Environment Setting by module command

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Changelog

- Sep. 6, 2019 first version
- Jan. 16, 2020 Update

Introduction

The aim of this document is to explain how to perform environmental settings using “module” command.

“module” command from Environment Modules is useful
(1) when preparing PATH and LD_LIBRARY_PATH environment variables before running application
and(2) when choosing compilers and libraries before building applications.

(You can prepare environment without “module” command.
“module” command is one of the options when setting environments in RCCS.)

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Default Environment

- Some of modules are already loaded just upon logon.
  (If custom setting is not employed.)
- Currently loaded modules can be listed by module list command.
- Environment variables (e.g. PATH) are also set accordingly.

```
[user@ccfep4 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2018update4   4) allinea/7.1
  2) pgilic                             5) cuda/9.1
  3) pgi/18.1
[user@ccfep4 ~]$ gcc -v
Using built-in specs.
COLLECT_GCC=gcc
COLLECT_LTO_WRAPPER=/usr/libexec/gcc/x86_64-redhat-linux/4.8.5/lto-wrapper
Target: x86_64-redhat-linux
Configured with: ../configure --prefix=/usr --mandir=/usr/share/man --infodir=/usr/share/info --with-
bugurl=http://bugzilla.redhat.com/bugzilla --enable-bootstrap --enable-shared --enable-threads=posix --
enable-checking=release --with-system-zlib --enable-__cxa_atexit --disable-libunwind-exceptions --
enable-gnu-unique-object --enable-linker-build-id --with-linker-hash-style=gnu --enable-
languages=c,c++,objc,obj-c++,java,fortran,ada,go,lto --enable-plugin --enable-initfini-array --disable-
libgcj --with-isl=/builddir/build/BUILD/gcc-4.8.5-20150702/obj-x86_64-redhat-linux/isl-install --with-
cloog=/builddir/build/BUILD/gcc-4.8.5-20150702/obj-x86_64-redhat-linux/cloog-install --enable-gnu-
indirect-function --with-tune=generic --with-arch_32=x86-64 --build=x86_64-redhat-linux
Thread model: posix
gcc version 4.8.5 20150623 (Red Hat 4.8.5-36) (GCC)
[user@ccfep4 ~]$ icc -v
icc version 18.0.5 (gcc version 4.8.5 compatibility)
[user@ccfep4 ~]$
```

Default modules
- Intel compilers (2018u4)
- PGI compilers
- CUDA 9.1 (nvcc)

(some details may be available by “module help (package name)” command)

Available Modules

- List of available modules can be accessed via “module avail” command.
- Please also check https://ccportal.ims.ac.jp/en/installed_applications.

```
[user@ccfep5]$ module avail

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/suite ------------------------------------------------------------------------------------------------------------
intel_parallelstudio/2015update1          intel_parallelstudio/2018update2          intel_parallelstudio/2019update5          scl/devtoolset-6
intel_parallelstudio/2017update4          intel_parallelstudio/2018update4(default) scl/devtoolset-3                          scl/devtoolset-7
intel_parallelstudio/2017update8          intel_parallelstudio/2019update1          scl/devtoolset-4                          scl/devtoolset-8

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/comp -------------------------------------------------------------------------------------------------------------
cuda/10.1             cuda/8.0              intel/15.0.1          intel/17.0.8          intel/18.0.5(default) intel/19.0.5          pgi/16.5              pgi/18.1(default)
cuda/7.5              cuda/9.1(default)     intel/17.0.4          intel/18.0.2          intel/19.0.1          julia/1.3.1           pgi/17.5

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/apl --------------------------------------------------------------------------------------------------------------
mpi/intelmpi/2017.3.196   mpi/intelmpi/2019.1.144   mpi/openmpi/2.1.3/gnu5.3  mpi/openmpi/2.1.3/intel17 mpi/openmpi/3.1.0/gnu5.3  mpi/openmpi/3.1.0/intel17 mpi/openmpi/4.0.0/gnu5.3  mpi/openmpi/4.0.0/intel17
mpi/intelmpi/2017.4.262   mpi/intelmpi/2019.5.281   mpi/openmpi/2.1.3/gnu6.3  mpi/openmpi/2.1.3/intel18 mpi/openmpi/3.1.0/gnu6.3  mpi/openmpi/3.1.0/intel18 mpi/openmpi/4.0.0/gnu6.3  mpi/openmpi/4.0.0/intel18
mpi/intelmpi/2018.2.199   mpi/intelmpi/5.0.2.044    mpi/openmpi/2.1.3/gnu7.3  mpi/openmpi/2.1.3/intel19 mpi/openmpi/3.1.0/gnu7.3  mpi/openmpi/3.1.0/intel19 mpi/openmpi/4.0.0/gnu7.3  mpi/openmpi/4.0.0/intel19
mpi/intelmpi/2018.4.274   mpi/openmpi/2.1.3/gnu4.8  mpi/openmpi/2.1.3/gnu8.3  mpi/openmpi/3.1.0/gnu4.8  mpi/openmpi/3.1.0/gnu8.3  mpi/openmpi/4.0.0/gnu4.8  mpi/openmpi/4.0.0/gnu8.3
mpi/intelmpi/2019         mpi/openmpi/2.1.3/gnu4.9  mpi/openmpi/2.1.3/intel15 mpi/openmpi/3.1.0/gnu4.9  mpi/openmpi/3.1.0/intel15 mpi/openmpi/4.0.0/gnu4.9  mpi/openmpi/4.0.0/intel15

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/apl_ex -----------------------------------------------------------------------------------------------------------
GRRM/11-g09                 espresso/5.1.2              genesis/1.3.0-CUDA          gromacs/2018.1/gnu          gromacs/2018.8/intel-CUDA   lammps/16Mar18/intel        openmolcas/20190604
GRRM/14-g09(default)        espresso/5.4                genesis/1.4.0               gromacs/2018.1/intel        gromacs/2019.2/gnu          lammps/16Mar18/intel-CUDA   orca/4.2.1
abinit/7.8.2                espresso/6.1                genesis/1.4.0-CUDA          gromacs/2018.3/gnu          gromacs/2019.2/gnu-CUDA     lammps/22Aug18/intel        psi4/1.1
abinit/8.8.3(default)       espresso/6.3(default)       gromacs/2016.1/intel        gromacs/2018.3/gnu-CUDA     gromacs/2019.2/intel        lammps/22Aug18/intel-CUDA   reactionplus/1.0
amber/16/bugfix10           gamess/2018Feb14            gromacs/2016.1/intel-CUDA   gromacs/2018.3/intel        gromacs/2019.2/intel-CUDA   lammps/22Aug18/intel-CUDA-volta siesta/3.1
amber/16/bugfix15           gamess/2018Sep30(default)   gromacs/2016.3/intel        gromacs/2018.3/intel-CUDA   gromacs/2019.4/gnu          lammps/7Aug19/intel         siesta/4.0.2(default)
amber/18/bugfix1            gamess/2019Sep30            gromacs/2016.3/intel-CUDA   gromacs/2018.6/gnu          gromacs/2019.4/gnu-CUDA     lammps/7Aug19/intel-CUDA    smash/2.2.0
amber/18/bugfix11-volta     gaussian/g09/b01            gromacs/2016.4/intel        gromacs/2018.6/gnu-CUDA     gromacs/2019.4/intel        molcas/8.2                  turbomole/7.2.1-MPI
amber/18/bugfix12           gaussian/g09/c01            gromacs/2016.4/intel-CUDA   gromacs/2018.6/intel        gromacs/2019.4/intel-CUDA   molpro                      turbomole/7.2.1-SMP
amber/18/bugfix16           gaussian/g09/d01            gromacs/2016.5/gnu          gromacs/2018.6/intel-CUDA   gromacs/5.1.4/intel         namd/2.11                   turbomole/7.2.1-serial
autodock/4.2.6              gaussian/g09/e01            gromacs/2016.5/gnu-CUDA     gromacs/2018.7/gnu          gromacs/5.1.4/intel-CUDA    namd/2.11-CUDA              turbomole/7.3-MPI(default)
cp2k/6.1.0/gnu              gaussian/g16/a03            gromacs/2016.5/intel        gromacs/2018.7/gnu-CUDA     gromacs/5.1.5/gnu           namd/2.13(default)          turbomole/7.3-SMP
cp2k/6.1.0/gnu-CUDA         gaussian/g16/b01            gromacs/2016.5/intel-CUDA   gromacs/2018.7/intel        gromacs/5.1.5/gnu-CUDA      namd/2.13-CUDA              turbomole/7.3-serial
cp2k/6.1.0/intel            gaussian/g16/c01            gromacs/2016.6/gnu          gromacs/2018.7/intel-CUDA   gromacs/5.1.5/intel         ntchem/2013-5.0-mpi         turbomole/7.4-MPI
cp2k/6.1.0/intel-CUDA       genesis/1.1.6               gromacs/2016.6/gnu-CUDA     gromacs/2018.8/gnu          gromacs/5.1.5/intel-CUDA    ntchem/2013-5.0-mpiomp      turbomole/7.4-SMP
crystal/14-104              genesis/1.1.6-CUDA          gromacs/2016.6/intel        gromacs/2018.8/gnu-CUDA     lammps/16Mar18/gnu          ntchem/2013-5.0-serial      turbomole/7.4-serial
dirac/18.0                  genesis/1.3.0               gromacs/2016.6/intel-CUDA   gromacs/2018.8/intel        lammps/16Mar18/gnu-CUDA     nwchem/6.8

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/apl_viewer -------------------------------------------------------------------------------------------------------
luscus/0.8.6 molden/5.7   nboview/2.0  vmd/1.9.3

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/apl_util ---------------------------------------------------------------------------------------------------------
allinea/7.1           cmake/2.8.12.2(default) cmake/3.8.2

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/lib --------------------------------------------------------------------------------------------------------------
boost/1.53.0(default)     boost/1.70.0              mkl/2017.0.3              mkl/2018.0.2              mkl/2019.0.1              spglib/1.11.1(default)
boost/1.59.0              mkl/11.2.1                mkl/2017.0.4              mkl/2018.0.4(default)     nccl/2.3.7-1+cuda9.1(default)

------------------------------------------------------------------------------------------------------------ /local/apl/lx/modules/misc -------------------------------------------------------------------------------------------------------------
inteldev intellic pgilic
[user@ccfep5]$
```

(Non-standard versions of GCC are available via scl/devtoolset modules.)

Loading & Switching modules

- If you want to switch version of a certain application, try module switch (module name).
- If you want to load new application, try module load (module name). Examples of switch & load for intel2017u8 & gcc7 are shown below.

```
[user@ccfep4 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2018update4   4) allinea/7.1
  2) pgilic                             5) cuda/9.1
  3) pgi/18.1
[user@ccfep4 ~]$ module switch intel_parallelstudio/2017update8
[user@ccfep4 ~]$ module load scl/devtoolset-7
[user@ccfep4 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2017update8   4) allinea/7.1
  2) pgilic                             5) cuda/9.1
  3) pgi/18.1                           6) scl/devtoolset-7
[user@ccfep4 ~]$ icc -v
icc version 17.0.8 (gcc version 7.0.0 compatibility)
[user@ccfep4 ~]$ gcc -v
Using built-in specs.
COLLECT_GCC=gcc
COLLECT_LTO_WRAPPER=/opt/rh/devtoolset-7/root/usr/libexec/gcc/x86_64-redhat-linux/7/lto-wrapper
Target: x86_64-redhat-linux
Configured with: ../configure --enable-bootstrap --enable-languages=c,c++,fortran,lto --prefix=/opt/rh/devtoolset-7/root/usr --
mandir=/opt/rh/devtoolset-7/root/usr/share/man --infodir=/opt/rh/devtoolset-7/root/usr/share/info --with-
bugurl=http://bugzilla.redhat.com/bugzilla --enable-shared --enable-threads=posix --enable-checking=release --enable-multilib -
-with-system-zlib --enable-__cxa_atexit --disable-libunwind-exceptions --enable-gnu-unique-object --enable-linker-build-id --
with-gcc-major-version-only --enable-plugin --with-linker-hash-style=gnu --enable-initfini-array --with-default-libstdcxx-
abi=gcc4-compatible --with-isl=/builddir/build/BUILD/gcc-7.3.1-20180303/obj-x86_64-redhat-linux/isl-install --enable-libmpx --
enable-gnu-indirect-function --with-tune=generic --with-arch_32=i686 --build=x86_64-redhat-linux
Thread model: posix
gcc version 7.3.1 20180303 (Red Hat 7.3.1-5) (GCC)
[user@ccfep4 ~]$
```

Switch to Intel 2017 u8 from 2018 u4

Load GCC 7 env (Software Collections employed)

(you can unload all the loaded modules by “module purge” command.)

Load Libraries and Utilities (1)

- Newer version of certain software (such as cmake & boost) are available at /local/apl/lx. They can also be loaded by “module”. This type of modules can be found at “lib” or “apl_util” category.

```
----------------- /local/apl/lx/modules/apl_util -------------------
allinea/7.1             cmake/2.8.12.2(default) cmake/3.8.2
                                  2.8.12 is /usr/bin/cmake, 3.8.2 is in /local/apl/lx
-------------------- /local/apl/lx/modules/lib ---------------------
boost/1.53.0(default)         mkl/2017.0.3              mkl/2019.0.1
boost/1.70.0                  mkl/2017.0.4              nccl/2.3.7-1+cuda9.1(default)
boost/1.59.0                  mkl/2018.0.2              spglib/1.11.1(default)
mkl/11.2.1                    mkl/2018.0.4(default)
 1.53.0 is system default one located at /usr/lib64/libboost*
```

```
[user@ccfep4 ~]$ module purge
[user@ccfep4 ~]$ module list
No Modulefiles Currently Loaded.
[user@ccfep4 ~]$ cmake --version
cmake version 2.8.12.2
[user@ccfep4 ~]$ module load intel_parallelstudio/2018update4
[user@ccfep4 ~]$ module load cmake/3.8.2
[user@ccfep4 ~]$ module load boost/1.70.0
[user@ccfep4 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2018update4   3) boost/1.70.0
  2) cmake/3.8.2
[user@ccfep4 ~]$ cmake --version
cmake version 3.8.2

CMake suite maintained and supported by Kitware (kitware.com/cmake).
[user@ccfep4 ~]$
```

Load Libraries and Utilities (2)

- Modules are prepared for normal applications such as Gromacs, Amber, and Gaussian. They can be used in job scripts of course. In addition, they may be useful on the interactive shell at frontend node (ccfep*) to run some utilities.

```
[user@ccfep8 ~]$ ambpdb
bash: ambpdb: command not found...
[user@ccfep8 ~]$ formchk
bash: formchk: command not found...
[user@ccfep8 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2018update4   4) allinea/7.1
  2) pgilic                             5) cuda/9.1
  3) pgi/18.1
[user@ccfep8 ~]$ module load amber/18/bugfix12
[user@ccfep8 ~]$ ambpdb
Error: 'prmtop': No such file or directory

Usage: ambpdb -p 'Top' -c 'Coords' [Additional Options]
       ambpdb -p 'Top' < 'AmberRestart' [Additional Options]
    -p 'Top'       Topology file (default: prmtop).
    -c 'Coords'    Coordinate file.
    'AmberRestart' Amber restart file from STDIN.
  PDB is written to STDOUT.
  Use '-h' or '--help' to see additional options.

[user@ccfep8 ~]$ module load gaussian/g16/b01
[user@ccfep8 ~]$ module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2018update4   5) cuda/9.1
  2) pgilic                             6) amber/18/bugfix12
  3) pgi/18.1                           7) gaussian/g16/b01
  4) allinea/7.1
[user@ccfep8 ~]$ formchk
 Checkpoint file?
```

“ambpdb” and “formchk” are not available on the default setting.

Load “amber18/bugfix12”

“ambpdb” becomes available (does not run correctly here, since input files are not prepared)

“formchk” becomes available once Gaussian module is loaded.

Tips: Note (1)

- If you omit version of the application upon loading, default version will be loaded.
- In some cases, some additional modules will be loaded automatically.

```
% module purge
% module load amber gaussian
info: purge all the modules
info: loading intel_parallelstudio/2017update8
info: loading cuda/9.1
% module list
Currently Loaded Modulefiles:
  1) intel_parallelstudio/2017update8   3) amber/18/bugfix12
  2) cuda/9.1                           4) gaussian/g16/b01
```

Automatically loaded modules

Tips: Note (2)

- If your login shell is “/bin/csh” and in the job script, you need to run the following command before using “module” command:
  “source /etc/profile.d/modules.csh” .
  (This is not necessary at the front-end node (ccfep*).)
- You cannot load multiple versions of single application.
  - If you try to load both of intel_parallelstudio/2018update4 and intel_parallelstudio/2017update8, it will fail.
  - Please use “switch” to change versions.
- Some applications (Anaconda for example) cannot be loaded by “module”. Please load settings files for them.

Tips: List of Compilers (Jan, 2020)

- Intel Parallel Studio 2019 Update 5 (icc/icpc/ifort 19.0.5)
- Intel Parallel Studio 2019 Update 1 (icc/icpc/ifort 19.0.1)
- Intel Parallel Studio 2018 Update 4 (icc/icpc/ifort 18.0.5) (default)
- Intel Parallel Studio 2018 Update 2 (icc/icpc/ifort 18.0.2)
- Intel Parallel Studio 2017 Update 8 (icc/icpc.ifort 17.0.8)
- Intel Parallel Studio 2017 Update 4 (icc/icpc/ifort 17.0.4)
- Intel Parallel Studio 2015 Update 1 (icc/icpc/ifort 15.0.1)
- GCC 4.8.5 (default; OS standard version)
- GCC 8.3.1 (Devtoolset-8 Software Collections (scl))
- GCC 7.3.1 (Devtoolset-7 Software Collections (scl))
- GCC 6.3.1 (Devtoolset-6 Software Collections (scl))
- GCC 5.3.1 (Devtoolset-4 Software Collections (scl))
- GCC 4.9.2 (Devtoolset-3 Software Collections (scl))
- CUDA 8.0.61 (nvcc)
- CUDA 9.1.85 (nvcc) (default)
- CUDA 10.1.243 (nvcc)