



Environment Modules

Nikolaos Nikoloutsakos

GRNET

Athens, 11 - 12 Dec. 2019



Contents

- 1 User Environment
- 2 Environment Modules
 - What are they ?
 - What modules exist
 - How to use them
 - Available Software
- 3 Compilers
 - MPI compilers
 - Compilation flags
 - Optimization flags



User Environment

- Login Shell

```
/bin/bash
```

```
echo $SHELL
```

- Environment Variables

```
env
```

```
printenv GRNET_ROOT; echo $GRNET_ROOT
```

- Default variables
 - ▶ \$GRNET_ROOT
 - ▶ \$HOME
 - ▶ \$WORKDIR



Working Directories

- `$HOME` your home directory under GPFS
 - ▶ Store your source code and build your executables here.
 - ▶ Users are NOT supposed to run jobs from this filesystem because of the low performance.
 - ▶ Emphasis is reliability over performance.
- `$WORKDIR` points to the `/work` or `/work2` filesystem under GPFS
 - ▶ Store large files here.
 - ▶ Change to this directory in your batch scripts and run jobs in this file system.
 - ▶ Emphasis performance rather than reliability, as a fast workspace for temporary storage.



Environment Modules

- All software on ARIS is available through modules.
- Provides a way to rationalize software and its environment variables
- **modules** way to manage user environment
- Dynamically set up environments for different applications **PATH**, **LD_LIBRARY_PATH** etc.
- One module for each software version
- Detects software dependencies and informs which modules must be loaded



ARIS work environment is organized in modules divided in 5 categories:

- **compilers:** GNU, Intel, Pgi, Cuda, ...
- **parallel:** IntelMPI, OpenMPI, mpiP, ...
- **libraries:** openBLAS, FFTW, NetCDF, ..
- **applications:** Gromacs, CP2K, WRF, R, Octave, ...
- **tools:** git, cmake, make, prace, ...



- When **loading** a module a set of environment variables will be set.
eg:
 - ▶ `PATH`, `MANPATH`, `LD_LIBRARY_PATH`, ...
- All modules set the *root* variable **MODULENAMEROOT**
 - ▶ this variable points to the root path installation of the software



What modules exist?

module avail

List available modules.

```
----- /apps/modulefiles/applications -----  
abinit/7.10.4(default)          namd/2.10/hybrid/normal  
bigdft/1.7.6(default)         namd/2.10/purempi/memopt  
cdo/1.7.0(default)            namd/2.10/purempi/normal  
code_saturne/4.0.1/intel      ncarg/6.3.0(default)
```



module avail <module>

List <module> available versions

```
/apps/modulefiles/compilers:  
gnu/4.9.2(default)  
gnu/4.9.3  
gnu/5.1.0  
gnu/5.2.0
```

Default version marked as **(default)**



- Default module version

- ▶ Almost all ARIS software packages have multiple versions marked as **(default)** In these case the commands:

```
module load MODULENAME
```

and

```
module load MODULENAME/DEFAULTVERSION
```

are equivalent.

- ▶ eg. current defaults

```
module load intel
```

and

```
module load intel/15.0.3
```

are the same



- ▶ Sometimes, after proper notification, the system defaults may change.
- ▶ In that case if you are using the `defaults`, it's recommended to re-compile you code.
- ▶ If you need to use a specific software version, please use it's relevant module version.



Use Modules

`module load/unload <module>`

Load/Unload <module> into the shell environment

`module switch <module1> <module2>`

Switch loaded module1 with module2.

`module list`

List loaded modules.

```
Currently Loaded Modulefiles:
```

```
1) gnu/4.9.2      2) intel/15.0.3  3) intelmpi/5.0.3
```



Examine a module

```
module show <module>
```

List all of the environment changes the <module> will make if loaded

```
-----  
/apps/modulefiles/compilers/gnu/4.9.2:  
  
module-whatis      Enable usage for the GNU Compiler Collection ver  
setenv             COMPILER_GNUROOT /apps/compilers/gnu/4.9.2  
prepend-path      PATH /apps/compilers/gnu/4.9.2/bin  
prepend-path      INCLUDE /apps/compilers/gnu/4.9.2/include  
prepend-path      LD_LIBRARY_PATH /apps/compilers/gnu/4.9.2/lib  
prepend-path      LD_LIBRARY_PATH /apps/compilers/gnu/4.9.2/lib64  
prepend-path      MANPATH /apps/compilers/gnu/4.9.2/share/man  
-----
```



Examine a module

- `setenv`: Set environment variable
- `prepend-path`: Prepend value to environment variable.
- `MODULENAMEROOT/include`, `MODULENAMEROOT/lib`

`module whatis <module>`

Display what is the module information

`module help <module>`

More specific help about <module>



Prereqs and Conflicts

- **PREREQS:** some modules have other modules as prerequisites, thus `prereqs` must be loaded first.

```
prereq    gnu/4.9.2
```

```
prereq    intel/15.0.3
```

- **CONFLICTS:** some modules should not be used together.



Available Software

<http://doc.aris.grnet.gr/software/>

Software Environment / Available Modules

ARIS DOCUMENTATION
Home
System Information -
Login and Data transfer
User Environment
Running Jobs -
SLURM - Job Script Template
Development Environment -
Software Environment -
Available Modules
Life Sciences
Computational Chemistry & Material Science
Weather Forecasting
Engineering
Numerical Libraries
Generic Data I/O Libraries
Visualization Software
High-level Languages
Remote Visualization
FAQ
System Messages
Contact

Software Environment

In this section we present an overview of installed software.

Software package	version	jobs	GPU	PIE
amcode	2.4.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
abnre	7.10.4, 7.10.5, 8.8.7, 8.0.8, 8.4.3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
alysm	20150917	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
arid	5.3.1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
arlis	3.10.2, 3.10.3, 3.11.34, 3.11.39	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
autobk	4.2.6	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
logfl	1.7.6, 1.7.7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
bnutils	2.25, 2.26, 2.27, 2.28, 2.29	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
bcact	1.98.0, 1.62.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
boonapp2	1.98.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>



Development Tools

- *Compilers*: GCC, INTEL, PGI
- *Parallel*: Intel MPI, OpenMPI
- *Debug*: gdb, gdb-ia , pgdbg, ddd
- *Profilers*: VTune, Scalasca, mpiP, gprof, pgprof



Table: Compilers

GNU	C	gcc
	C++	g++
	Fortran	gfortran
Intel	C	icc
	C++	icpc
	Fortran	ifort
PGI	C	pgcc
	C++	pgc++
	Fortran	pgfortran



Compilers

module avail

All available compilers check for "compilers" section

```
----- /apps/modulefiles/compilers -----  
binutils/2.25          gnu/5.1.0          intel/17.0.4  
binutils/2.26          gnu/5.2.0          intel/17.0.5  
binutils/2.27          gnu/5.3.0          intel/18.0.0  
binutils/2.28          gnu/5.4.0          intel/18.0.1  
binutils/2.29(default) gnu/5.5.0          java/1.7.0  
clang/5.0.0(default)  gnu/6.1.0          java/1.8.0(default)  
cuda/6.5.14           gnu/6.2.0          pgi/15.5  
cuda/7.0.28           gnu/6.3.0          pgi/16.10  
cuda/7.5.18           gnu/6.4.0          pgi/16.4  
cuda/8.0.27           gnu/7.1.0          pgi/16.5  
cuda/8.0.44           gnu/7.2.0          pgi/16.7  
cuda/8.0.61(default) intel/15.0.3(default) pgi/16.9  
cuda/9.1.85           intel/15.0.6          pgi/17.1
```



MPI versions

module avail

Check for "parallel" section

```
----- /apps/modulefiles/parallel -----  
intelmpi/2017.0      openmpi/1.10.0/gnu    openmpi/2.0.0/intel  
intelmpi/2017.1      openmpi/1.10.0/intel  openmpi/2.0.1/gnu  
intelmpi/2017.2      openmpi/1.10.1/gnu    openmpi/2.0.1/intel  
intelmpi/2017.3      openmpi/1.10.1/intel  openmpi/2.0.2/gnu  
intelmpi/2017.4      openmpi/1.10.2/gnu    openmpi/2.0.2/intel  
intelmpi/2017.5      openmpi/1.10.2/intel  openmpi/2.0.3/gnu  
intelmpi/2018.0      openmpi/1.10.3/gnu    openmpi/2.0.3/intel  
intelmpi/2018.1      openmpi/1.10.3/intel  openmpi/2.1.0/gnu  
intelmpi/5.0.3(default) openmpi/1.10.4/gnu    openmpi/2.1.0/intel  
intelmpi/5.1.1       openmpi/1.10.4/intel  openmpi/2.1.1/gnu  
intelmpi/5.1.2       openmpi/1.10.5/gnu    openmpi/2.1.1/intel  
intelmpi/5.1.3       openmpi/1.10.5/intel  openmpi/2.1.2/gnu
```



Intel MPI

Language	wrapper
C	mpiicc
C++	mpicpc
Fortran	mpifort

Launcher

`srun`



module avail intelmpi

```
----- /apps/modulefiles/parallel -----  
intelmpi/2017.0      intelmpi/2017.5      intelmpi/5.1.2  
intelmpi/2017.1      intelmpi/2018.0      intelmpi/5.1.3  
intelmpi/2017.2      intelmpi/2018.1      intelmpi/5.1.3.258  
intelmpi/2017.3      intelmpi/5.0.3(default)  
intelmpi/2017.4      intelmpi/5.1.1
```

module list

```
Currently Loaded Modulefiles:  
  1) gnu/4.9.2          2) intel/15.0.3      3) intelmpi/5.0.3
```



(gnu) mpicc -show

```
gcc -I/apps/compilers/intel/impi/5.0.3.048/intel64/include -L/apps/compilers/intel/impi/5.0.3.048/intel64/lib/release_mt -L/apps/compilers/intel/impi/5.0.3.048/intel64/lib -Xlinker --enable-new-dtags -Xlinker -rpath -Xlinker /apps/compilers/intel/impi/5.0.3.048/intel64/lib/release_mt -Xlinker -rpath -Xlinker /apps/compilers/intel/impi/5.0.3.048/intel64/lib -Xlinker -rpath -Xlinker /opt/intel/mpi-rt/5.0/intel64/lib/release_mt -Xlinker -rpath -Xlinker /opt/intel/mpi-rt/5.0/intel64/lib -lmpifort -lmpi -lmpigi -ldl -lrt -lpthread
```

(intel) mpiicc -show

```
icc -I/apps/compilers/intel/impi/5.0.3.048/intel64/include -L/apps/compilers/intel/impi/5.0.3.048/intel64/lib/release_mt -L/apps/compilers/intel/impi/5.0.3.048/intel64/lib -Xlinker --enable-new-dtags -Xlinker -rpath -Xlinker /apps/compilers/intel/impi/5.0.3.048/intel64/lib/release_mt -Xlinker -rpath -Xlinker /apps/compilers/intel/impi/5.0.3.048/intel64/lib -Xlinker -rpath -Xlinker /opt/intel/mpi-rt/5.0/intel64/lib/release_mt -Xlinker -rpath -Xlinker /opt/intel/mpi-rt/5.0/intel64/lib -lmpifort -lmpi -lmpigi -ldl -lrt -lpthread
```



OpenMPI

Language	wrapper
C	mpicc
C++	mpicxx
Fortran	mpifort, mpif90

Launcher

`srun`



module avail openmpi

```
----- /apps/modulefiles/parallel -----  
openmpi/1.10.0/gnu(default) openmpi/1.8.5/intel  
openmpi/1.10.0/intel        openmpi/1.8.7/gnu  
openmpi/1.8.5/gnu          openmpi/1.8.7/intel
```



```
module load openmpi/1.10.1/intel
```

```
Currently Loaded Modulefiles:
```

```
1) gnu/4.9.2          3) intelmpi/5.0.3
2) intel/15.0.3      4) openmpi/1.10.1/intel
```

```
mpicc -show
```

```
icc -I/apps/parallel/openmpi/1.10.1/intel/include -pthread -Wl,-rpath -Wl,/apps/parallel/openmpi/1.10.1/intel/lib -Wl,--enable-new-dtags -L/apps/parallel/openmpi/1.10.1/intel/lib -lmpi
```



```
module load openmpi/1.10.1/gnu
```

```
Currently Loaded Modulefiles:
```

- | | |
|-----------------|-----------------------|
| 1) gnu/4.9.2 | 3) intelmpi/5.0.3 |
| 2) intel/15.0.3 | 4) openmpi/1.10.1/gnu |

```
mpicc -show
```

```
gcc -I/apps/parallel/openmpi/1.10.1/gnu/include -pthread -Wl,-rpath -Wl,/apps/parallel/openmpi/1.10.1/gnu/lib -Wl,--enable-new-dtags -L/apps/parallel/openmpi/1.10.1/gnu/lib -lmpi
```



CUDA

module avail cuda

```
----- /apps/modulefiles/compiler -----  
cuda/6.5.14          cuda/8.0.27          cuda/9.1.85  
cuda/7.0.28          cuda/8.0.44  
cuda/7.5.18          cuda/8.0.61(default)
```

- TESLA K40: `nvcc -arch=compute_35 -code=sm_35 ...`
- OpenCL: `-I $CUDAROOT/CL -lOpenCL`



Suggested Flags

- GNU `gcc -O3 -mavx -march=ivybridge`
- INTEL `icc -O3 -xCORE-AVX-I`
- PGI `pgcc -O4 -tp=sandybridge`