Software Management

The INCD software is managed using a tool called modules. This tool allows the user to load the correct environment (PATH, LD_LIBRARY_PATH, etc) for each specific software package. The main commands are explained in the next sections.

List of available Software

- All software available to INCD users is usable using modules, the presented list is context depended, some groups have customized environment bundles showed only to them:

```
[jpina@hpc7 ~]$ module avail


----------------------------------------------------------------------------------- /cvmfs/sw.el7/modules/LIP
-----------------------------------------------------------------------------------
clhep/2.3.4.3     delphes/3.4.2pre15 geant/4.10.03     lhapdf/6.1.6     pythia/6.4.26     pythia/8.2.35
root/6.08.00     root/6.16.00
delphes/3.4.1     fastjet/3.3.0     hepmc/2.6.9     madgraph/2.6.0     pythia/6.4.28     root/5.34.36
root/6.10.02     root/6.16.00-RUBEN
delphes/3.4.2pre10 geant/4.10.02.p01 heptoptagger/2.0  madgraph/2.6.1     pythia/8.2.15     root/6.04.02
root/6.14.06     xroot/4.3.0


----------------------------------------------------------------------------------- /cvmfs/sw.el7/modules/soft
-----------------------------------------------------------------------------------
aster-13.1.0          cmake-3.5.2          gcc63/netcdf-fortran/4.4.4 hdf5-1.8.16
ngspice/30          r-3.2.5          udocker/1.0.4
blat-36.2          cuda-8.0          gcc63/ngspice/30     homer-4.8     openmpi/2.1.0          r-
3.5.2          udocker/1.1.0
boost-1.55          cuda-9.0          gcc63/openmpi/2.1.0     kallisto-0.43.0     openmpi-
1.10.2     rt          udocker/1.1.0-devel
bowtie2-2.3.0          DATK          gcc63/openmpi-1.10.2     macs-1.4.2          openmpi-
2.1.0          sbcl-1.3.4          udocker/1.1.1
clang/7.0.0          fastqc-0.11.5          gcc63/openmpi-2.1.0     matlab/R2018a
parallel/20180622          schism/5.4.0          weblogo-2.8.2
clang/ngspice/30     fftw-3.3.4          gcc63/r-3.4.2     mpich-3.2          plumed-2.2.1
sicer-1.1          wine/4.2
clhep-2.2.0.8          fftw-3.3.5          gcc63/schism/5.4.0     mvapich2-1.8          python/3.7.2
```

```
star-2.5.2b

clhep-2.3.1.1          gcc-4.8          gcc-6.3          netcdf/4.6.1          python-2.7.11          teste

clhep-2.3.2.2          gcc63/mpich-3.2          gcc-7.3          netcdf2/4.6.1          python-3.5.1

trimmomatic-0.33

cmake/3.11.2          gcc63/netcdf/4.6.1          gromacs-4.6.7          netcdf-fortran/4.4.4          python-

3.5.4          udocker/1.0.2

...
```

Show / list module information

* Using this option will show the following information:

```
[jpina@hpc7 ~]$ module show gcc63/ngspice/30

----------------------------------------------------------------

/cvmfs/sw.el7/modules/soft/gcc63/ngspice/30:


module-whatis□ Sets up NGSpice

system□□ test -d /cvmfs/sw.el7/ar/ix_5400/gcc63/ngspice/30

----------------------------------------------------------------
```

Summary

software[1]	Location[2]	software	availability	complex software[3]	type of compiler[4]
gromacs-4.6.7	/cvmfs/sw.el7/modules/LIP	Gromacs 4.6.7	usable by everyone	no	OS default (gcc -V)
clang/7.0.0	/cvmfs/sw.el7/modules/soft	AMD compiler	usable by everyone	no	clang 7.0.0
gcc63/r-3.4.2	/cvmfs/sw.el7/modules/soft	R software compiled with gcc 6.3	usable by everyone	yes	gcc 6.3

[1] these are just examples and the full list of available software can be accessed by logging-in into the login machine and run command 'module avail'
[2] Path of the installed software. No action needed from the user
[3] This means if a software is composed by more than one module (compiler + software + modules)
[4] At INCD software can be compiled using several types of compilers (gcc, cland (AMD), Intel etc)

Load Software

- Please select a name using previous command

```
module load gcc63/ngspice/30
```

Loaded software

- How to list your loaded modules

```
[jpina@hpc7 ~]$ module list
Currently Loaded Modulefiles:
  1) gcc-6.3         2) gcc63/ngspice/30
```

- On this example two different software gcc 6.3 plus ngsipe 3.9.

Unload software

```
[jpina@hpc7 ~]$ module list
Currently Loaded Modulefiles:
  1) gcc-6.3         2) gcc63/ngspice/30
[jpina@hpc7 ~]$ module unload gcc63/ngspice/30
[jpina@hpc7 ~]$ module list
Currently Loaded Modulefiles:
  1) gcc-6.3
[jpina@hpc7 ~]$ module unload gcc-6.3
[jpina@hpc7 ~]$ module list
No Modulefiles Currently Loaded.
```

- Do no unload gcc-6.3 or ngspice will stop working because this software was compiled against gcc 6.3.

Help

- List usefull comands for modules software

```
[jpina@hpc7 ~]$ module help

Modules Release 3.2.10 2012-12-21 (Copyright GNU GPL v2 1991):
```

```
Usage: module [ switches ] [ subcommand ] [subcommand-args ]
```

> **NOTE** only free software is available to **ALL** users at INCD. For non-free software please contact the **INCD support helpdesk**

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