Software Catalog

Below is a table of all custom compiled software available on the new side of cluster (gplogin2/3) via lmod.

If compiling an app from source see Compiler Variants.

If compiling an MPI app from source see OpenMPI Variants.

This serves as a quick reference on how to load any package based on its prerequisite compiler if any.

Software	Indepedent	GNU prerequisite	Intel prerequisite
anaconda/2 anaconda/3	ml anaconda/2 ml anaconda/3		
arpack-ng/3.5.0	ml arpack-ng/3.5.0		ml intel/2018.2 arpack-ng/3.5.0
avogadro/1.2	ml avogadro/1.2		
castep/19.1		ml intel/2018.3 openmpi/4.0.1 castep/19.1	
cp2k/4.1 cp2k/5.1	ml cp2k/4.1 ml cp2k/5.1		
dftbplus/18.1			ml intel/2018.2 dftbplus/18.1
fftw/3.3.6-pl2 fftw/3.3.8		ml gnu/7.2.0 fftw/3.3.6-pl2 ml gnu/8.2.0 fftw/3.3.8 (09/06)	ml intel/2018.0 fftw/3.3.6-pl2 ml intel/2018.3 fftw/3.3.8 (09/06)
gamess/2018.R3			ml intel/2018.3 openmpi/3.1.1 gamess/2018.R3 ml intel/2018.3 openmpi/3.1.2 gamess/2018.R3 ml intel/2018.3 openmpi/3.1.2-slim gamess/2018.R3

gaussian/09 gaussian/16	ml gaussian/09 ml gaussian/16		
gerris/1.3.2		ml gnu/8.2.0 openmpi/3.1.1 gerris/1.3.2 ml gnu/8.2.0 openmpi/3.1.2 gerris/1.3.2 ml gnu/8.2.0 openmpi/3.1.2-slim gerris/1.3.2	
gromacs/2018.3		ml gnu/7.3.0 openmpi/3.0.1 gromacs/2018.3	
hdf5/1.8.21 hdf5/1.10.2		ml gnu/8.2.0 hdf5/1.8.21 ml gnu/8.2.0 openmpi/3.1.1 hdf5/1.8.21 ml gnu/8.2.0 openmpi/3.1.2 hdf5/1.8.21 ml gnu/7.3.0 hdf/1.10.2 ml gnu/7.3.0 openmpi/3.0.1 hdf5/1.10.2	ml intel/2018.3 hdf5/1.8.21 ml intel/2018.3 openmpi/3.1.1 hdf5/1.8.21 ml intel/2018.3 openmpi/3.1.2 hdf5/1.8.21 ml intel/2018.2 hdf/1.10.2 ml intel/2018.2 openmpi/3.0.1 hdf5/1.10.2
hwloc/1.11.10 hwloc/1.11.11 hwloc/2.0.1 hwloc/2.0.2 hwloc/2.0.3	ml hwloc/1.11.10 ml hwloc/1.11.11 ml howloc/1.11.12 ml hwloc/2.0.1 ml hwloc/2.0.2 ml hwloc/2.0.3 (compiled w/ gnu/4.8.5)		
idl/8.1	ml idl/8.1		
julia/0.6.4 julia/0.7.0 julia/1.0.0 julia/1.1.0	ml julia/0.6.4 ml julia/0.7.0 ml julia/1.0.0 ml julia/1.1.0		
matlab/R2017b matlab/R2018b	ml matlab/R2017b ml matlab/R2018b		
miniconda/2/own miniconda/3/own	ml miniconda/2/own ml miniconda/3/own		
molden/5.7	ml molden/5.7		

namd/2.10_REST namd/2.12 namd/2.13b1		ml gnu/7.2.0 openmpi/3.0.1a namd/2.10_REST ml gnu/7.2.0 openmpi/3.0.1a namd/2.12	ml intel/2018.3 openmpi/3.1.2 namd/2.13b1
ncl/6.3.0 ncl/6.4.0 ncl/6.5.0	ml ncl/6.3.0 ml ncl/6.4.0 ml ncl/6.5.0		
netcdf/4.4.1.1 netcdf/4.6.1 netcdf/4.7.0		ml gnu/8.2.0 netcdf/4.4.1.1 ml gnu/8.2.0 openmpi/3.1.1 netcdf/4.4.1.1 ml gnu/8.2.0 openmpi/3.1.2 netcdf/4.4.1.1 ml gnu/8.2.0 openmpi/3.1.2-slim netcdf/4.4.1.1 ml gnu/8.3.0 netcdf/4.7.0 ml gnu/8.3.0 openmpi/4.0.1 netcdf/4.7.0	ml intel/2018.3 netcdf/4.4.1.1 ml intel/2018.3 openmpi/3.1.1 netcdf/4.4.1.1 ml intel/2018.3 openmpi/3.1.2 netcdf/4.4.1.1 ml intel/2018.3 openmpi/3.1.2-slim netcdf/4.4.1.1 ml intel/2018.2 netcdf/4.6.1 ml intel/2018.2 openmpi/3.0.1 netcdf/4.6.1 ml intel/2018.3 netcdf/4.7.0 ml intel/2018.3 openmpi/4.0.1 netcdf/4.7.0
openblas/0.2.20- openmp_64 openblas/0.2.20-openmp openblas/0.2.20-single_64 openblas/0.2.20-single openblas/0.2.20- pthreads_64 openblas/0.2.20-pthreads		ml gnu/7.2.0 openblas/0.2.20- openmp_64 ml gnu/7.2.0 openblas/0.2.20-openmp ml gnu/7.2.0 openblas/0.2.20-single_64 ml gnu/7.2.0 openblas/0.2.20-single ml gnu/7.2.0 openblas/0.2.20- pthreads_64 ml gnu/7.2.0 openblas/0.2.20-pthreads	

openmpi/1.10.7 openmpi/2.1.1 openmpi/2.1.2 openmpi/3.0.1a openmpi/3.0.1 openmpi/3.1.1 openmpi/3.1.2 openmpi/3.1.2-slim		ml gnu/7.2.0 openmpi/1.10.7 ml gnu/7.2.0 openmpi/2.1.2 ml gnu/7.2.0 openmpi/3.0.1a ml gnu/7.3.0 openmpi/3.0.1 ml gnu/8.2.0 openmpi/3.1.1 ml gnu/8.2.0 openmpi/3.1.2 ml gnu/8.2.0 openmpi/3.1.2-slim	ml intel/2018.0 openmpi/1.10.7 ml intel/2017.2 openmpi/2.1.1 ml intel/2017.2 openmpi/2.1.2 ml intel/2018.0 openmpi/3.0.1a ml intel/2018.2 openmpi/3.0.1 ml intel/2018.2 openmpi/3.1.1, ml intel/2018.3 openmpi/3.1.1 ml intel/2018.3 openmpi/3.1.2 ml intel/2018.3 openmpi/3.1.2-slim
pio/2.3.1		ml gnu/8.2.0 openmpi/3.1.1 pio/2.3.1 ml gnu/8.2.0 openmpi/3.1.2 pio/2.3.1	ml intel/2018.2 openmpi/3.0.1 pio/2.3.1 ml intel/2018.3 openmpi/3.1.1 pio/2.3.1 ml intel/2018.3 openmpi/3.1.2 pio/2.3.1
pnetcdf/1.9.0 pnetcdf/1.10.0		ml gnu/7.3.0 openmpi/3.0.1 pnetcdf/1.9.0 ml gnu/8.2.0 openmpi/3.1.1 pnetcdf/1.10.0 ml gnu/8.2.0 openmpi/3.1.2 pnetcdf/1.10.0	ml intel/2018.2 openmpi/3.0.1 pnetcdf/1.9.0 ml intel/2018.3 openmpi/3.1.1 pnetcdf/1.10.0 ml intel/2018.3 openmpi/3.1.2 pnetcdf/1.10.0
python/2.7.14 python/3.6.4	ml python/2.7.14 ml python/3.6.4		
qchem/5.0		ml gnu/7.2.0 openmpi/1.10.7 qchem/5.0	
qespresso/6.3			ml intel/2018.3 openmpi/3.1.1 qespresso/6.3 ml intel/2018.3 openmpi/3.1.2 qespresso/6.3
turbomole/7.2-official turbomole/7.2.1-official turbomole/7.3-beta turbomole/7.3-official		ml turbomole/7.2-official ml turbomole/7.2.1-official ml turbomole/7.3-beta ml turbomole/7.3-official	

udunits/2.2.26	ml udunits/2.2.26 (compiled w/ gnu/4.8.5)		
vmd/1.9.3	ml vmd/1.9.3		

One can generate a list of all available custom installed software via `ml spider`
Then `ml spider <package>` to get details on all variants of a given package.
The later is how the above table was generated!

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