Installed Software

Software installed on Computerome

At Computerome we maintain an extensive and ever growing list of software available to our users.

This page describes how to use the software packages installed on the Computerome cluster.

To use this software you must first log in to the system, see **SSH login to Computerome 2.0**.

Using modules

Software installed on Computerome is managed using **modules** as described in the Environment Modules Project.

Modules provide a mechanism to set/unset all environment variables related to a given package in one UNIX shell command.
Modules definitions are contained in so-called **modulefiles** located in several directories. The directory structure is dependent on the system.

Modules are activated by default for users on Computerome.

Listing and finding modules

Computerome utilities for modules

To help in finding tools, we have created a module 'computerome_utils' with a handful of small utilities - currently (2020.09.30):

```
moduleavail <string> - list available environment modules
moduleapropos [-i] <string> - search for string in module information
modulewhatis <string> - list module information
findintools [-i] <string> - search for string across all applications (modules, perl, anaconda, R)
findinanaconda [-i] <string> - search for string in Anaconda packages
findinperl [-i] <string> - search for string in Perl packages
findinr [-i] <string> - search for string in R packages
```

Just load it and try it out

$ module load tools computerome_utils/2.0

`module avail`

To list your currently available modules, type:

```
$ module avail
```

The command will per default list something similar to this:

```
$ module avail
------------------------------------------------------------------------------- /cm/local/modulefiles
------------------------------------------------------------------------------
cluster-tools/8.2  cmd   cmsub  freeipmi/1.6.2  ipmitool/1.8.18  module-git   ngs   openldap  python36  tools
cm-cloud-copy/8.2  cmsh  dot    gcc/8.2.0       lua/5.3.5        module-info  null  python2   shared

------------------------------------------------------------------- /cm/local/.modulefiles_cache/shared
/modulefiles -------------------------------------------------------------------
blacs/openmpi/gcc/64/1.1patch03  cuda10.1/blas/10.1.243      default-environment               hwloc/1.
11.11                            openblas/dynamic(default)
blas/gcc/64/3.8.0                cuda10.1/fft/10.1.168       fftw2/openmpi/gcc/64/double/2.1.5  intel-tbb-oss
/ia32/2019_20190410oss     openblas/dynamic/0.2.20
bonnie++/1.97.3                  cuda10.1/fft/10.1.243       fftw2/openmpi/gcc/64/float/2.1.5   intel-tbb-oss
/intel64/2019_20190410oss  openmpi/gcc/64/1.10.7
cm-pmix3/3.1.4                   cuda10.1/nsight/10.1.168    fftw3/openmpi/gcc/64/3.3.8         iozone
/3_482                            openmpi/gcc/64/4.0.2
cuda/toolkit/10.1/10.1.168       cuda10.1/nsight/10.1.243    gdb/8.2                            lapack/gcc/64/3.
8.0                     scalapack/openmpi/gcc/64/2.0.2
cuda/toolkit/10.1/10.1.243       cuda10.1/profiler/10.1.168  globalarrays/openmpi/gcc/64/5.7    mpich/ge/gcc/64
/3.3                     sge/2011.11p1
cuda/toolkit/101/10.1.168        cuda10.1/profiler/10.1.243  hdf5/1.10.1                        mvapich2/gcc/64
/2.3                     slurm/18.08.8
cuda/toolkit/101/10.1.243        cuda10.1/toolkit/10.1.168   hdf5_18/1.8.20                     netcdf/gcc/64/4.
6.1
cuda10.1/blas/10.1.168           cuda10.1/toolkit/10.1.243   hpl/2.2                            netperf/2.7.0

------------------------------------------------------------------- /cm/local/.modulefiles_cache/tools
/modulefiles -------------------------------------------------------------------
454/2.9                                depot_tools/20160809                    intel/perflibs
/2018_update2              netphorest_human/2.1           samblaster/0.1.24
abawaca/20170520                       diamond/0.7.9                           intel/perflibs
/2018_update3              netsurfp/1.0b                  samclip/0.2
abctoolbox/20090930                    diamond/0.8.31                          intel/perflibs
/2018_update4              netsurfp/1.0d                  samstat/1.5.1
abra2/2.20                             diamond/0.9.13                          intel/perflibs
/2019                      nettle/3.5.1                   samtools/0.1.18
abricate/0.5                           diamond/0.9.24                          intel/perflibs
/2019_update2              netturnp/1.0a                  samtools/0.1.19
abricate/0.8.7                         diginorm/20131102                       intel/perflibs
/2019_update3              new_fugue/20100602             samtools/1.2
abyss/2.0.2                            disco/1.0                               intel/perflibs
/2019_update5              newick-utils/1.6               samtools/1.3.1
abyss/2.1.5                            discovar/52188                          intel/redist/2017.
2.174                  nextflow/0.31.1               samtools/1.4
activetcl/8.6.8.0                      discovar/52488                          intel/redist
/2017_update4                nextflow/19.03.0-edge          samtools/1.4.1
AdapterRemoval/2.1.3                   discovardenovo/52488                    intel/redist
/2018                        nextflow/19.07.0               samtools/1.5
adapterremoval/2.1.3                   discovarexp/52242                       intel/redist
/2018_update1                nextflow/19.09.0-edge          samtools/1.6
AdapterRemoval/2.1.7                   dissect/1.2                             intel/redist
/2018_update3                ngb/2.5.1.374.1                samtools/1.7
adapterremoval/2.1.7                   dlcpar/1.0                              intel/redist
/2018_update5                ngless/0.7.1                   samtools/1.8
AdapterRemoval/2.2.0                   docker-compose/1.21.2                   intel/redist
/2019                        ngless/0.8.1                   samtools/1.9
adapterremoval/2.2.0                   dos2unix/7.3.1                          intel/redist
/2019_update2                ngless/0.9.1                   sas/DEPRECATED/9.4
AdapterRemoval/2.2.1a                  dos2unix/7.4.0                          interop/1.
1.8                            ngmlr/0.2.7                    satsuma/3.0
adapterremoval/2.2.1a                  drop-seq_tools/2.0.0                    interproscan/5.11-
```

```
51.0                    ngsadmix/32                    savvy/1.2.0
AdapterRemoval/2.2.2                       dropest/0.8.5                              interproscan/5.13-
52.0                    ngsqctoolkit/2.3.3             sbcl/1.3.17
adapterremoval/2.2.2                       dropest/20190401                           interproscan/5.17-
56.0                    ngstools/20180814              scaffold/4.9.0
AdapterRemoval/2.2.4                       dssp/2.0.4                                 interproscan/5.19-
58.0                    ngstools/20190624              scalpel/0.5.2
adapterremoval/2.2.4                       dssp/2.2.1                                 interproscan/5.22-
61.0                    nim/0.16.0                     schmutzi/1.5.5.5
admixture/1.3.0                            duphold/0.1.5                              interproscan/5.25-
64.0                    nim/1.0.0                      schmutzi/20161010
admixture/1.23                             ea-utils/1.1.2-806                         interproscan/5.32-
71.0                    ninja/1.8.2                    scipion-dev/1.1F
adolc/2.5.2                                eager-gui/1.92.37                          interproscan/5.36-
75.0                    ninja/1.9.0                    scipion/1.0
adxv/1.9.10                                eagle/2.3.5                                ioapi/3.
1                                nlopt/2.4.2                    scipion/1.0.0
adxv/1.9.11                                eclipse-cpp/2018-09                        iozone/3.
434                              nnlinplayer/1.0                scipion/1.0.1
adxv/1.9.12                                eclipse-parallel/2018-09                   iperf/2.
0.5                               nodejs/8.9.1_LTS               scipion/1.1
agouti/0.3.3.1-gc8bd255                    edirect/7.50                               iperf/3.
0.11                              nodejs/9.2.0                   scipion/1.2
albula/3.2.0-2                             effectorp/1.0                              iperf/3.
1                                 nodejs/10.1.0                  scipion/2.0.0
ale/20130717                               effectorp/2.0                              ipn/0.
581                                 nodejs/10.16.0_LTS             scratch-1d/1.1
alfred/0.1.17                              eggnog-mapper/0.12.7                       iqsub/1.
0                                 nodejs/12.6.0                  screen/4.6.2
allelecount/3.2.3                          eggnog-mapper/0.99.3                       iqtree/1.
5.5                              novocaller/20190521            scwrl/4.0
allelecount/3.3.1                          eggnog-mapper/1.0.3                        iqtree/1.
6.1                              novocraft/3.03.02              searchgui/2.8.5
:
```

Regular users should focus on modules located under **`/cm/local/modulefiles`**, in particular those highlighted above: **`tools`**, **`ngs`**, **`shared`** and **`use.own`**. These can be loaded using the using the command:

```
$ module load <module name>
```

where **<module name>** can be **tools**, **ngs**, **shared**, **use.own** etc.

You can limit the number of listed modules, by adding the first letter(s) of the modulename to the **`module avail`** command.

```
$ module avail f
------------------------------------------------------------------------------- /cm/local/modulefiles
------------------------------------------------------------------------------
freeipmi/1.6.2

------------------------------------------------------------------- /cm/local/.modulefiles_cache/shared
/modulefiles ------------------------------------------------------------------
fftw2/openmpi/gcc/64/double/2.1.5  fftw2/openmpi/gcc/64/float/2.1.5  fftw3/openmpi/gcc/64/3.3.8

------------------------------------------------------------------- /cm/local/.modulefiles_cache/tools
/modulefiles ------------------------------------------------------------------
falcon/0.3.0           fastp/0.19.4           fasttree/2.1.8                fftw/3.3.6-pl1
firebird/CS/2.5.7.27050-0     flye/2.4.2                  frogs/2.0.0
falcon/20160621        fastphylo/1.0.1        fasttree/2.1.9                fftw/3.3.6-pl2
firebird/SS/2.5.7.27050-0     foldx/4                     frustratometer/2.0
falcon_zip/20180716    fastq-tools/0.8        fasttree/2.1.10               fftw/3.3.7                firefox
/67.0                  foldx/4_expires20190409      funannotate/1.1.1
famseq/1.0.3           fastqc/0.11.2          fastuniq/1.1                  fftw/3.3.8                fithic
/1.0.1                  fpocket/3.1.2               funannotate/1.2.0
fasta/36.3.8e          fastqc/0.11.4          fastx_toolkit/0.0.14(default)  fgbio/0.8.1
fix_assembly_errors/20180508  fpocket/3.1.3               funannotate/1.3.2
fasta/36.3.8g          fastqc/0.11.5          fchmm/1.0.0                   fgbio/1.0.0               flash
/1.2.11                  fraggenescan/1.30            funannotate/1.3.4
fastani/1.1            fastqc/0.11.7          fdt/0.25                      fgwas/0.3.6
flashpca/2.0                  freebayes/1.0.2-33-gdbb6160  funannotate/1.5.1
fastme/2.1.5           fastqc/0.11.8          fdupes/1.6.1                  figtree/1.4.4             fltk/1.
3.3                    freebayes/1.1.0-50-g61527c5  funannotate/1.6.0
fastml/3.1             fastqtl/2.184          feh/3.1                       filezilla/3.44.2          fltk/1.
3.4-2                  freebayes/1.2.0-2-g29c4002   fuseq/1.1.2
fastNGSadmix/20190716  fastsimcoal/2.6.0.3     ffmpeg/4.1.3                  find-clumpiness/0.2.3.1   fltk/1.
3.5                    freesasa/1.1                fusionmap/20150331
fastp/0.12.2           faststructure/20150319  fftw/3.3.4                    fineradstructure/20180529  flye/2.
3.7                    freetype/2.9.1
```

module whatis

To get basic information on the modulefiles, you can use **`module whatis [modulefile...]`**.

```
$ module whatis tools ngs gcc anaconda3/4.4.0
------------------------------------------------------------------------------- /cm/local/modulefiles
------------------------------------------------------------------------------
              tools: Adds cached /services/tools modules

------------------------------------------------------------------------------- /cm/local/modulefiles
------------------------------------------------------------------------------
                ngs: Adds cached NGS modules

------------------------------------------------------------------------------- /cm/local/modulefiles
------------------------------------------------------------------------------
          gcc/8.2.0: adds GNU Cross Compilers to your environment variables

------------------------------------------------------------------- /cm/local/.modulefiles_cache/tools
/modulefiles ------------------------------------------------------------------
          gcc/4.9.4: GCC 4.9.4 - GNU Compiler Collection
          gcc/5.4.0: GCC 5.4.0 - GNU Compiler Collection
          gcc/6.2.0: GCC 6.2.0 - GNU Compiler Collection
          gcc/7.2.0: GCC 7.2.0 - GNU Compiler Collection
          gcc/8.2.0: GCC 8.2.0 - GNU Compiler Collection

------------------------------------------------------------------- /cm/local/.modulefiles_cache/tools
/modulefiles ------------------------------------------------------------------
     anaconda3/4.4.0: Anaconda3 4.4.0 - Python 3 distribution for scientific computing
```

module apropos

To search for a particular string in the basic information on the modulefiles, you can use **`module apropos <string>`**.

This is the **only** module sub-command which currently does for case insensitive module parameter evaluation.

```
$ module apropos genome
---------------------------------------------------------------------- /cm/local/.modulefiles_cache/tools
/modulefiles ----------------------------------------------------------------------------
agouti/0.3.3.1-gc8bd255: AGOUTI 0.3.3.1-gc8bd255 - Annotated Genome Optimization Using Transcriptome Information
    allpathslg/52415: ALLPATHS-LG 52415 - short read genome assembler
    allpathslg/52488: ALLPATHS-LG 52488 - short read genome assembler
     anicalculator/1: ANIcalculator 1 - compute gANI,AF values between two genomes
          arcs/1.0.0: ARCS 1.0.0 - Scaffolding genome sequence assemblies using 10X Genomics GemCode/Chromium
data
          arcs/1.1.0: ARCS 1.1.0 - Scaffold genome sequence assemblies using 10x Genomics data
  argweaver/20150629: ARGweaver 20150629 - Sampling and manipulating genome-wide ancestral recombination graphs
      ascatngs/4.2.1: ascatNgs 4.2.1 - Somatic copy number analysis using paired end wholegenome sequencing
         baypass/2.1: BayPass 2.1 - Genome-Wide Scan for Adaptive Differentiation and Association Analysis with
population-specific covariables
       bedops/2.4.14: BEDOPS 2.4.14 - fast, highly scalable and easily-parallelizable genome analysis toolkit
       bedops/2.4.35: BEDOPS 2.4.35 - fast, highly scalable and easily-parallelizable genome analysis toolkit
     bedtools/2.22.1: bedtools 2.22.1 - powerful toolset for genome arithmetic
     bedtools/2.26.0: bedtools 2.26.0 - powerful toolset for genome arithmetic
     bedtools/2.27.1: bedtools 2.27.1 - powerful toolset for genome arithmetic
     bedtools/2.28.0: bedtools 2.28.0 - powerful toolset for genome arithmetic
          bmagwa/1.0: BMAGWA 1.0 - Bayesian Model Averaging in Genome-wide Association Studies
 bmagwa/2.0-20121210: BMAGWA 2.0-20121210 - Bayesian Model Averaging in Genome-wide Association Studies
            bpga/1.3: BPGA 1.3 - tool for ultra-fast pan-genome analysis of microbes
    brat_ng/20150505: BRAT NextGen 20150505 - Bayesian analysis of recombinations in whole-genome DNA sequence
data
breakdancer/1.1_2011_02_21: BreakDancer 1.1_2011_02_21 - Perl/Cpp package that provides genome-wide detection
of structural variants from next generation paired-end sequencing reads
busco/3.0.1_20170529: BUSCO 3.0.1_20170529 - Assessing genome assembly and annotation completeness with
Benchmarking Universal Single-Copy Orthologs
busco/3.0.2b_20170717: BUSCO 3.0.2b_20170717 - Assessing genome assembly and annotation completeness with
Benchmarking Universal Single-Copy Orthologs
           bwa/0.6.1: BWA 0.6.1 - Burrows-Wheeler Aligner, mapping low-divergent sequences against a large
reference genome
     bwa/0.7.6a-r433: BWA ExaScience 0.7.6a-r433 - Burrows-Wheeler Aligner (ExaScience fork), mapping low-
divergent sequences against a large reference genome
          bwa/0.7.10: BWA 0.7.10 - Burrows-Wheeler Aligner, mapping low-divergent sequences against a large
reference genome
          bwa/0.7.12: BWA 0.7.12 - Burrows-Wheeler Aligner, mapping low-divergent sequences against a large
reference genome
          bwa/0.7.15: BWA 0.7.15 - Burrows-Wheeler Aligner, mapping low-divergent sequences against a large
reference genome
         bwa/0.7.16a: BWA 0.7.16a - Burrows-Wheeler Aligner, mapping low-divergent sequences against a large
reference genome
       cbrc_last/861: CBRC LAST 861 - Genome-Scale Sequence Comparison
       cbrc_last/963: CBRC LAST 963 - Genome-Scale Sequence Comparison
 cdsgff2seq/20070813: cdsgff2seq 20070813 - read GFF, genome fasta; write CDS sequence, aa translation (with
check for exon phase). write gene/exon offset subranges
clonalframeml/20170927: ClonalFrameML 20170927 - Efficient Inference of Recombination in Whole Bacterial Genomes
    codingquarry/2.0: CodingQuarry 2.0 - highly accurate hidden Markov model gene prediction in fungal genomes
using RNA-seq transcripts
  control-freec/11.5: Control-FREEC 11.5 - Copy number and genotype annotation in whole genome and whole exome
sequencing data
 cortex_var/1.0.5.21: cortex_var 1.0.5.21 - genome assembly and variation analysis from sequence data
        das_tool/1.0: DAS_Tool 1.0 - Tool for genome-resolved metagenomics
      das_tool/1.1.1: DAS_Tool 1.1.1 - Tool for genome-resolved metagenomics
           disco/1.0: Disco 1.0 - Multi-threaded Distributed Memory Overlap-Layout-Consensus (OLC) Metagenome
Assembler
      discovar/52188: DISCOVAR 52188 - assemble genomes and find variants
      discovar/52488: DISCOVAR 52488 - assemble genomes and find variants
discovardenovo/52488: DISCOVAR de novo 52488 - assemble genomes and find variants
   discovarexp/52242: DISCOVAR de novo - assemble genomes and find variants
         dissect/1.2: DISSECT 1.2 - massive genome analysis tool
eggnog-mapper/0.12.7: EggNOG-mapper 0.12.7 - Fast genome-wide functional annotation through orthology assignment
eggnog-mapper/0.99.3: EggNOG-mapper 0.99.3 - Fast genome-wide functional annotation through orthology assignment
 eggnog-mapper/1.0.3: EggNOG-mapper 1.0.3 - Fast genome-wide functional annotation through orthology assignment
eggnog-mapper/20170307: EggNOG-mapper 20170307 - Fast genome-wide functional annotation through orthology
assignment
estimate_genome_size.pl/0.05: estimate_genome_size.pl 0.05 - Scripts to estimate genome size and coverage from
kmer distribution generated by jellyfish
```

Example using `module apropos`

```
$ module apropos netMHC
------------------------------------------------------------------------ /cm/local/.modulefiles_cache/tools
/modulefiles ------------------------------------------------------------------------
         netmhc/3.0c: NetMHC 3.0c - Prediction of peptide-MHC class I binding using artificial neural networks
(ANNs)
         netmhc/3.4a: NetMHC 3.4a - Prediction of peptide-MHC class I binding using artificial neural networks
(ANNs)
         netmhc/4.0a: NetMHC 4.0a - Prediction of peptide-MHC class I binding using artificial neural networks
(ANNs)
        netmhcii/2.3: NetMHCII 2.3 - predicts binding of peptides to HLA-DR, HLA-DQ, HLA-DP and mouse MHC class
II alleles
    netmhciipan/3.1a: NetMHCIIpan 3.1a - predicts binding of peptides to MHC class II molecules
     netmhciipan/3.2: NetMHCIIpan 3.2 - predicts binding of peptides to MHC class II molecules
      netmhcpan/2.8a: NetMHCpan 2.8a - Prediction of peptide-MHC class I binding using artificial neural
networks (ANNs)
      netmhcpan/3.0a: NetMHCpan 3.0a - Prediction of peptide-MHC class I binding using artificial neural
networks (ANNs)
      netmhcpan/4.0a: NetMHCpan 4.0a - Prediction of peptide-MHC class I binding using artificial neural
networks (ANNs)
$ module load netmhciipan/3.1a
```

`module display`

Further information is available with **`module display [modulefile...]`**.

```
$ module display RepeatMasker/4.0.6
-------------------------------------------------------------------
/cm/local/.modulefiles_cache/tools/modulefiles/RepeatMasker/4.0.6:

module-whatis   {RepeatMasker 4.0.6 - screens DNA sequences for interspersed repeats and low complexity DNA
sequences}
conflict        RepeatMasker
prereq          perl
prereq          trf
prereq          ncbi-rmblastn hmmer
prepend-path    PATH /services/tools/RepeatMasker/4.0.6/util
prepend-path    PATH /services/tools/RepeatMasker/4.0.6
prepend-path    PERL5LIB /services/tools/RepeatMasker/4.0.6
setenv          REPEATMASKER /services/tools/RepeatMasker/4.0.6

RepeatMasker is a program that screens DNA sequences for interspersed repeats and low complexity DNA sequences.
The output of the program is a detailed annotation of the repeats that are present in the query sequence as
well as a modified version of the query sequence in which all the annotated repeats have been masked (default:
replaced by Ns). Currently over 56% of human genomic sequence is identified and masked by the program. Sequence
comparisons in RepeatMasker are performed by one of several popular search engines including nhmmer,
cross_match, ABBlast/WUBlast, RMBlast and Decypher. RepeatMasker makes use of curated libraries of repeats and
currently supports Dfam ( profile HMM library derived from Repbase sequences ) and Repbase, a service of the
Genetic Information Research Institute.
-------------------------------------------------------------------
```

`This command will also list conflict (modules which` **`conflict`** `with this) and prereq (modules which` **`must be loaded`** `t o use this).`

Listing software not included as modules

Sometimes, the software you are looking for will **not** have its own module, but comes as part of a module.

The most common examples of this are **Anaconda (python) packages**, **Perl-modules**, and **R packages**. In these cases, `module display` will inform you how you can find further information.

Anaconda (python) packages

```
$ module display anaconda3/4.4.0
-------------------------------------------------------------------
/services/tools/modulefiles/anaconda3/4.4.0:

module-whatis    anaconda3 4.4.0 - Python 2 distribution for scientific computing
conflict         anaconda3
conflict         anaconda
prepend-path     PATH /services/tools/anaconda3/4.4.0/bin
prepend-path     MANPATH /services/tools/anaconda3/4.4.0/share/man
prepend-path     PYTHONPATH /services/tools/anaconda3/4.4.0/bin
prepend-path     PYTHONPATH /services/tools/anaconda3/4.4.0/lib
prepend-path     PYTHONPATH /services/tools/anaconda3/4.4.0/lib/python2.7
setenv           ANACONDAHOME /services/tools/anaconda3/4.4.0
setenv           QT_PLUGIN_PATH

To list currently installed Python packages, use command 'pip list' or 'pip list | grep -i <packagename>'
-------------------------------------------------------------------

$ module load anaconda3/4.4.0
$ pip list
Package                           Version             Location
--------------------------------- ------------------- ------------------------------
-etworkx                          2.4
-otocore                          1.10.80
-penpyxl                          2.6.2
-ytest                            3.3.2
absl-py                           0.7.1
adjustText                        0.7.3
agate                             1.6.1
agate-dbf                         0.2.0
agate-excel                       0.2.2
agate-sql                         0.5.3
ago                               0.0.9
aioeasywebdav                     2.2.0
aiohttp                           2.2.5
alabaster                         0.7.10
albatradis                        x.y.z
alchy                             2.2.2
alembic                           1.0.11
altair                            4.1.0
altgraph                          0.15
anaconda-client                   1.6.3
anaconda-navigator                1.6.2
anaconda-project                  0.6.0
ansible                           2.5.0
appdirs                           1.4.3
apsw                              3.9.2.post1
...
```

Perl-modules

```
$ module display perl/5.20.2
-------------------------------------------------------------------
/services/tools/modulefiles/perl/5.20.2:

module-whatis    Perl 5.20.2 - highly capable, feature-rich programming language
conflict         perl
conflict         perl_LEGACY
prepend-path     PATH /services/tools/perl/5.20.2/bin
prepend-path     MANPATH /services/tools/perl/5.20.2/man
prepend-path     PERL5LIB /services/tools/perl/5.20.2/lib/5.20.2

To list currently installed Perl modules, use command 'cpan -l'
-------------------------------------------------------------------

$ module load perl/5.20.2
$ cpan -l
arybase 0.07
Fcntl   1.11
re      0.26
NDBM_File       1.12
Socket  2.013
Opcode  1.27
B       1.48
POSIX   1.38_03
SDBM_File       1.11
Storable        2.49_01
Config  5.020002
DynaLoader      1.25
Cwd     3.48_01
...
```

R packages

```
$ module display R/3.2.5
-------------------------------------------------------------------
/services/tools/modulefiles/R/3.2.5:

module-whatis    R 3.2.5 - software environment for statistical computing and graphics
conflict         R
prereq   gcc
prepend-path     PATH /services/tools/R/3.2.5/bin
prepend-path     MANPATH /services/tools/R/3.2.5/share/man
prepend-path     LD_LIBRARY_PATH /services/tools/R/3.2.5/lib64/R/library
prepend-path     LD_LIBRARY_PATH /services/tools/R/3.2.5/lib64/R/lib
prepend-path     INCLUDE_PATH /services/tools/R/3.2.5/lib64/R/include
prepend-path     CPATH /services/tools/R/3.2.5/lib64/R/include
prepend-path     PKG_CONFIG_PATH /services/tools/R/3.2.5/lib64/pkgconfig
setenv           RSCRIPTBINDIR /services/tools/R/3.2.5/bin

Use the following R commands to list installed packages:
> packinfo <- installed.packages()
> packinfo[,c("Package","Version")]
-------------------------------------------------------------------

$ module load gcc/5.2.0 R/3.2.5
$ R
> packinfo <- installed.packages()
> packinfo[,c("Package","Version")]
                                          Package
abind                                     "abind"
acepack                                   "acepack"
ada                                       "ada"
adabag                                    "adabag"
ade4                                      "ade4"
AER                                       "AER"
affxparser                                "affxparser"
...
                                          Version
abind                                     "1.4-5"
acepack                                   "1.4.1"
ada                                       "2.0-5"
adabag                                    "4.1"
ade4                                      "1.7-5"
AER                                       "1.2-5"
affxparser                                "1.42.0"
...
```

Using module output with other commands

`module` commands write their output to **STDERR** (where 'normal' commands write to **STDOUT**). So if you, for instance, use `grep` after a `module` command, the result might not be quite what you expected.

```
$ module load tools
$ module whatis | grep sequence
cluster-tools/7.0    : Adds cluster-tools to your environment
cmd                  : Adds the CMDaemon binaries to your path.
dot                  : adds `.' to your PATH environment variable
freeipmi/1.3.4       : adds FREEIPMI to your environment variables
ipmitool/1.8.13      : adds IPMItool to your environment variables
module-git           : get this version of the module sources from SourceForge.net
module-info          : returns all various module-info values
mvapich2/mlnx/gcc/64/2.0: adds MVAPICH2-gcc to your environment variables
ngs                  : adds NGS modules
null                 : does absolutely nothing
openldap             : Adds the CMDaemon binaries to your path.
openmpi/mlnx/gcc/64/1.8.4rc1: adds OpenMPI to your environment variables
shared               : adds shared modules
tools                : adds /services/tools modules
use.own              : adds your own modulefiles directory to MODULEPATH
version              : Changes the MODULE_VERSION environment variable
acml/gcc/64/5.3.1    : adds ACML to your environment variables
acml/gcc/fma4/5.3.1  : adds ACML to your environment variables
acml/gcc/mp/64/5.3.1 : adds ACML to your environment variables
acml/gcc/mp/fma4/5.3.1: adds ACML to your environment variables
...list goes on and on and on...
```

You must remember to redirect STDERR (the **2>&1** below):

```
$ module whatis 2>&1 | grep sequence
FastTree/2.1.8       : FastTree 2.1.8 - A-M-L phylogenetic trees from alignments of nucleotide or protein
sequences
RepeatMasker/4.0.5   : RepeatMasker 4.0.5 - screens DNA sequences for interspersed repeats and low complexity
DNA sequences
beagle-lib/20150407  : BEAGLE 20150407 - general purpose library for evaluating the likelihood of sequence
evolution on trees
bowtie2/2.2.4        : Bowtie 2 2.2.4 - ultrafast and memory-efficient aligning of sequencing reads to long
reference sequences
bowtie2/2.2.5        : Bowtie 2 2.2.5 - ultrafast and memory-efficient aligning of sequencing reads to long
reference sequences
bwa/0.7.10           : Burrows-Wheeler Aligner 0.7.10 - mapping low-divergent sequences against a large
reference genome
bwa/0.7.12           : Burrows-Wheeler Aligner 0.7.12 - mapping low-divergent sequences against a large
reference genome
cd-hit/4.5.4         : CD-HIT 4.5.4 - program for clustering and comparing protein or nucleotide sequences
cd-hit/4.6.1         : CD-HIT 4.6.1 - program for clustering and comparing protein or nucleotide sequences
hmmer/3.1b2          : HMMER 3.1b2 - biosequence analysis using profile hidden Markov models
interproscan/5.11-51.0: InterProScan 5.11-51.0 - scan protein and nucleic sequences against InterPro's
signatures
ncbi-blast/2.2.30+   : BLAST 2.2.30+ - Basic Local Alignment Search Tool, finds regions of local similarity
between sequences
sortmerna/2.0        : SortMeRNA 2.0 - biological sequence analysis tool for filtering, mapping and OTU-picking
NGS reads
trf/4.07b            : Tandem Repeats Finder 4.07b - program to locate and display tandem repeats in DNA
sequences
trinityrnaseq/2.0.6  : Trinity 2.0.6 - De novo Assembly of transcript sequences from Illumina RNA-Seq data
usearch/7.0.1090     : USEARCH 7.0.1090 - Ultra-fast sequence analysis with high-throughput search and
clustering
usearch/8.0.1623     : USEARCH 8.0.1623 - Ultra-fast sequence analysis with high-throughput search and
clustering
velvet/1.2.10        : Velvet 1.2.10 - sequence assembler for very short reads
vsearch/1.1.3        : VSEARCH 1.1.3 - multithreaded tool for processing metagenomic sequences
```

Adding and removing modules

`module load`

To add one or more modules, use **`module load [modulefile...]`**.

Modules listed **without** version information (like `tools`) reference a new **set of modulefiles**, so if you for instance load **`tools`** and **`ngs`** modules, you will get access to a massive list of extra modulefiles.

```
$ module load tools ngs
$ module avail
...ignoring parts of listing for readability...
-------------------------------------------------- /cm/local/.modulefiles_cache/modulefiles
--------------------------------------------------
anaconda3/2.1.0                  hdf5/1.10.0                      plink2/1.90beta3
anaconda3/2.2.0                  hdf5/1.8.15p1                    plumed/2.2.1
anaconda3/4.4.0                  hisat2/2.0.1-beta                polysolver/1.0
anaconda3/2.1.0                  hkl2map/0.3.i-beta               poppler/0.45.0
anaconda3/2.2.0                  hlaminer/1.3                     pplacer/1.1.alpha17
anaconda3/4.4.0                  hlareporter/1.0.3                prank/140603
anarci/1.0                       hla-vbseq/20150729               preseq/1.0.2
annovar/2015jun17                hmmer/2.3.2                      price/1.2
ansys/16.2                       hmmer/3.1b2                      prinseq-lite/0.20.4
ansys/17.0                       htslib/1.2.1                     prodigal/2.6.2
ansys/17.1                       htslib/1.3.1                     progressivecactus/20160427
apache-maven/3.3.3               idba/1.1.1(default)              prokka/1.11
...long listing left out...

------------------------------------------------ /cm/local/.modulefiles_cache/ngs/modulefiles
------------------------------------------------
bcl2fastq/2.17.1.14              ncbi-blast/2.2.26                SPAdes/3.7.0
bedtools/2.22.1(default)         ncbi-blast/2.2.30+               SPAdes/3.8.0
bwa/0.7.10(default)              ncbi-blast/2.2.31+               sratoolkit/2.4.5-2
circos/0.64                      ncbi-tools/current(default)      sratoolkit/2.5.7
circos/0.67-7(default)           netmhciipan/3.1a                 srnaworkbench/4.0-alpha
circos-tools/0.21                netmhcpan/2.8a                   srnaworkbench/4.1-alpha
cope/1.2.5                       netsurfp/1.0b                    ssake/3.8.3
cufflinks/2.2.1                  ngsqctoolkit/2.3.3               tabix/0.2.6
ensembl-tools/78(default)        PBSuite/15.2.20                  tabix/1.2.1(default)
express/1.5.1                    pear/0.9.6                       trf/4.07b
...long listing left out...
```

Modules listed **with** version information (like `gcc/4.8.2`) reference a **particular version** of a tool.
Generally, it is recommended to always include the **version** when loading a tool; if you **do not** specify version, the **`(default)`** will be loaded if any is available - otherwise the command will print an error.

```
$ module load gcc
$ which gcc
/cm/shared/apps/gcc/4.8.2/bin/gcc
$ module load anaconda3/2.1.0
$ which python
/services/tools/anaconda-2.1.0/bin/python
```

Modules will report any `conflict` and missing `prereq`

```
$ module load RepeatMasker/4.0.6
RepeatMasker/4.0.6(37):ERROR:151: Module 'RepeatMasker/4.0.6' depends on one of the module(s) 'perl/5.8.9 perl
/5.20.2 perl/5.20.1'
RepeatMasker/4.0.6(37):ERROR:102: Tcl command execution failed: prereq perl
```

If you get such a message, you can use **`module display` command** for further information.

```
$ module display RepeatMasker/4.0.6
-------------------------------------------------------------------
/services/tools/modulefiles/RepeatMasker/4.0.6:

module-whatis    RepeatMasker 4.0.6 - screens DNA sequences for interspersed repeats and low complexity DNA
sequences
conflict         RepeatMasker
prereq   perl
prereq   trf
prereq   ncbi-rmblastn
prepend-path     PATH /services/tools/RepeatMasker/4.0.6
prepend-path     PERL5LIB /services/tools/RepeatMasker/4.0.6
-------------------------------------------------------------------
```

module list

Verify which modules are loaded

```
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) anaconda3/2.1.0
```

module switch

To switch loaded modulefile1 with modulefile2, use **`switch [modulefile1] modulefile2`**
If **modulefile1** is not specified, then it is assumed to be the currently loaded module with the same **root name** as **modulefile2**.

```
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) anaconda3/2.1.0
$ module switch anaconda3/2.1.0 anaconda3/4.4.0
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) anaconda3/4.4.0
```

```
$ module switch anaconda3/2.2.0
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) anaconda3/2.2.0
```

```
$ module switch anaconda3/2.2.0 perl/5.20.2
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) perl/5.20.2
```

module unload

To remove one or more modules, use **`module unload [modulefile...]`**

```
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2        2) tools            3) ngs              4) perl/5.20.2
$ module unload perl ngs
$ module list
Currently Loaded Modulefiles:
  1) gcc/4.8.2   2) tools
```

module purge

In case all modules need to be unloaded at once use:

```
$ module purge
$ module list
No Modulefiles Currently Loaded.
```

Managing modules in your login environment

You should keep the number of modules that you load in your login environment to an **absolute minimum**, usually limited to only **`tools`** and/or **`ngs`**. Having too many modules loaded can potentially cause problems with pre-requirements and/or conflicts, affecting or even breaking your environment.

It is possible to permanently add, manipulate and remove modules in your login environment, by using the **`module init...`** family of commands.

Use <tab>-completion to list the sub-commands:

```
$ module init<tab><tab>
initadd      initclear    initlist     initprepend  initrm       initswitch
```

initadd modulefile...

Add modulefile(s) to the shell's initialization file in the user's home directory.

initprepend modulefile [modulefile...]

Does the same as initadd but prepends the given modules to the beginning of the list.

initrm modulefile...

Remove modulefile(s) from the shell's initialization files.

initswitch modulefile1 modulefile2

Switch modulefile1 with modulefile2 in the shell's initialization files.

initlist

List all of the modulefiles loaded from the shell's initialization file.

initclear

Clear all of the modulefiles from the shell's initialization files.

Further information is available in MAN page for 'module'

```
$ man module
```

Modules in batch jobs

With permanent module settings described above submit a batch job with standard `qsub` command.

First add anaconda2/2.2.0 (which includes Python 2.7) to your login environment:

```
$ module initadd tools anaconda2/2.2.0
```

Start a new login shell to activate the updated environment, and run your script:

```
$ qsub script.py
```

with an example `script.py`::

```
#!/usr/bin/env python

from ase import Hartree
print Hartree
```

You can also enable the required modules for a given batch job (depending on the shell this may work only when permanent modules settings related to those modules are **NOT** present in you shell startup scripts).
This feature is useful mostly for developers when comparing different versions of a code, or for making sure that a given software will be used during the whole computational project.

Examples are given below:

Create the following `myscript.sh` script::

```
#!/bin/sh
module load tools
module load anaconda2/2.2.0          # For Python 2.7
module load unison
module load ncbi-blast

python script.py
```

You submit this script with::

```
$ qsub myscript.sh
```

Modules in Perl

With our standard Perl, `module load tools perl`, we have included a PM Env::Modulecmd that provides an automated interfaces to the `module` com mand directly from inside Perl scripts.

Using personal modules

The recommended place to keep personal modules is under **`~/privatemodules`**. To enable this directory use the following command::

```
$ module load use.own
```

and to disable it::

```
$ module unload use.own
```

Computerome provides commented templates in directory **`/services/tools/modulefiles/.template_simple/`**.

Please read the online Man page of MODULEFILE for further information.

Requesting software

To request installation of new software (or other version of existing software), please send a mail from your department mail to Computerome support - preferably including a descriptive subject line, incl. tool name, and information on where the requested software can be obtained (Home-page, download information, etc.):

Subject: Software request - NewBrilliantTool

```
Hi,
I would like to use NewBrilliantTool on Computerome, it is available from:
http://<some_url>/software/NewBrilliantTool
```

User installed software

Individual users can also install own software in their **Project** (for sharing inside the project) or **HOME** (for strictly personal use) directory.

This is **only** recommended for software that is actively being developed or maintained at Computerome.
Regular software should preferably be available through the standard modules structure.

Tips and Tricks

Unable to render {include} The included page could not be found.