

# Software Catalog

Below is a table of all custom compiled software available on the new side of cluster (glogin2/3) via Imod.

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> <a href="#">anaconda/3</a>	ml anaconda/2 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 openmpi/4.0.1 castep/19.1	
<a href="#">cp2k/4.1</a> <a href="#">cp2k/5.1</a>	ml cp2k/4.1 ml cp2k/5.1		
<a href="#">dftbplus/18.1</a>			ml intel/2018.2 dftbplus/18.1
<a href="#">fftw/3.3.6-pl2</a> <a href="#">fftw/3.3.8</a>		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)
<a href="#">gamess/2018.R3</a>			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

<a href="#">gaussian/09</a> gaussian/16	ml gaussian/09 ml gaussian/16		
<a href="#">gerris/1.3.2</a>		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	
<a href="#">gromacs/2018.3</a>		ml gnu/7.3.0 openmpi/3.0.1 gromacs/2018.3	
hdf5/1.8.21 <a href="#">hdf5/1.10.2</a>		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
<a href="#">hwloc/1.11.10</a> 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)		
<a href="#">idl/8.1</a>	ml idl/8.1		
<a href="#">julia/0.6.4</a> <a href="#">julia/0.7.0</a> <a href="#">julia/1.0.0</a> <a href="#">julia/1.1.0</a>	ml julia/0.6.4 ml julia/0.7.0 ml julia/1.0.0 ml julia/1.1.0		
<a href="#">matlab/R2017b</a> matlab/R2018b	ml matlab/R2017b ml matlab/R2018b		
<a href="#">miniconda/2/own</a> miniconda/3/own	ml miniconda/2/own ml miniconda/3/own		
<a href="#">molden/5.7</a>	ml molden/5.7		

<a href="#">namd/2.10_REST</a> <a href="#">namd/2.12</a> <a href="#">namd/2.13b1</a>		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 <a href="#">ncl/6.5.0</a>	ml ncl/6.3.0 ml ncl/6.4.0 ml ncl/6.5.0		
<a href="#">netcdf/4.4.1.1</a> <a href="#">netcdf/4.6.1</a> <a href="#">netcdf/4.7.0</a>		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
<a href="#">openblas/0.2.20-</a> openmp_64 openblas/0.2.20-openmp openblas/0.2.20-single_64 openblas/0.2.20-single openblas/0.2.20- pthread_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- pthread_64 ml gnu/7.2.0 openblas/0.2.20-pthreads	

<p>openmpi/1.10.7  openmpi/2.1.1  openmpi/2.1.2  openmpi/3.0.1a  openmpi/3.0.1  openmpi/3.1.1  <a href="#">openmpi/3.1.2</a>  openmpi/3.1.2-slim</p>		<p>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</p>	<p>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</p>
<p><a href="#">pio/2.3.1</a></p>		<p>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</p>	<p>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</p>
<p><a href="#">pnetcdf/1.9.0</a>  pnetcdf/1.10.0</p>		<p>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</p>	<p>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</p>
<p>python/2.7.14  python/3.6.4</p>	<p>ml python/2.7.14  ml python/3.6.4</p>		
<p><a href="#">qchem/5.0</a></p>		<p>ml gnu/7.2.0  openmpi/1.10.7 qchem/5.0</p>	
<p><a href="#">gespresso/6.3</a></p>			<p>ml intel/2018.3  openmpi/3.1.1  gespresso/6.3  ml intel/2018.3  openmpi/3.1.2  gespresso/6.3</p>
<p>turbomole/7.2-official  turbomole/7.2.1-official  turbomole/7.3-beta  <a href="#">turbomole/7.3-official</a></p>		<p>ml turbomole/7.2-official  ml turbomole/7.2.1-official  ml turbomole/7.3-beta  ml turbomole/7.3-official</p>	

<a href="#">udunits/2.2.26</a>	ml udunits/2.2.26 (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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