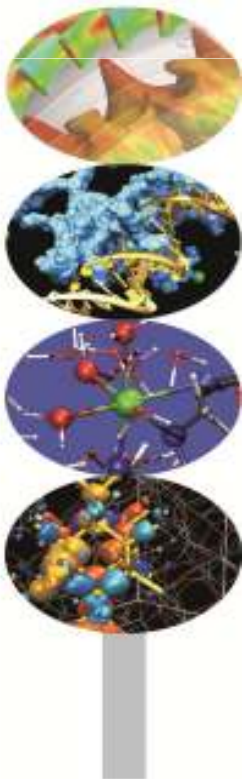
CINECA SCAI
SuperComputing Applications and Innovation

Software modules and programming environment

SCAI User Support



Marconi User Guide
https://wiki.u-gov.it/confluence/display/SCAIUS/UG3.1%3A+MARCONI+UserGuide

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Modules

Set module variables

- module load <module_name>

Show module variables, prereq (compiler and libraries) and conflict

- module show <module_name>

Give info about the software, the batch script, the available executable variants (e.g, single precision, double precision)

- module help <module_name>

Modules

Set the variables of the module and its dependencies (compiler and libraries)

- module load autoload <module name>

module load <compiler_name>

module load <library _name>

module load <module_name>

Profiles and categories

- The modules are
  - organized by functional category (compilers, libraries, tools, applications,…).
  - collected in different profiles (base, advanced, …..)
- The profile is a group of modules that share something

Profiles

- Programming profiles
  - They contain only **compilers, libraries and tools** modules used for compilation, debugging, profiling and pre-proccessing activity

BASE

Basic compilers, libraries and tools (gnu, intel, intelmpi, openmpi--gnu, math libraries, profiling and debugging tools, rcm,…)

ADVANCED

Advanced compilers, libraries and tools (pgi, openmpi--intel, ….)

Profiles

- Production profiles
  - They contain only **libraries, tools and applications** modules used for production activity
  - They match the most important scientific domains. For this reason we call them “domain” profiles:

CHEM
PHYS
LIFESC
BIOINF
ENG

Profiles

Programming and production and profile

- ARCHIVE
  - It contains all old versions of applications and tools and the old versions of compilers and libraries not used by other modules

Profiles

- BASE profile is the default. It is automatically loaded after login:

```
module av
```

To use a module of BASE profile you have only to load the module:

```
module load autoload <module_name>
```

To use a module placed under others profiles, you have to load preventively the corresponding profile:

```
module load profile/<profile_name>
module load autoload <module_name>
```

To list all loaded profiles use the following command:

```
module list
```

Mappa dei moduli

- modmap command
  - -all
    Print the full modules map: all profiles, all categories defined for each profile, all modules available for each category
  - -profiles
    Print all profiles available
  - -categories
    Print all categories available
  - -p <profile name>
    Print all modules available for the selected profile
  - -c <category name>
    Print all modules available for the selected category
  - -m <module name>
    Print all versions of the selected module

Mappa dei moduli

- NAMD - use example:

Find out all available NAMD versions and the profiles where they are located

```
modmap -m namd
```

Load the profile where NAMD of my personal interest is located

```
module load profile/chem    or
module load profile/archive
```

Load NAMD module

```
module load autoload namd
```

Load a specific version if more NAMD versions are available

```
module load autoload namd/<version>
```

Compilers

modmap -c compilers

Profiles: base

gnu

5.3
6.1

intel

pe-xe-2016--binary—binary

intelmpi

5.1

openmpi

1.10--gnu—6.1

python

3.5.1

Profiles: advanced

pgi

16.3

For each compiler more versions can be available into the specific profile. The default module is the latest version

INTEL

- List of compilers:

ifort: Fortran77 and Fortran90 compiler
icc: C compiler
cpc: C++ compiler

- Example of usage:

module load intel

icc -o my_exe prog.c
ifort -o my_exe prog.f90

GNU

- List of compilers:

gfortran: GNU Fortran compiler
gcc: GNU C compiler
g++: GNU C++ compiler

- Example of usage:

```
module load gnu
gcc -o a.out foo.c
```

IntelMpi

- List of wrappers using INTEL compilers:

mpiifort (Fortran MPI wrapper)
mpiicc (C MPI wrapper)
mpiicpc (C++ MPI wrapper)

- List of wrappers using GNU compilers:

mpif77,mpif90: (Fortran MPI wrapper)
mpicc: (C MPI wrapper)
mpicxx: (C++ MPI wrapper)

- Example of usage:

```
module load autoload intelmpi
mpiicc -o my_mpi_exe mpi_prog.c
```

Openmpi--gnu

- List of wrappers:

mpif77,mpif90: (Fortran MPI wrapper)
mpicc: (C MPI wrapper)
mpicxx: (C++ MPI wrapper)

- Example of usage:

```
module load autoload openmpi
mpicc -o my_mpi_exe mpi_prog.c
```

Python and its packages

PYTHON

- module load python
  - python

- PACKAGES
- 1. module load python
  - /…/site-packages → they contain only basic packages

- 2. module load <module_name>

- module load numpy
- module load scipy
- module load ipython
- module load cython

Python and its packages

- 3. VIRTUALENV to create isolated *Python* environments. Follow these steps:

using python interpreter from the module

- module load python

create a virtualenv, basically just a new directory (my_venv) containing all you need

- virtualenv my_venv

activate the new virtualenv

- source my_venv/bin/activate

now you can pip install whatever you need

- pip install **matplotlib**

when you are done working

- deactivate

Python and its packages

if you want to dump all the pip installed modules on your virtualenv

- pip freeze > requirements.txt

if you want to recreate tha same virtualenv

- pip install -r requirements.txt

if you want to remove the virtualenv

- rm -rf my_venv

Libraries

modmap -c libraries

Profiles: base

- blas
- boost
- fftw
- hdf5
- lapack
- mkl
- mpi4py
- netcdf
- numpy
- scalapack
- scipy
- szip
- zlib

Libraries

- The available libraries are compiled with **intel compiler** when they need a good performance, otherwise they are compiled with **gnu compiler** in order to ensure the the compatibility gnu/intel

- For each library more versions can be available into the specific profile. The default module is the latest and parallel version

- HDF5 - USE EXAMPLE

```
module load autoload hdf5
module load autoload szip
module load autoload zlib
```

$ icc **-I$HDF5_INC** input.c **-L$HDF5_LIB -lhdf5 -L$SZIP_LIB -lsz -L$ZLIB_LIB -lz**

Tools

modmap -c tools

Profiles: base

- cmake
- rcm
- scalasca
- superc
- totalview
- valgrind
- vtune

For each tool only one module is available into the specific profile. It is the latest version. The older versions are available into archive profile

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Applications

modmap -c applications

Profiles: eng

abaqus
ansys
openfoam
starccm++

Profile: chem

abinit
adf
amber
cp2k
cpmd
crystal
dl_poly
g09
gromacs
lammps
molcas
namd
nwchem
plumed
pyfrag
qe
siesta
vasp
yambo

Profile: bioinf

r

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Applications

- For each application only one module is available into the specific domain. It is the latest version. The older versions are available into archive profile

- For the same application more variants can be available and they differ for the executable name into the corresponding module

Gromacs EXAMPLE:

module load gromacs

→ executables:

mdrun
mdrun_mpi
mdrun_mpi_plumed