

# 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  |
|--|----------------------------------|---|---|
| <a href="#">anaconda/2</a><br><a href="#">anaconda/3</a>     | ml anaconda/2<br>ml anaconda/3   |   |   |
| <a href="#">arpack-ng/3.5.0</a>                              | ml arpack-ng/3.5.0               |   | ml intel/2018.2 arpack-ng/3.5.0   |
| <a href="#">avogadro/1.2</a>                                 | ml avogadro/1.2                  |   |   |
| <a href="#">castep/19.1</a>                                  |                                  | ml intel/2018.3<br>openmpi/4.0.1 castep/19.1                      |   |
| <a href="#">cp2k/4.1</a><br><a href="#">cp2k/5.1</a>         | ml cp2k/4.1<br>ml cp2k/5.1       |   |   |
| <a href="#">dftbplus/18.1</a>                                |                                  |   | ml intel/2018.2<br>dftbplus/18.1  |
| <a href="#">fftw/3.3.6-pl2</a><br><a href="#">fftw/3.3.8</a> |                                  | ml gnu/7.2.0 fftw/3.3.6-pl2<br>ml gnu/8.2.0 fftw/3.3.8<br>(09/06) | ml intel/2018.0 fftw/3.3.6-pl2<br>ml intel/2018.3<br>fftw/3.3.8 (09/06)   |
| <a href="#">gamess/2018.R3</a>                               |                                  |   | ml intel/2018.3<br>openmpi/3.1.1<br>gamess/2018.R3<br>ml intel/2018.3<br>openmpi/3.1.2 gamess/2018.R3<br>ml intel/2018.3<br>openmpi/3.1.2-slim gamess/2018.R3 |
| <a href="#">gaussian/09</a><br><a href="#">gaussian/16</a>   | ml gaussian/09<br>ml gaussian/16 |   |   |

|   |  |  |   |
|---|--|--|---|
| <a href="#">gerris/1.3.2</a>  |  | ml gnu/8.2.0 openmpi/3.1.1<br>gerris/1.3.2<br>ml gnu/8.2.0 openmpi/3.1.2<br>gerris/1.3.2<br>ml gnu/8.2.0<br>openmpi/3.1.2-slim<br>gerris/1.3.2   |   |
| <a href="#">gromacs/2018.3</a>  |  | ml gnu/7.3.0 openmpi/3.0.1<br>gromacs/2018.3   |   |
| <a href="#">hdf5/1.8.21</a><br><a href="#">hdf5/1.10.2</a>  |  | ml gnu/8.2.0 hdf5/1.8.21<br>ml gnu/8.2.0 openmpi/3.1.1<br>hdf5/1.8.21<br>ml gnu/8.2.0 openmpi/3.1.2<br>hdf5/1.8.21<br>ml gnu/7.3.0 hdf/1.10.2<br>ml gnu/7.3.0 openmpi/3.0.1<br>hdf5/1.10.2 | ml intel/2018.3 hdf5/1.8.21<br>ml intel/2018.3<br>openmpi/3.1.1 hdf5/1.8.21<br>ml intel/2018.3<br>openmpi/3.1.2 hdf5/1.8.21<br>ml intel/2018.2 hdf/1.10.2<br>ml intel/2018.2<br>openmpi/3.0.1 hdf5/1.10.2 |
| <a href="#">hwloc/1.11.10</a><br><a href="#">hwloc/1.11.11</a><br><a href="#">hwloc/2.0.1</a><br><a href="#">hwloc/2.0.2</a><br><a href="#">hwloc/2.0.3</a> | ml hwloc/1.11.10<br>ml hwloc/1.11.11<br>ml howloc/1.11.12<br>ml hwloc/2.0.1<br>ml hwloc/2.0.2<br>ml hwloc/2.0.3<br>(compiled w/ gnu/4.8.5) |  |   |
| <a href="#">idl/8.1</a>   | ml idl/8.1   |  |   |
| <a href="#">julia/0.6.4</a><br><a href="#">julia/0.7.0</a><br><a href="#">julia/1.0.0</a><br><a href="#">julia/1.1.0</a>                                    | ml julia/0.6.4<br>ml julia/0.7.0<br>ml julia/1.0.0<br>ml julia/1.1.0   |  |   |
| <a href="#">matlab/R2017b</a><br><a href="#">matlab/R2018b</a>  | ml matlab/R2017b<br>ml matlab/R2018b   |  |   |
| <a href="#">miniconda/2/own</a><br>miniconda/3/own  | ml miniconda/2/own<br>ml miniconda/3/own   |  |   |
| <a href="#">molden/5.7</a>  | ml molden/5.7  |  |   |
| <a href="#">namd/2.10_REST</a><br><a href="#">namd/2.12</a><br><a href="#">namd/2.13b1</a>  |  | ml gnu/7.2.0<br>openmpi/3.0.1a<br>namd/2.10_REST<br>ml gnu/7.2.0<br>openmpi/3.0.1a namd/2.12   | ml intel/2018.3<br>openmpi/3.1.2<br>namd/2.13b1   |
| <a href="#">ncl/6.3.0</a><br><a href="#">ncl/6.4.0</a><br><a href="#">ncl/6.5.0</a>   | ml ncl/6.3.0<br>ml ncl/6.4.0<br>ml ncl/6.5.0   |  |   |

|   |  |   |   |
|---|--|---|---|
| <a href="#">netcdf/4.4.1.1</a><br><a href="#">netcdf/4.6.1</a><br><a href="#">netcdf/4.7.0</a>  |  | ml gnu/8.2.0 netcdf/4.4.1.1<br>ml gnu/8.2.0 openmpi/3.1.1 netcdf/4.4.1.1<br>ml gnu/8.2.0 openmpi/3.1.2 netcdf/4.4.1.1<br>ml gnu/8.2.0 openmpi/3.1.2-slim netcdf/4.4.1.1<br>ml gnu/8.3.0 netcdf/4.7.0<br>ml gnu/8.3.0 openmpi/4.0.1 netcdf/4.7.0     | ml intel/2018.3 netcdf/4.4.1.1<br>ml intel/2018.3 openmpi/3.1.1 netcdf/4.4.1.1<br>ml intel/2018.3 openmpi/3.1.2 netcdf/4.4.1.1<br>ml intel/2018.3 openmpi/3.1.2-slim netcdf/4.4.1.1<br>ml intel/2018.2 netcdf/4.6.1<br>ml intel/2018.2 openmpi/3.0.1 netcdf/4.6.1<br>ml intel/2018.3 netcdf/4.7.0<br>ml intel/2018.3 openmpi/4.0.1 netcdf/4.7.0 |
| <a href="#">openblas/0.2.20-openmp_64</a><br><a href="#">openblas/0.2.20-openmp</a><br><a href="#">openblas/0.2.20-single_64</a><br><a href="#">openblas/0.2.20-single</a><br><a href="#">openblas/0.2.20-pthreads_64</a><br><a href="#">openblas/0.2.20-pthreads</a> |  | ml gnu/7.2.0 openblas/0.2.20-openmp_64<br>ml gnu/7.2.0 openblas/0.2.20-openmp<br>ml gnu/7.2.0 openblas/0.2.20-single_64<br>ml gnu/7.2.0 openblas/0.2.20-single<br>ml gnu/7.2.0 openblas/0.2.20-pthreads_64<br>ml gnu/7.2.0 openblas/0.2.20-pthreads |   |
| openmpi/1.10.7<br>openmpi/2.1.1<br>openmpi/2.1.2<br>openmpi/3.0.1a<br>openmpi/3.0.1<br>openmpi/3.1.1<br><a href="#">openmpi/3.1.2</a><br>openmpi/3.1.2-slim   |  | ml gnu/7.2.0 openmpi/1.10.7<br>ml gnu/7.2.0 openmpi/2.1.2<br>ml gnu/7.2.0 openmpi/3.0.1a<br>ml gnu/7.3.0 openmpi/3.0.1<br>ml gnu/8.2.0 openmpi/3.1.1<br>ml gnu/8.2.0 openmpi/3.1.2<br>ml gnu/8.2.0 openmpi/3.1.2-slim                               | ml intel/2018.0 openmpi/1.10.7<br>ml intel/2017.2 openmpi/2.1.1<br>ml intel/2017.2 openmpi/2.1.2<br>ml intel/2018.0 openmpi/3.0.1a<br>ml intel/2018.2 openmpi/3.0.1<br>ml intel/2018.2 openmpi/3.1.1, ml intel/2018.3 openmpi/3.1.1<br>ml intel/2018.3 openmpi/3.1.2<br>ml intel/2018.3 openmpi/3.1.2-slim                                      |

|  |  |   |   |
|--|--|---|---|
| <a href="#">pio/2.3.1</a>  |  | ml gnu/8.2.0 openmpi/3.1.1<br>pio/2.3.1<br>ml gnu/8.2.0 openmpi/3.1.2<br>pio/2.3.1  | ml intel/2018.2<br>openmpi/3.0.1 pio/2.3.1<br>ml intel/2018.3<br>openmpi/3.1.1 pio/2.3.1<br>ml intel/2018.3<br>openmpi/3.1.2 pio/2.3.1                        |
| <a href="#">pnetcdf/1.9.0</a><br><a href="#">pnetcdf/1.10.0</a>  |  | ml gnu/7.3.0 openmpi/3.0.1<br>pnetcdf/1.9.0<br>ml gnu/8.2.0 openmpi/3.1.1<br>pnetcdf/1.10.0<br>ml gnu/8.2.0 openmpi/3.1.2<br>pnetcdf/1.10.0 | ml intel/2018.2<br>openmpi/3.0.1<br>pnetcdf/1.9.0<br>ml intel/2018.3<br>openmpi/3.1.1<br>pnetcdf/1.10.0<br>ml intel/2018.3<br>openmpi/3.1.2<br>pnetcdf/1.10.0 |
| <a href="#">python/2.7.14</a><br><a href="#">python/3.6.4</a>  | ml python/2.7.14<br>ml python/3.6.4          |   |   |
| <a href="#">qchem/5.0</a>  |  | ml gnu/7.2.0<br>openmpi/1.10.7 qchem/5.0  |   |
| <a href="#">qespresso/6.3</a>  |  |   | ml intel/2018.3<br>openmpi/3.1.1<br>qespresso/6.3<br>ml intel/2018.3<br>openmpi/3.1.2<br>qespresso/6.3  |
| <a href="#">turbomole/7.2-official</a><br><a href="#">turbomole/7.2.1-official</a><br><a href="#">turbomole/7.3-beta</a><br><a href="#">turbomole/7.3-official</a> |  | ml turbomole/7.2-official<br>ml turbomole/7.2.1-official<br>ml turbomole/7.3-beta<br>ml turbomole/7.3-official                              |   |
| <a href="#">udunits/2.2.26</a>   | ml udunits/2.2.26<br>(compiled w/ gnu/4.8.5) |   |   |
| <a href="#">vmd/1.9.3</a>  | 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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