works and nice examples

The Lmod official web site

The TCL/C classical module web site

Tracking Module Usage

Questions and discussion: