

Oscar Software Modules

List and instructions for software modules available on the Oscar cluster.

- [Currently Available Modules](#)
- [Oscar: Sage](#)
- [Oscar: MATLAB](#)
- [Oscar: Mathematica](#)

Currently Available Modules

If you require a software package that is not currently available on the Oscar cluster, please [contact ICERM's IT staff](#) and we will work with CCV to get the software installed.

This list is current as of November 10, 2021. To see the most up to date list of software modules, log into your Oscar account and run the command `module avail`.

```
~~~~~ category:
~~~~~
bxh_xcede_tools/1.11.14  confocal/1.0      potfit/20201014
cesm_post_process/Oct18  pigz/2.4
~~~~~ category: Microstructure modeling ~~~~~
oof2/2.1.17
~~~~~ category: access controlled ~~~~~
Molpro/2012.1.15
Molpro/2015_gcc
Molpro/2015_serial
Molpro/2018.2_ga
Molpro/2019.2
Molpro/2019.2_ga
Molpro/2020.1
Molpro/2020.1_ga
Molpro/2020.1_openmpi_4.0.5_gcc_10.2_slurm20
gaussian/g09
gaussian/g09-D01
gaussian/g09-D01-TEST
vasp/5.4.1
vasp/5.4.1_debug
vasp/5.4.1_mvapich2-2.3.5_intel_2020.2_slurm20
vasp/5.4.4
vasp/5.4.4_intel
vasp/5.4.4_mvapich2-2.3.5_intel_2020.2_slurm20
vasp/5.4.4_openmpi_4.0.5_gcc_10.2_slurm20
vasp/5.4.4a
vasp/6.1.1_ompi405_yqi27
vasp/6.1.1_openmpi_4.0.5_intel_2020.2_yqi27_slurm20
```

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vasp/6.1.1_yqi27
~~~~~ category: graph partitioning ~~~~~

metis/5.1.0  parmetis/4.0.3  scotch/6.0.4
~~~~~ category: image processing
~~~~~

multinest/3.10  openslide/3.4.1  pstokes/1.0
~~~~~ category: libraries
~~~~~

astropy/3.2.1  cudnn/7.4      flann/1.8.4    lapack/3.7.0
astroquery/3.0.9  cudnn/7.6      hnn/1.0        mumps/5.0.2
blas/3.7.0      cudnn/7.6.5    horovod/0.16    mumps/5.0.2-seq
cudnn/5.1       cudnn/8.1.0    horovod/0.19.5  pcl/1.9.1
cudnn/6.0       cudnn/8.2.0    lapack/3.4.2    pcl/1.9.1_nurbs
cudnn/7.0       dlib/19.17     lapack/3.6.0    scalapack/2.0.2
~~~~~ category: library
~~~~~

openslide-python/1.1.1
~~~~~ category: machine learning
~~~~~

keras/2.0.9     keras/2.1.3_py3  nccl/2.8.4
keras/2.1.1     nccl/2.4.7
~~~~~ category: math
~~~~~

gsl/1.15  gsl/2.3  gsl/2.5
~~~~~ category: package
~~~~~

subread/1.6.2
~~~~~ category: software
~~~~~

mriconvert/2.1.0
~~~~~ category: utility
~~~~~

mriconvert/2.1.0
~~~~~ category: visualization
~~~~~

mayavi/4.6.0
~~~~~ category: (none)
~~~~~

HiC-Pro/2.7.8      jo/1.4      repeatmasker/4.1.0
HiC-Pro~/2.10.0    libsodium/1.0.17  repeatmodeler/1.0.11

```

awscli/1.0	mumax/3.9.3	sdl2/2.0.12
basilisk/1.0	ncl/6.4.0	siesta/3.2
canu/1.7.1	neuron/7.5	siesta/4.1
dropest/0.86	neuron/7.7	skewer/0.2.1
fiji/2017-java6	neuron/7.7_mpi	squashfs/4.3
fiji/2020	nvidia-driver/440.33.01	tmux/2.8
fmri/20.0.0	pdflib/7.0.5	topcat/4.7
fv/5.5	pypy/6.0.0_2.7	transrate/1.0.3
gcm-core/2.0.498	pypy/6.0.0_3.5	vscode/1.22
grads/2.2.0	pypy/7.3.0_3.6	zstd/1.5.0
hotnet/1.0	repeatmasker/4.0.7	

~~~~~ category: Applied Maths

~~~~~  
oof2/2.1.17

~~~~~ category: Astrophysics

~~~~~  
polychord/1.0 polychord/2.0

~~~~~ category: Bioinformatics

~~~~~  
MultiQC/1.0 muscle/3.8.31

~~~~~ category: CAD

~~~~~  
freecad/0.18 librecad/2.0

~~~~~ category: Chemistry

~~~~~  
dalton/2018.0

dalton/2018.0_mvapich2-2.3.5_intel_2020.2_slurm20

~~~~~ category: Computer Architecture ~~~~~

risc/1.0

~~~~~ category: EDA tools

~~~~~  
cadence/IC06.18.090 cadence/IC6.1.8.33 incisive/15.20.085

~~~~~ category: Executable for ceckpointings ~~~~~

dmtcp/2.6.0

~~~~~ category: Flag for CMAKE for fast build ~~~~~

ninja/1.9.0

~~~~~ category: GENETEICS

~~~~~  
eigensoft/6.0

~~~~~ category: Genomic

```
~~~~~
Genrich/0.5  mcscanx/1.0
~~~~~ category: Genomic Library
~~~~~
redundans/1.0
~~~~~ category: Genomics
~~~~~
baypass/2.2  beast/2.5.2  kissplice/2.5.1
beast/1.10.4  kissplice/2.5.0
~~~~~ category: Genomics Sequencing Alignment ~~~~~
qualimap/2.2.1
~~~~~ category: Graphics
~~~~~
beagle/1.0.0
~~~~~ category: Helper function type ~~~~~
datamash/1.3
~~~~~ category: I/O
~~~~~
cdo/1.9.8
cdo/1.9.9
hdf5/1.10.0
hdf5/1.10.1_mvapich2-2.3.5_gcc_10.2_slurm20
hdf5/1.10.1_parallel
hdf5/1.10.5
hdf5/1.10.5_fortran
hdf5/1.10.5_mvapich2-2.3.5_intel_2020.2_slurm20
hdf5/1.10.5_openmpi_3.1.3_gcc
hdf5/1.10.5_openmpi_3.1.6_gcc
hdf5/1.10.5_openmpi_4.0.0_gcc
hdf5/1.10.5_openmpi_4.0.5_gcc_10.2_slurm20
hdf5/1.10.5_parallel
hdf5/1.10.7_hpcx_2.7.0_intel_2020.2_slurm20
hdf5/1.10.7_openmpi_4.0.5_gcc_10.2_slurm20
hdf5/1.10.7_openmpi_4.0.5_intel_2020.2_slurm20
hdf5/1.12.0_hpcx_2.7.0_intel_2020.2
hdf5/1.12.0_hpcx_2.7.0_intel_2020.2_slurm20
hdf5/1.12.0_openmpi_4.0.5_intel_2020.2_slurm20
jasper/1.900.1-intel
nco/4.6.6
nco/4.8.2
```

nco/4.9.3
netcdf/3.6.3
netcdf/4.4.1.1_gcc
netcdf/4.4.1.1_intel
netcdf/4.4.1.1_pgi
netcdf/4.7.0_intel2019.3
netcdf/4.7.4_gcc8.3
netcdf/4.7.4_gcc_10.2_hdf5_1.10.5
netcdf/4.7.4_intel_2020.2_hdf5_1.12.0
sqlite/3.25.2
sqlite/3.31.1
udunits/1.12.11
udunits/2.2.24
~~~~~ category: IDE  
~~~~~  
meshlab/20190129_qt59 spyder/3.3.5
~~~~~ category: Image processing and visualization ~~~~~  
opencv-python/4.1.0.25  
~~~~~ category: Library for optimizer ~~~~~  
numbbo/2.3_python2 numbbo/2.3_python3
~ category: Material science: <https://icet.materialsmodeling.org/overview.html> ~
icet/0.3
~~~~~ category: Medical imaging  
~~~~~  
mricrogl/1.0 mricrogl/1.2.20210317
~~~~~ category: Multifunctional Wavefunction Analyzer ~~~~~  
multiwfn/3.3.9  
~~~~~ category: Numerical Library  
~~~~~  
ngsolve/6.2.1901  
~~~~~ category: Numerical Solver  
~~~~~  
dedalus/2.1810  
dedalus/2.1905  
dedalus/2.1905\_openmpi\_4.05\_gcc\_10.2\_slurm20  
dedalus/Sep2019  
nektar++/4.5.0  
~~~~~ category: Quantum Monte Carlo  
~~~~~  
casino/2.13

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~~~~~ category: Tool for Image Manipulation ~~~~~
netpbm/10.47.71
~~~~~ category: Utility
~~~~~
globus/1.11
~~~~~ category: Visualization Package Qt's Python API ~~~~~
pyqt/4.12.1
~~~~~ category: X
~~~~~
turbovnc/2.1.1 turbovnc/2.2.1 turbovnc/2.2.6 turbovnc/2.2.b1
~~~~~ category: astronomy
~~~~~
ares/0.1      iraf/2.16      sextractor/2.8.6
ares/0.5      iraf/2.16.1+2018.11.01 supermongo/2.4.34
ccfits/2.5    lsst/14.0      swarp/2.38
cfitsio/3.450  planck_likelihood/3.0 theli/1.9.5
cfitsio/3.48   planck_likelihood/3.01 wcstools/3.9.5
ds9/7.6       scamp/2.0.4
galfit/3.0.5   sextractor/2.19.5
~~~~~ category: astrophysics
~~~~~
fiat/Oct2019
~~~~~ category: astropy computing
~~~~~
astropy/3.2.1
~~~~~ category: astroquery computing
~~~~~
astroquery/3.0.9
~~~~~ category: benchmark
~~~~~
elbencho/2.0-1
~~~~~ category: binary for genome studies ~~~~~
bedGraphToBigWig/1.04
~~~~~ category: bio
~~~~~
SNAP/2013-11-29 mira/4.0.2
abyss/2.1.1 mne/0.17.0
ale/20140120 moseq2/0.1.2
aliview/1.25 moseq2/0.2.0
amplisat/20170208 mothur/1.39.5

```

|                   |                       |
|-------------------|-----------------------|
| angsd/0.920       | mrBayes/3.2.6         |
| anvio/5.2         | mriqc/0.15.2          |
| anvio/5.5         | msmc/1.0.0            |
| anvio/6.1         | msmc/1.1.0            |
| anvio/7           | msmc/2.1.2            |
| arb/6.0.6         | msprime/0.7.0         |
| augustus/3.3      | msprime/0.7.2         |
| bamcleave/Oct2018 | msprime/0.7.4         |
| bamtools/2.3.0    | mummer/4.0.0.beta2    |
| bamtools/2.4.1    | namd/2.11-multicore   |
| bbmap/38.23       | namd/2.13b1-multicore |
| bbtools/38.12     | nda-tools/1.0         |
| bcftools/1.10.2   | nextclip/1.3.1        |
| bcftools/1.13     | nextgenmap/0.5.2      |
| bcftools/1.9      | nipype/1.5.0          |
| bcl2fastq/2.20.0  | nseg/20181012         |
| bedops/2.4.35     | nvtop/1.1.0           |
| bedtools/2.25.0   | obitools/1.2.12       |
| bedtools/2.26.0   | octopus/0.7.4         |
| beeline/1.0       | oligotyping/2.0       |
| biolite/1.0.0     | omero/5.6.2           |
| biomed/1.0        | opera/2.0.6           |
| biopython/1.66    | orthomcl/2.0.9        |
| biopython/1.73    | paml/4.8              |
| bismark/0.20.0    | pandaseq/2.11         |
| blast/2.2.30+     | paris/1.1.3           |
| blast/2.6.0+      | paup/4.0a157          |
| blast/2.7.1+      | paup/4.0a166          |
| blast/2.8.1+      | paup/4.0a168          |
| blast/2.9.0+      | pbsuite/15.8.24       |
| blat/36x2         | pcangsd/0.98          |
| bowtie/1.2.0      | picard-tools/2.17.11  |
| bowtie/2.4.1      | picard-tools/2.9.2    |
| bowtie2/2.3.0     | pilon/1.22            |
| bowtie2/2.3.5.1   | pilon/1.24            |
| bowtie2/2.4.2     | plink/1.07            |
| braker/2.1.0      | plink/1.90            |
| busco/3.0.2       | plink/2.00            |
| bwa/0.7.15        | polyphen/2.2.2        |
| cabana/1.0        | poolparty/0.8         |



|                                        |                    |
|----------------------------------------|--------------------|
| cabana/1.1_hpcx_2.7.0_gcc_10.2_slurm20 | popoolation2/1.201 |
| cantera/5.9.7                          | prinseq/0.20.4     |
| ccp4/7.0                               | prodigal/2.6.3     |
| circlator/1.5.5                        | psmc/0.6.5         |
| conn/16b                               | psmc/0.6.5a        |
| conn/18a                               | pymol/2.2b         |
| conn/18b                               | qctool/2.0         |
| conn/18b_runtime                       | qiime/1.9.1        |
| conn/18b_standalone                    | quast/5.0.0        |
| conn/19c                               | raremetal/4.14.1   |
| conn/20b                               | raxml/8.2.10       |
| conn/20b_standalone                    | raxml-ng/0.9.0     |
| connectome_workbench/1.3.1             | recon/1.08         |
| connectome_workbench/1.3.2             | repeatscout/1.0.5  |
| connectome_workbench/1.4.2             | revbayes/1.0.5     |
| cpac/1.0.1                             | revbayes/1.0.6     |
| cpac/1.5.0                             | rmblastn/2.10.0    |
| cufflinks/2.2.1                        | rmblastn/2.6.0     |
| cutadapt/1.14                          | rsem/1.3.1         |
| dada2/1.4.1                            | salmon/0.11.3      |
| dada2/1.8                              | salmon/0.8.2       |
| dbg2olc/Sep2018                        | salmon/1.0.0       |
| dendropy/4.2.0                         | salmon/1.2.0       |
| diamond/0.9.12                         | salmon/1.3.0       |
| diamond/0.9.24                         | samblaster/0.1.24  |
| diamond/2.0.8                          | samtools/0.1.18    |
| dida/1.0.1                             | samtools/1.10      |
| diffreps/1.55.6                        | samtools/1.12      |
| dlcpar/1.1                             | samtools/1.13      |
| edge-pro/1.3.1                         | samtools/1.2       |
| eems/1.0                               | samtools/1.3.1     |
| emboss/6.6.0                           | samtools/1.4.1     |
| entap/0.8.1-beta                       | samtools/1.9       |
| entap/0.8.4-beta                       | schrodinger/2017-3 |
| exonerate/2.2.0                        | schrodinger/2020-1 |
| fastme/2.1.5                           | schrodinger/2020-3 |
| fastqc/0.11.5                          | schrodinger/2021-1 |
| fastsimcoal/2                          | schrodinger/2021-3 |
| fasttree/2.1.10                        | selscan/1.2.0a     |
| fasttree/2.1.11                        | seqkit/0.10.1      |

|                        |                     |
|------------------------|---------------------|
| fastuniq/1.1           | seqtk/1.3           |
| fastx-toolkit/2.6      | sga/0.10.15         |
| fgap/1.8.1             | sift/6.2.1          |
| fgbio/0.6.1            | sift4g/2.0.0        |
| figtree/1.4.4          | sjaracne/0.2.0      |
| flashpca/2.0           | skesa/1.68          |
| freebayes/1.1.0        | slicer/4.10.0       |
| freebayes/1.2.0        | slim/3.1            |
| garlic/1.1.6           | slim/3.2.1          |
| gatk/4.0.9.0           | slim/3.3            |
| gatk/4.1.6.0           | snippy/Oct2017      |
| gatk/4.2.2.0           | spades/3.10.1       |
| gdcclient/1.4.0        | spades/3.13.0       |
| genemark/4.33          | span/0.10.0.4787    |
| guppy/4.0.11           | spm/spm12           |
| guppy/4.2.2            | spm/spm12_7771      |
| guppy/5.0.7            | sprint/0.1.8        |
| hapbin/1.3.0           | sratoolkit/2.10.5   |
| hisat2/2.1.0           | sratoolkit/2.11.0   |
| hmmer/3.1b2            | sratoolkit/2.8.2-1  |
| homer/4.10             | stacks/2.2          |
| hotnet2/1.2.1          | stampy/1.0.32       |
| htseq/0.11.1           | star/2.6.1b         |
| htseq/0.9.1            | star/2.7.2a         |
| idba/1.1.3             | star/2.7.3a         |
| idemp/20180928         | starfusion/1.7.0    |
| ilash/1.0.0            | starfusion/1.8.1    |
| ilash/1.0.2            | stringtie/1.3.3b    |
| interproscan/5.26-65.0 | stringtie/1.3.4d    |
| interproscan/5.27-66.0 | tabix/0.2.6         |
| interproscan/5.28-67.0 | tablemaker/2.1.1    |
| interproscan/5.32-71.0 | taxonkit/0.3.0      |
| interproscan/5.33-72.0 | tophat/2.1.1        |
| iq-tree/1.6.7          | transabyss/2.0.1    |
| iq-tree/2.0.6          | transindel/20181017 |
| jellyfish/1.1.11       | trf/4.09            |
| jellyfish/2.2.10       | trimal/1.4          |
| kneaddata/0.6.1        | trimgalore/0.5.0    |
| kraken/2.0.7-beta      | trimmomatic/0.36    |
| kraken/2.0.9-beta      | trinity/2.11.0      |

|                                |                       |                  |                   |
|--------------------------------|-----------------------|------------------|-------------------|
| kraken/2.1.2                   | trinity/2.4.0         |                  |                   |
| last/956                       | trinity/2.8.4         |                  |                   |
| macs/2.1.1                     | usearch/5.2.32        |                  |                   |
| macs/2.2.6                     | usearch/8.1.1861      |                  |                   |
| mafft/7.310-with-extensions    | varscan/2.3.9         |                  |                   |
| maker/2.31.10                  | vcftools/0.1.16       |                  |                   |
| marsbar/0.42                   | velvet/1.2.10         |                  |                   |
| maxbin2/2.2.5                  | velvet/1.2.10a        |                  |                   |
| megahit/1.1.3                  | vep/101               |                  |                   |
| meraculous/2.2.6               | vep/104               |                  |                   |
| metabat/2.12.1                 | viennarna/2.4.9       |                  |                   |
| metaphlan/2.6.0                | vmd/1.9.3             |                  |                   |
| metavelvet/1.2.01              | vsearch/2.11.1        |                  |                   |
| migrate/3.6.11                 | weblogo/2.8.2         |                  |                   |
| ~~~~~ category: bio packages   |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| bwameth/0.10                   |                       |                  |                   |
| ~~~~~ category: bioinformatics |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| umitools/1.0.0                 |                       |                  |                   |
| ~~~~~ category: biology        |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| haplostrips/1.2.1              | htslib/1.9            | meme/5.0.5       | mmsplice/0.2.7    |
| htslib/1.13                    | libBigWig/0.4.4       | meme/5.3.0       | wiggletools/1.2.3 |
| ~~~~~ category: build tool     |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| scons/3.0.1                    |                       |                  |                   |
| ~~~~~ category: cave           |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| gigapixelviewer/alpha          | minvr/dev_ben         | vrg3d/265_compat |                   |
| minvr/0.3master                | planetaryviewer/alpha | vrg3d/265_demos  |                   |
| minvr/0.4                      | scalable/20150828     | vrpn/7.33        |                   |
| minvr/beta                     | scalable/opengl32+    |                  |                   |
| minvr/beta-bleeding            | vrg3d/265             |                  |                   |
| ~~~~~ category: chemistry      |                       |                  |                   |
| ~~~~~                          |                       |                  |                   |
| Molpro/2012.1.15               |                       |                  |                   |
| Molpro/2015_gcc                |                       |                  |                   |
| Molpro/2015_serial             |                       |                  |                   |
| Molpro/2018.2_ga               |                       |                  |                   |

Molpro/2019.2  
Molpro/2019.2\_ga  
Molpro/2020.1  
Molpro/2020.1\_ga  
Molpro/2020.1\_openmpi\_4.0.5\_gcc\_10.2\_slurm20  
ambertools/amber16  
ambertools/amber16-gpu  
ambertools/amber17  
ambertools/amber17\_lic  
ambertools/amber21  
ase/3.13.0  
ase/3.19.1  
ase/3.8.1  
bagel/1.2.2  
cp2k/7.1  
cp2k/8.1.0  
crossrate/2016.3.23  
dacapo/2.7.16\_mvapich2\_intel  
dice/1.0  
elk/5.2.14  
gaussian/g09  
gaussian/g09-D01  
gaussian/g09-D01-TEST  
gaussview/14Aug20  
gromacs/2016.6  
gromacs/2018.2  
gromacs/2018.2\_gpu  
gromacs/2018.2\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
gromacs/2020.1  
gromacs/2020.1\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
gromacs/2020.4\_gpu  
gromacs/2020.4\_gpu\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
gromacs/2020.4\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
hande/1.1.1  
hande/1.1.1\_64  
hande/1.1.1\_debug  
hotbit/10mar17  
lammps/11Aug17\_serial  
lammps/29Oct20\_openmpi\_4.0.5\_gcc\_10.2\_slurm20  
medea/3.2.3.0

molden/5.7  
mrcc/2014-intel  
mrcc/2014-intel-threaded  
mrcc/2018-intel  
mrcc/2018-intel-threaded  
mrcc/2020  
n2p2/1.0.0  
n2p2/2.0.0  
n2p2/2.0.0\_hpcx  
nbo/7.0  
nwchem/6.8-openmpi  
nwchem/7.0  
nwchem/7.0.2\_mvapich2-2.3.5\_intel\_2020.2\_slurm20  
openbabel/2.4.1  
openbabel/3.0.0  
openmolcas/18.09.617  
orca/4.0.1.2  
orca/4.1.1  
orca/4.2.1  
orca/5.0.0  
orca/5.0.1  
prophet/augustegm\_1.2  
pyscf/1.4.7  
pyscf/1.6.3  
qchem/5.0.2  
qchem/5.0.2-openmpi  
qmcpack/3.10.0\_openmpi\_4.0.5\_intel\_2020.2\_slurm20  
qmcpack/3.7.0  
qmcpack/3.9.1  
qmcpack/3.9.1\_openmpi\_3.1.6  
qmcpack/3.9.2\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
qmcpack/3.9.2\_intel\_2020  
qmcpack/3.9.2\_openmpi\_4.0.0\_gcc\_8.3\_slurm20  
qmcpack/3.9.2\_openmpi\_4.0.0\_gcc\_8.3\_slurm20\_complex  
qmcpack/3.9.2\_openmpi\_4.0.1\_gcc  
qmcpack/3.9.2\_openmpi\_4.0.4\_gcc  
qmcpack/3.9.2\_openmpi\_4.0.5\_intel\_2020.2\_slurm20  
quantumespresso/6.1  
quantumespresso/6.3  
quantumespresso/6.4

quantumpresso/6.4.1  
quantumpresso/6.4\_openmpi\_4.0.0\_gcc\_8.3\_slurm20  
quantumpresso/6.4\_openmpi\_4.0.5\_intel\_2020.2\_slurm20  
quantumpresso/6.4\_openmpi\_4.0.5\_intel\_slurm20  
quantumpresso/6.5  
quantumpresso/6.5\_openmpi\_4.0.5\_intel\_slurm20  
quantumpresso/6.6  
quantumpresso/6.6\_openmpi\_4.0.5\_intel\_2020.2\_slurm20

rotd/2014-11-15\_mvapich2

schrodinger/2017-3

schrodinger/2020-1

schrodinger/2020-3

schrodinger/2021-1

schrodinger/2021-3

sharc/2.0

sharc/2.1.1

sharc/2.1.1\_intel

vasp/5.4.1

vasp/5.4.1\_debug

vasp/5.4.1\_mvapich2-2.3.5\_intel\_2020.2\_slurm20

vasp/5.4.4

vasp/5.4.4\_intel

vasp/5.4.4\_mvapich2-2.3.5\_intel\_2020.2\_slurm20

vasp/5.4.4\_openmpi\_4.0.5\_gcc\_10.2\_slurm20

vasp/5.4.4a

vasp/6.1.1\_ompi405\_yqi27

vasp/6.1.1\_openmpi\_4.0.5\_intel\_2020.2\_yqi27\_slurm20

vasp/6.1.1\_yqi27

xcrysden/1.5.60

~~~~~ category: class

~~~~~

class/1435

~~~~~ category: clients

~~~~~

aspera/3.8.1

~~~~~ category: climate

~~~~~

cesm/1.2.1 cesm/2.1.1 esmf/8.0.0 esmf/8.1.0b11

cesm/1.2.2 esmf/7.1.0r esmf/8.0.0b esmf/8.1.9b17

~~~~~ category: compilers

```

~~~~~
Xvfb/1.20.12      gcc/10.2      java/8u111
clang/3.9.1       gcc/4.5.4     java/jdk-11.0.11
clang/7.0.0       gcc/4.7.2     java/jdk-12.0.2
clang/7.1.0       gcc/4.9.4     kokkos/3.3.1
cuda/10.0.130     gcc/5.4       kokkos/3.4.1
cuda/10.1.105     gcc/6.2       llvm/11.0.1
cuda/10.2         gcc/6.3       llvm/3.8.1
cuda/11.1.1       gcc/7.2       llvm/4.0.0
cuda/11.1.1_intel_2020 gcc/8.3       llvm/6.0.1
cuda/11.3.1       intel/2011.11.339 llvm/7.1.0
cuda/7.5.18       intel/2013.1.106 nag/6.2
cuda/8.0.61       intel/2017.0  nag/mb16i25dnl
cuda/9.0.176      intel/2018.1  pgi/16.7
cuda/9.1.85.1     intel/2019.3  pgi/2019
cuda/9.2.148      intel/2020.2  swig/3.0.10
~~~~~ category: computer architecture ~~~~~

llvmpopenmp/1.0 llvmpopenmp/2.0
~~~~~ category: containers
~~~~~

singularity2/2.5.2
~~~~~ category: cross webbrowser web application development environment ~~~~~

chromedriver/2.46
~~~~~ category: data analysis(http://www.mega-nerd.com/) ~~~~~

libsnd/1.0.28
~~~~~ category: data science
~~~~~

catboost/0.8.1 manureadr/1.0 pandas/py_3.6.6
catboost/0.8.1_py3 pandas/py_3.5.2
~~~~~ category: data structure library ~~~~~

dcm2bids/2.1.4
~~~~~ category: debugging and profiling ~~~~~

forge/18.2.3 forge/19.1.2 forge/21.0.2
~~~~~ category: dev
~~~~~

googletest/1.8.0 qemu/4.1.0
~~~~~ category: devel
~~~~~

bazel/0.23.0 glew/1.13.0 opengl/nvidia-375.66
bazel/0.25.2 glew/2.1.0 opengl/nvidia-390.30

```

```
bazel/0.4.4 opengl/mesa-12.0.6 opengl/nvidia-410.72
bazel/0.5.4 opengl/mesa-18.3.3 protobuf/3.4.1
bazel/1.2.1 opengl/nvidia protobuf/3.6.0_gcc5.4
~~~~~ category: editor
~~~~~

emacs/26.3 neovim/0.4.4
~~~~~ category: engineering
~~~~~

abaqus/2017 comsol/5.6
abaqus/2021 mentor-calibre/2020.1_36.18
abaqus/2021.1 spectre/191
abaqus/2021.1_intel17 su2/7.0.2
abaqus/6.12sp2 synopsys/2018.06
ansys/18.1 synopsys/2020.06
assura/04.16.107 synopsys/L_2016.03-SP2
comsol/5.2
~~~~~ category: fMRI
~~~~~

brainiak/Feb2018
~~~~~ category: fonts
~~~~~

freetype/2.7.1
~~~~~ category: gene and species tree ~~~~~
phyldog/1.0
~~~~~ category: genetics
~~~~~

megacc/10.1.8
~~~~~ category: genomic
~~~~~

admixture/1.3.0  glactools/1.0.7    pybigwig/0.3.15
deeptools/3.2.1  partitionfinder/2.1.1  pysam/0.15.2
deeptoolsintervals/0.1.7  py2bit/0.3.0    pyslim/1.0
~~~~~ category: genomics
~~~~~

cellranger/3.1.0  cellranger/arc-1.0.1 faststructure/1.0
cellranger/5.0.1  chromopainter/0.0.4  relernn/6Dec2019
cellranger/6.0.0  clustal_omega/1.2.4
~~~~~ category: graphics
~~~~~

campari/3.0      gnuplot/5.2.3      inkscape/Sep-2019
```



~~~~~ category: image

~~~~~

c3d/1.0.0 imagej/1.52a leptonica/1.79.0 openexr/2.2.1

ffmpeg/3.2.4 imagemagick/7.0.7 libgd/2.2.5

ffmpeg/4.0.1 isis/3.5.1 libgit/1.1.0

~~~~~ category: image converter

~~~~~

mriconvert/2.1.0

~~~~~ category: image processing

~~~~~

libgif/5.1.9 libjpeg-turbo/2.0.2 openjpeg/2.3.1

libjpeg/9.0 mayavi/4.6.0 openslide-python/1.1.1

~~~~~ category: languages

~~~~~

R/3.3.2 julia/1.0 miniconda/4.10

R/3.4.0 julia/1.0.2 perl/5.16.0

R/3.4.3 julia/1.1.0 perl/5.18.2

R/3.4.3\_mkl julia/1.2.0 perl/5.24.1

R/3.4.4 julia/1.4.1 perl/5.30.0

R/3.5.2 julia/1.4.2 perl/5.8.9

R/3.6.0 julia/1.5.0 python/2.7.12

R/3.6.3 julia/1.5.1 python/2.7.12\_clean

R/4.0.0 julia/1.5.2 python/2.7.16

R/4.0.3 julia/1.5.3 python/3.5.2

R/4.0.5 julia/1.5.4 python/3.6.6

R/4.1.0 julia/1.6.0 python/3.6.6\_test

anaconda/2-4.3.0 julia/1.6.1 python/3.6.8\_gcc8.3

anaconda/2-5.3.0 julia/1.6.2 python/3.7.4

anaconda/2020.02 julia/1.6.3 python/3.8.12\_gcc8.3

anaconda/3-4.3.0 lua/5.3.4 python/3.9.0

anaconda/3-5.2.0 maple/16 qt/3.3.8b

golang/1.15.6 maple/20 qt/3.3.8b-51

golang/1.16.6 materialstudio/2020 qt/5.10.1

golang/1.17.1 mathematica/10.3.1 qt/5.12

idl/8.5.1 mathematica/11.0 qt/5.12.0

idl\_DEEPS/8.7.2 mathematica/12.0 qt/5.13.1

java/8u111 matlab/R2016a qt/5.14.2

java/jdk-11.0.11 matlab/R2017a qt/5.7.0

java/jdk-12.0.2 matlab/R2017b qt/5.9.0

julia/0.5.1 matlab/R2018a ruby/2.4.0

|             |               |              |
|-------------|---------------|--------------|
| julia/0.6.1 | matlab/R2018b | rust/1.45.1  |
| julia/0.6.4 | matlab/R2019a | rust/1.50.1  |
| julia/0.7.0 | matlab/R2021a | scala/2.12.2 |

~~~~~ category: lib  
~~~~~

lftp/4.8.4  
~~~~~ category: libraries  
~~~~~

Xvfb/1.20.12  
acml/5.2.0-gfortran  
agalma/1.0.0  
armadillo/9.200.4  
assimp/4.1.0  
assimp/5.0.0  
blast-legacy/2.2.26  
boost/1.44.0  
boost/1.49.0  
boost/1.55  
boost/1.57  
boost/1.62.0-intel  
boost/1.63.0  
boost/1.68  
boost/1.69  
boost/1.75.0\_openmpi\_4.0.5\_intel\_2020.2\_slurm20  
boost/1.76.0\_hpcx\_2.7.0\_gcc\_10.2\_slurm20  
boost/1.76.0\_hpcx\_2.7.0\_intel\_2020.2\_slurm20  
bzip2/1.0.2  
c-blosc/1.16.3  
cdhit/4.6.8  
cuda/10.0.130  
cuda/10.1.105  
cuda/10.2  
cuda/11.1.1  
cuda/11.1.1\_intel\_2020  
cuda/11.3.1  
cuda/7.5.18  
cuda/8.0.61  
cuda/9.0.176  
cuda/9.1.85.1  
cuda/9.2.148

ea-utils/1.04.807  
fabm/1.0.2  
fastq-tools/0.8  
fftw/2.1.5  
fftw/2.1.5-double  
fftw/3.3.6  
fftw/3.3.8  
fftw/3.3.8a  
freeglut/3.0.0  
geos/3.4.2  
geos/3.7.1  
geos/3.8.1  
gerris/1.0  
global\_arrays/5.6.1  
global\_arrays/5.6.1\_i8  
global\_arrays/5.6.1\_openmpi\_2.0.3  
global\_arrays/5.8\_openmpi\_4.0.5\_gcc\_10.2\_slurm20  
gmp/6.1.2  
gsl/1.15  
gsl/2.3  
gsl/2.5  
igraph/0.7.1  
keras/2.0.9  
keras/2.1.1  
keras/2.1.3\_py3  
lemon/1.3.1  
leveldb/1.20  
libcutensor/10.2  
libflint/2.7.1  
libint/2.5.0  
libpng12/1.2.57  
libspatialindex/1.9.3  
libtiff/4.0.10  
libxc/4.3.4  
libzip/0.9-3.1.el6  
lp\_solve/5.5.2.5  
metis/5.1.0  
mpfr/3.1.5  
mpfr/4.0.2  
mpi4py/3.0.1\_py3.6.8

mxnet/1.3.0  
node.js/14.16.0  
node.js/6.10.3  
occa/1.2  
openblas/0.2.19  
openblas/0.2.8  
openblas/0.3.7  
opencv/3.2.0  
opencv/3.4.1  
parmetis/4.0.3  
pcre2/10.35  
phylobales/1.8b  
proj/4.9.3  
proj/5.2.0  
proj/7.0.0  
pytorch/1.3.1  
sparsehash/2.0.2  
suiteparse/4.5.4  
sysstat/12.5.4  
tensorflow/1.1.0\_cpu  
tensorflow/1.1.0\_gpu  
tensorflow/1.13.1\_cpu\_py3  
tensorflow/1.13.1\_gpu  
tensorflow/1.13.1\_gpu\_keras  
tensorflow/1.13.1\_gpu\_py3  
tensorflow/1.14.0\_gpu\_py36  
tensorflow/1.4.1\_cpu  
tensorflow/1.4.1\_cpu\_py3  
tensorflow/1.4.1\_gpu  
tensorflow/1.4.1\_gpu\_py3  
tensorflow/1.4.1\_gpu\_py3\_cuda9.1  
tensorflow/1.5.0\_cpu\_py3  
tensorflow/1.5.0\_gpu  
tensorflow/1.5.0\_gpu\_py3  
tensorflow/2.0.0\_cpu\_py37  
tensorflow/2.0.0\_gpu\_py37  
theano/1.0.1\_py3  
transdecoder/5.4.0  
v8/3.14.5  
voro++/0.4.6

vrpn/7.33

whatshap/Sep2018

xeyes/1.0

xz/5.2.4

yaml-cpp/0.6.2

yaml-cpp/0.6.2\_intel2019.3

yaml-cpp/0.6.3\_intel\_2020.2

zlib/1.2.11

~~~~~ category: library

~~~~~

catch2/2.3          matplotlib/2.2.4      pmclib/1.1

dcmstk/3.6.6          multineat/3.10      pstokes/1.0

dotnet/5.0.202      nccl/2.4.7          sprng/5.0

easydict/1.7          nccl/2.8.4          statsmodels/0.9.0

fastq\_screen/0.13.0   openslide/3.4.1

gsutil/350          p7zip/16.02

~~~~~ category: machine learning

~~~~~

1/1.01                  py-faster-rcnn/July2018

1/2.03                  rapidjson/1.1.0

attend2u/20180216          scikit-learn/0.19.1

cuda/5.1                  scikit-learn/0.21.2

cuda/6.0                  sciml\_class/pytorch-21.06

cuda/7.0                  tensorflow/1.1.0\_cpu

cuda/7.4                  tensorflow/1.1.0\_gpu

cuda/7.6                  tensorflow/1.13.1\_cpu\_py3

cuda/7.6.5                  tensorflow/1.13.1\_gpu

cuda/8.1.0                  tensorflow/1.13.1\_gpu\_keras

cuda/8.2.0                  tensorflow/1.13.1\_gpu\_py3

deeparg/Jan2019                  tensorflow/1.14.0\_gpu\_py36

deeparg/Oct2018                  tensorflow/1.4.1\_cpu

deeplabcut/1.01                  tensorflow/1.4.1\_cpu\_py3

deeplabcut/2.03                  tensorflow/1.4.1\_gpu

deeplabcut/2.1.4                  tensorflow/1.4.1\_gpu\_py3

deeplabcut/2.1.9                  tensorflow/1.4.1\_gpu\_py3\_cuda9.1

deeplabcut/2.2                  tensorflow/1.5.0\_cpu\_py3

dlib/19.17                  tensorflow/1.5.0\_gpu

flann/1.8.4                  tensorflow/1.5.0\_gpu\_py3

hnn/1.0                  tensorflow/2.0.0\_cpu\_py37

horovod/0.16                  tensorflow/2.0.0\_gpu\_py37

```

horovod/0.19.5          tf-horovod/1.0
pcl/1.9.1               xgboost/1.3.3
pcl/1.9.1_nurbs
~~~~~ category: math
~~~~~

atlas/3.10.3            lapack/3.7.0            ripser/0.5.3
blas/3.7.0              macaulay2/1.12-1        rss/1.0
cgal/3.14.1             magma/V2.23-10          sage/8.7
fenics/2017.1           magma/V2.25-5           sage/9.0
fenics/2018.1.0         magma/V2.25-5-gpu       scalapack/2.0.2
gap/4.9.1               magma-gpu/2.4.0         sympy/1.4
gmsh/3.0.1              magma-gpu/2.5.4_volta   trlan/2010.09
lapack/3.4.2            nlopt/2.5.0
lapack/3.6.0            numpy/intel_1.15.1
~~~~~ category: misc
~~~~~

mark/Dec18              mysql/8.0.13
mysql/5.7.28            netcdf4-python/4.1.4.2
~~~~~ category: ml
~~~~~

bonito/0.3.1
~~~~~ category: model
~~~~~

gotm/5.0_qingli gotm/5.3
~~~~~ category: molecular dynamics
~~~~~

mdanalysis/0.19.2
~~~~~ category: mpi
~~~~~

mpi/cave_mvapich2_2.3b_gcc
mpi/cave_mvapich2_2.3b_intel
mpi/cave_mvapich2_2.3rc2_gcc
mpi/hpcx_2.7.0_gcc_10.2_slurm20
mpi/hpcx_2.7.0_intel_2020.2_slurm20
mpi/mpich3.3a3_intel_2020.2
mpi/mvapich2-2.3.5_gcc_10.2_slurm20
mpi/mvapich2-2.3.5_intel_2017.0_slurm20
mpi/mvapich2-2.3.5_intel_2020.2_slurm20
mpi/openmpi_2.0.3_intel_2020.2_slurm20
mpi/openmpi_3.1.6_gcc

```

```
mpi/openmpi_3.1.6_gcc_10.2_slurm20
mpi/openmpi_4.0.0_gcc
mpi/openmpi_4.0.1_gcc
mpi/openmpi_4.0.4_gcc
mpi/openmpi_4.0.4_gcc_8.3_slurm20
mpi/openmpi_4.0.5_gcc_10.2_slurm20
mpi/openmpi_4.0.5_intel_2020.2_cuda_9.1.85_slurm20
mpi/openmpi_4.0.5_intel_2020.2_slurm20
mpi/openmpi_4.1.1_gcc_10.2_slurm20
osu-mpi/5.3.2
osu-mpi/5.6.2_mvapich2-2.3a_gcc
~~~~~ category: mri
~~~~~

afni/17.1.00      freesurfer/6.0.0
afni/18.2.06      freesurfer/6.0.0_rh7
afni/19.0.17      freesurfer/6.0.0_rh7-30-Nov-2018
afni/19.3.08      freesurfer/7.1.1
afni/19.3.10      fsl/5.0.10
afni/20.0.03      fsl/6.0.0
afni/20.1.06      fsl/6.0.3
afni/21.2.04      mmvt/2020-06
ants/2.1.0        mricron/05-2016
ants/2.3.1        mricron/12-2012
ants/2.3.4        mricron/2019-09
dsi/april2019     tortoise/3.1.0
~~~~~ category: neuro
~~~~~

dtitk/2.3.1  qit/1.0  qit/2.0  qit/Jun21
~~~~~ category: neuroscience
~~~~~

sct/4.2.2
~~~~~ category: numerical optimization ~~~~~
bayop/1.0
~~~~~ category: other
~~~~~

sbt/1.2.3
~~~~~ category: package
~~~~~

ffte/6.0 fftf/6.0/mpi
~~~~~ category: performance
```

~~~~~

ior/2.10.3	ipm/2.0.6_r
ior/3.0.1	osu-mpi/5.3.2
ior/3.2.1	osu-mpi/5.6.2_mvapich2-2.3a_gcc
ipm/2.0.6	papi/5.4.3

~~~~~ category: physics

~~~~~

casa/5.1.2
geant/4.10.04.p01
geant/4.10.3
geant/4.10.5
geant/4.9.4.p04
gpaw/0.10.0
gpaw/1.2.0
gpaw/1.2.0_hpcx_2.7.0_gcc
gpaw/1.2.0_mvapich2-2.3a_gcc
gpaw/20.10.0_hpcx_2.7.0_intel_2020.2_slurm20
gpaw/20.10_hpcx_2.7.0_intel_2020.2_slurm20
gpaw/21.1.0_hpcx_2.7.0_gcc_10.2_slurm20
gpaw/21.1.0_openmpi_4.0.5_gcc_10.2_slurm20
gpaw/21.1.0a_openmpi_4.0.5_gcc_10.2_slurm20
hoomd/2.9.0
jdftx/1.4.2
lumericalfdtd/8.16.982
mcx/20180525
mcxlab/2017.7
mujoco-py/1.50.1.23
pymultinest/2.9
root/6.10

~~~~~ category: profiling and debugging ~~~~~

|                |                           |
|----------------|---------------------------|
| cube/4.3.4     | ncdu/1.14                 |
| ddd/3.3.12     | scalasca/2.3.1_intel      |
| gdb/7.12.1     | scorep/3.0_intel_mvapich2 |
| gperftools/2.5 | valgrind/3.12.0           |

~~~~~ category: python

~~~~~

numpydoc/0.9.1	pytables/3.5.2	six/1.12.0
plotly/3.9.0	python_igraph/0.7.1	

~~~~~ category: python library

~~~~~



```

wx/1.0
~~~~~ category: software
~~~~~

annovar/2018Apr16 orthofinder/2.2.7 orthofinder/2.3.3
~~~~~ category: software management
~~~~~

maven/3.2.2 maven/3.8.1
~~~~~ category: solvers
~~~~~

eigen/3.2.2
eigen/3.3.2
eigen/3.4.0
mcl/12.135
mineos/1.0
mumps/5.0.2
mumps/5.0.2-seq
openfoam/4.1
openfoam/4.1a
openfoam/7.0_hpcx_2.7.0_gcc_10.2_slurm20
pari/2.11.2
pastix/5.2.3
petsc/3.14.2_hpcx_2.7.0_gcc_10.2_slurm20
petsc/3.14.2_hpcx_2.7.0_intel_2020.2_slurm20
petsc/3.14.2_mpich3.3a3_intel_2020.2
petsc/3.7.5
petsc/3.7.7
petsc/3.8.3
polyrate/17C
scotch/6.0.4
suiteparse/4.5.4
trilinos/12.12.1
~~~~~ category: stat
~~~~~

seaborn/0.10.0
~~~~~ category: statistical analysis package ~~~~~

glmnet/1.0
~~~~~ category: statistics
~~~~~

JAGS/4.2.0 R/3.6.3 caffe/1.0_with_cudnn
JAGS/4.3.0 R/4.0.0 mallet/2.0.8rc3

```

R/3.3.2	R/4.0.3	rstudio/1.0.44
R/3.4.0	R/4.0.5	rstudio/1.1.463
R/3.4.3	R/4.1.0	rstudio/1.4.1103
R/3.4.3_mkl	SAS/9.4M6	stata/14
R/3.4.4	SAS/9.4b	stata/15
R/3.5.2	caffe/1.0	wfu_pickatlas/3.0.5b
R/3.6.0	caffe/1.0_CPU_ONLY	

~~~~~ category: sys

~~~~~

dos2unix/7.4.0

~~~~~ category: system

~~~~~

wayland/1.18.0	xfce/4.10	xfce/4.16
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wayland-protocols/1.20 xfce/4.12

~~~~~ category: tex

~~~~~

pandoc/2.9.2.1

~~~~~ category: text editing

~~~~~

texstudio/2.12.16

~~~~~ category: tool

~~~~~

dcm2niix/25.0

~~~~~ category: tool kit

~~~~~

subread/1.6.2

~~~~~ category: tools

~~~~~

idr/2.0.2 omero/5.6.2

~~~~~ category: utilities

~~~~~

atom/1.19.3	git/2.10.2
bamaddrg/20180928	git/2.20.2
binutils/2.29.1	git/2.29.2
binutils/2.31	h4cf/1.2
chrome/55.0	h5py/2.9.0
chrome/73.0	intltool/0.51.0
cmake/3.10.1	itstool/2.0.4
cmake/3.15.4	json_cpp/1.9.4
cmake/3.20.0	json_fortran/8.1.0

cmake/3.6.3	kallisto/0.46.1
cmake/3.8.0	libevent/2.1.8
colordiff/1.0.18	libwnck/3.24.1
comsol/5.2	mercurial/5.1
comsol/5.6	ncurses/6.2
cppunit/1.14.0	pdftk/2.02
curl/7.61.1	perf-tools/2.7
cvs/1.11.23	rclone/1.51.0
depot_tools/Jan2019	rsync/3.1.3
engineering/19.10.237	spfft/0.9.12
engineering/calibre2020.1_36	sublime/2.0.2
express/1.5.1	svn/1.8.17
fileZilla/3.10.0	svn/1.9.5
firefox/56.0.2	texinfo/4.13a
firefox/59.0.2	texlive/2018
firefox/66.0.3	vim/8.1
firefox/68.0	vim/8.1_py3
firefox/87.0	vnc-apps/7.2
ghostscript/9.21	xxdiff/4.0.1

~~~~~ category: utility

~~~~~

redis/6.2.4

~~~~~ category: version record for large files ~~~~~

gitlfs/2.7.1

~~~~~ category: vision

~~~~~

opencv/3.2.0     scikit-image/0.13.1     tesseract/3.05.00

opencv/3.4.1     scikit-image/0.15.0     tesseract/4.00.00

~~~~~ category: visualization

~~~~~

atomeye/3.0

basemap/1.2.0

blender/2.78

blender/2.79

blender/2.90.1

cartopy/0.16.0

cartopy/0.17.0

cave-demo/yurt

cave-utils/yurt

caviar/1.0

ferret/7.1  
gdal/2.1.3  
gdal/2.4.0  
gdal/3.0.4  
gephi/0.9.2  
gimp/2.8.22  
gimp/2.9.6  
glm/0.9.9  
glm/0.9.9.5  
grace/5.1.25  
graphviz/2.40.1  
minvr/0.3master  
minvr/0.4  
minvr/beta  
minvr/beta-bleeding  
minvr/dev\_ben  
ncview/2.1.7  
openscad/2015.03-3  
openscenegraph/3.4.0  
osgearth/2.7  
ovito/2.8.2  
ovito/2.9.0  
paraview/5.1.0  
paraview/5.1.0\_yurt  
paraview/5.4.1  
paraview/5.6.0\_no\_scalable  
paraview/5.6.0\_yurt  
paraview/5.8.0  
paraview/5.8.0\_mesa  
paraview/5.8.0\_release  
paraview/5.8.1\_openmpi\_4.0.5\_intel\_2020.2\_slurm20  
paraview/5.9.0  
photoscan/1.3.0  
pyshp/2.0.1  
shapely/1.6.4  
tecplot/2017  
tecplot/2017R3  
tecplot/2018R2  
tecplot/2019R1  
unity/Unity-2017.3.0b1

unity/unity-editor-2017.2.0f3

visit/2.13.2

visit/2.7.2

vmd/1.9.3

vrg3d/265

vrg3d/265\_compat

vrg3d/265\_demos

vtk/5.6.1

vtk/7.1.1

vtk/7.1.1a

vtk/8.1.0

xcrysden/1.5.60

~~~~~ category: vizualization

~~~~~

metashape/1.5.4

~~~~~ category: weather

~~~~~

wrf/3.6.1

wrf/4.2.1\_hpcx\_2.7.0\_intel\_2020.2\_slurm20

~~~~~ category: workshop

~~~~~

workshop/1.0 workshop/3.0

# Oscar: Sage

## Loading and Launching Sage

1. Once authenticated to Oscar, use the following commands at the command line.
2. Start an interactive job by using the `interact` command. This command can take additional parameters to extend the resources and time allotted to the node as well as the partition that the node operates on.
3. The Sage module provides containers. To load them use `module load sage-container/10.3`.
4. To start the container use `apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-container-10.3-avpqipfsnbneig726l72jrgdmlrivg4m/sage.sif`
5. Once inside the container's shell use `sage` to launch the Sage console.

## Sage on Oscar OnDemand

The easiest way to run Sage on Oscar OnDemand is to run sage in an interactive job via the terminal in your OnDemand session.

Use the `interact` command with parameters for your specific job to start the interactive session, then load your modules and run the sage binary (steps 2-4 above).

```
interact -n 2 -m 32g -t 04:00:00 -f 'haswell|broadwell|skylake'
```

## Using Sage with Batch Scripts

*Thanks to Trevor Hyde from Summer@ICERM 2019 for these instructions.*

One method for running computations with Sage on Oscar is to write a script and use the slurm batch scheduler to have Oscar run your script. This requires two pieces:

1. A shell script to configure and submit your batch job to the cluster.

2. Your Sage code/program you'd like to run.

# Example Batch Script

## sage-batch.sh

```
#!/bin/bash

#SBATCH -J test_program
#SBATCH --array=0-9
#SBATCH -t 1:00:00
#SBATCH --mem=8G

#SBATCH -e data/<oscar-username>/test_output/test%a.err
#SBATCH -o data/<oscar-username>/test_output/test%a.out

module load sage-container/10.3

apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-
container-10.3-avpqiipfsnbneig726l72jrgdmlrivg4m/sage.sif

sage test_program.sage $SLURM_ARRAY_TASK_ID
```

- `#!/bin/bash` tells the system this is a bash (shell) script.
- `#SBATCH -J test_program` sets the name of the job which appears when you check the status of your jobs.
- `#SBATCH --array=0-9` is an easy way of doing parallel computations. In this case it says our job will run on 10 different nodes, each node will be passed a parameter and we have specified that the parameters will take the values 0 through 9. You can specify several ranges or even list individual parameters if you prefer.
- `#SBATCH -t 1:00:00` specifies a time limit in `HH:MM:SS` for each node. Once this time runs out your program will stop running on that node. Be careful setting the time limit too high as doing so may make it take a long time for your job to get scheduled to run. Before starting a big computation try to do some smaller tests to see how long you expect to need.
- `#SBATCH --mem=8G` specifies how much memory each node gets. Standard exploratory accounts get 123GB total to use at any one time. So if you allocate too much per job, fewer jobs will run at once. On the other hand, if you allocate too little and a computation needs more than it has, then it will terminate. If this happens an “out of memory” error will show up in the `.err` file for that node.

- `#SBATCH -e data/<ccv-username>/test_output/test%a.err` and `#SBATCH -o data/<ccv-username>/test_output/test%a.out` specify where the error messages and output for each computation should be sent. You should store these files in your user folder, not on the submit node. We each have a folder inside the `data` directory which you can see from the submit node. In this example I have created a folder titled `test_output` where I'm putting both of these files. **You need to make these folders before you run the computation otherwise the output will be dumped into the void!** The `%a` will get replaced with the array parameter. So for example, since we set our array parameters to be `0-9` there will be 10 nodes running and each of them gets a number between 0 and 9; this node corresponding to the parameter 7 will create two files `test7.err` and `test7.out`.
- `module load sage-container/10.3` loads the sage container into the node.
- `apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-container-10.3-avpqi pfsnbneig726l72jrgdmlrivg4m/sage.sif` initiates the container's Sage console shell.

Everything after this in the script happens as if you typed it yourself onto the command line.

- In our example, we want to run sage code, so the line `sage test_program.sage` `$SLURM_ARRAY_TASK_ID` runs our example sage program `test_program.sage`.
- The file needs to have the `.sage` extension.
- You should write this file in a text editor, not in a Jupyter notebook (although you can first write and test your program in a Jupyter notebook and then copy and paste it into a new file when it's ready).
- This program is written to accept one input and I have passed it `$SLURM_ARRAY_TASK_ID` which is the array parameter passed to each node. You can use this parameter to select which input parameters to run your program on.

## Example Sage Program

### `test_program.sage`

```
import sys

def fun_math(message):
 print message
 sys.stdout.flush()

job_id = int(sys.argv[1])
fun_math('hi this is a test')
fun_math('my job id is' + str(job_id))
```



- In the Sage program, you first define all of your functions and then you include the code you want to run.
- Import `sys` so you can access the array parameter passed to your function from the node. This is accessed in this case by `sys.argv[1]`. Make sure you explicitly coerce to be an integer if you want to use it as an integer; it's a string by default.
- The output of the `print` command is appended to the `.out` file for this node as a new line.
- Notice the line `sys.stdout.flush()` included in the function. This makes the program immediately send whatever output it has to the output file when called. Otherwise the program won't output **anything** until it has completely finished running. If each node is running 100 potentially long computations and it finishes the first 99 but then times out on the 100th computation, and you don't include any `sys.stdout.flush()` commands, everything will be lost when time runs out.

## Submitting the Batch Job

- To run this batch program go back to the submit node and type `sbatch` `<NAME_OF_BATCH_FILE>`. In our example here, our batch file is called `sage-batch.sh`, so we simply type `sbatch sage-batch.sh`. Slurm will return a line that tells you your job has been submitted together with a job id number.
- To check the progress of your jobs type `myq` from anywhere on Oscar. This will show you what jobs you have running, how much time they have left, and which jobs are still waiting to run. Be patient, sometimes it takes a minute for things to get started.
- If you realize your code is never going to finish or that you've made some terrible mistake, you can cancel a batch job by typing `scancel <JOB_ID>`. You can specify a single node or just put the general job id for the whole run and cancel everything.

# Oscar: MATLAB

## Loading and Launching MATLAB

1. Open the Terminal and use the following commands at the command line.
2. `module avail matlab` to list all the available matlab versions.
3. `module load matlab/R2018a` to load matlab. This command should return the confirmation “*module loaded*”.
4. `matlab` to launch the MATLAB app.

## Installing MATLAB Packages such as YALMIP

MATLAB script packages, such as YALMIP, can be installed directly by the user on their Oscar account. These instructions assume you are using Oscar via the VNC client.

1. Open the Terminal on your VNC session.
2. Navigate to your home folder by typing `cd ~`
3. `mkdir -p MATLAB`
4. `wget -O yalmip.zip https://github.com/yalmip/yalmip/archive/master.zip`
5. `unzip yalmip.zip`
6. In MATLAB, add the YALMIP-master directory to your path.
  1. In the MATLAB file browser, navigate to the MATLAB folder you created in your home folder. `cd ~/MATLAB`
  2. Right click on the YALMIP-master folder.
  3. Select Add to Path > Selected Folders and Subfolders. This adds the YALMIP folders to your path.

7. To save your MATLAB path, use the savepath command in the MATLAB command prompt.

```
savepath ~/MATLAB/pathdef.m
```

YALMIP also requires a solver like SDPT3. The steps below add SDPT3 to MATLAB.

1. Open the Terminal.

2. `cd ~/MATLAB`

3. `wget -O sdpt3.zip https://github.com/sqlp/sdpt3/archive/master.zip`

4. `unzip sdpt3.zip`

5. In MATLAB, add the sdpt3 directory to your path.

1. In the MATLAB file browser, navigate to the MATLAB folder you created in your home folder. `cd ~/MATLAB`

2. Right click on the sdpt3-master folder.

3. Select Add to Path > Selected Folders and Subfolders. This adds the SDPT3 folders to your path.

6. To update/save your MATLAB path, use the savepath command in the MATLAB command prompt. `savepath ~/MATLAB/pathdef.m`

# Oscar: Mathematica

## Loading and Launching Mathematica

1. Open the Terminal and use the following commands at the command line.
2. `module avail mathematica` to list all the available mathematica versions.
3. `module load mathematica/11.0` to load mathematica. This command should return the confirmation *"module loaded"*.
4. `mathematica` to launch the Mathematica app.