NSCC ASPIRE 2A Software List

Last Updated: 12 May 2023

ASPIRE2A uses Red Hat Enterprise Linux 8 (RHEL) as its operating system (OS). Cray environment will be loaded by default.

Additional software may have been installed since this page was updated.

Type module list to see currently loaded modules.

Type module av to see the available modules on ASPIRE2A.

1. Applications:	2. Software Libraries	3. Cray Programming Environment
A abyss/2.3.2 ambertools/22 aocc/3.2.0 aocc/4.0.0 arm-forge/21.1.2 arm-forge/21.1.3 B bazel/4.2.2 bcftools/1.15.1 beast/1.10.4 beast/2.6.7 bedtools/2.30.0 berkeleygw/3.0.1 berkeleygw/3.0.1-b2 berkeleygw/3.0.1-b73 bowtie/1.1.2 bowtie/2.4.5 bwa/0.7.17 C cdo/2.0.5 cmake/3.23.1 cp2k/9.1 cp2k/2022.1 cuda/10.0 cuda/11.2 cuda/11.6.2 cylc/7.9.6 D doxygen/1.9.6 E eccodes/2.16.0 emacs/26.3	A aocl/3.1.0-aocc3.2 aocl/3.1.0-gcc11.1 aocl/3.2.0-aocc3.2 aocl/3.2.0-gcc11.2 aocl/4.0.0-aocc4.0 aocl/4.0.0-gcc11.2 atlas/3.10.3-hpe B beagle-lib/3.1.2-gcc11 beagle-lib/3.1.2-gcc11-cuda11 blis/0.8.1-hpe boost/1.76.0-gnu11 boost/1.81.0 C cudnn/10.0-7.6.5.32 cudnn/11.2-8.1.1.33 cudnn/11.6-8.4.0.27 E eigen/3.3.9 eigen/3.4.0 F fftw/3.3.4-intel fftw/3.3.10-gcc11 fftw/3.3.10-gcc11-ompi4 fftw/3.3.10-icc22-cmpi fftw/3.3.10-icc22-ompi4 flex/2.6.4 G g2clib/1.6.0 gdal/2.2.4 gdal/2.4.4 geos/3.10.1	A atp/3.14.10 C cce/13.0.2 cpe/22.04 cpe-cuda/22.04 cray-ccdb/4.12.10 cray-cti/2.15.10 cray-dsmml/0.2.2 cray-dyninst/12.0.0 cray-fftw/3.3.8.13 cray-hdf5/1.12.1.1 cray-hdf5-parallel/1.12.1.1 cray-libpals/1.1.6 cray-libsci/21.08.1.2 cray-mpich/8.1.15 cray-mpich-abi/8.1.15 cray-mpich-abi-pre-intel-5.0/8.1.15 cray-mpich-ucx/8.1.15 cray-mrnet/5.0.1 cray-netcdf/4.8.1.1 cray-netcdf-hdf5parallel/4.8.1.1 cray-openshmemx/11.5.3.beta cray-pals/1.1.6 cray-parallel-netcdf/1.12.2.1 craype/2.7.15 craype-accel-amd-gfx908 craype-accel-amd-gfx90a craype-accel-host craype-accel-nvidia70 craype-accel-nvidia80 craype-dl-plugin-py3/20.11.1 craype-network-none craype-network-ofi craype-network-ucx craype-x86-milan

F
fcm/2021.05.0
ffmpeg/5.0.1

G
gatk/4.2.6.1
gcc/8.5.0-nscc
gcc/9.5.0-nscc
gcc/10.3.0-nscc
gcc/11.2.0-nscc
gcc/11.3.0-nscc
gcc/12.1.0-nscc
gcc/12.2.0-nscc
ghostscript/9.25
git/2.39.2
go/1.18.1
grace/5.1.25
grads/2.2.1
graphviz/7.0.5
gromacs/2021.4-cuda-hpe
gromacs/2021.4-hpe
gromacs/2022.1
gromacs/2022.1-gpu

I
intel/2022.0.2
intel/2022.1.0
intel/2023.0.0
intel/2023.1.0
intel-classic/2022.0.2
intel-classic/2022.1.0
intel-classic/2023.0.0
intel-classic/2023.1.0
intel-oneapi/2022.0.2
intel-oneapi/2022.1.0
intel-oneapi/2023.0.0
intel-oneapi/2023.1.0

J
java/1.8.0_332-openjdk
java/11.0.15-openjdk
java/17.0.3.1-jdk
java/17.0.6-jdk
java/18.0.1.1-jdk
java/18.0.2.1-jdk
java/19.0.2-jdk
julia/1.7.2

L
lammps/23Jun2022_update1
lammps/23Jun2022_update1-gpu
lammps/29Sep2021_update3

M
gmp/6.2.1
grib_api/1.25.0
gsl/2.7.1-gcc11
gsl/2.7.1-hpe

H
hdf5/1.8.17-intel
hdf5/1.8.23-parallel-icc22-vmpi2
hdf5/1.10.5
hdf5/1.10.8-parallel-icc22-cmpi
hdf5/1.12.1-parallel-icc22-cmpi
hdf5/1.12.1-parallel-icc22-ompi4
hdf5/1.12.1-parallel-icc23-cmpi
hdf5/1.12.2-parallel-icc22-cmpi
hdfeos5/1.16

J
jasper/1.900.1
jasper/2.0.14
jpeg/9c

L
lapack/3.11-cray
lapack/3.11-intel

M
mkl/2022.0.2
mkl/2022.1.0
mkl/2023.0.0
mkl/2023.1.0

N
nccl/11.6-2.12.10-1

O
oasis3-mct/2.8
openblas/0.3.21-icc22
openblas/0.3.23
openjpeg/1.5.2
openjpeg/2.4.0

P
pcre2/10.42
petsc/3.16.5-hpe
proj/4.9.3
proj/8.1.1

Q
qt/5

R
readline/8.2
craype-x86-milan-x
craype-x86-rome
craype-x86-trento
craypkg-gen/1.3.24
cray-pmi/6.0.17
cray-pmi/6.1.1
cray-pmi-lib/6.0.17
cray-python/3.9.7.1
cray-R/4.1.2.0
cray-stat/4.11.9

G
gcc/10.3.0
gcc/11.2.0
gcc/8.1.0
gdb4hpc/4.13.10

L
libfabric/1.11.0.4.125

P
papi/6.0.0.14
perftools
perftools-base/22.04.0

V
valgrind4hpc/2.12.7

matlab/2022bup4_runtime
meld/3.16.4
miniforge3/23.10
mrtrix/3.0.3
mumax/3.10-gpu
mvapich/2.3.7-hpe
mvapich/2.3.7-icc22

N
namd/2.14
namd/3.0b3_net_smp
nasm/2.15.05
ncbi-blast/2.13.0
ncl/6.6.2
nco/5.0.6
ncview/2.1.7
nedit/5.7
nek5000/19.0
nektar/5.2.0
nextflow/22.04.0
nqstat/default
nqstat/nqstat-v1
numactl/2.0.14
nvhpc/22.3
nvhpc/22.5
nvhpc/22.11
nvhpc-byo-compiler/22.3
nvhpc-nompi/22.3
nvidia/22.3
nvidia/22.5
nvidia/22.11
nwchem/7.0.2

O
octave/7.1.0
openfoam/2112
openfoam/2112-hpe
openmpi/4.1.2-hpe
openmpi/4.1.4-aocc4.0
openmpi/4.1.5-aocc4
openmpi/4.1.5-gcc11
openmpi/4.1.5-icc22

P
python/2.7.18
python/3.7.13
python/3.8.13
python/3.9.12
python/3.10.4
python/3.10.9
python/3.11.3-gcc10
pytorch/1.11.0-hpe
pytorch/1.11.0-hpe-gpu
pytorch/1.11.0-py3
pytorch/1.11.0-py3-gpu

S
scalapack/2.2.0-icc22-cmpi-openblas
scalapack/2.2.0-icc22-ompi4-mkl22
scalapack/2.2.0-icc23-cmpi-mkl23
sparsehash/2.0.4-gcc11
swig/4.1.1
szip/2.1.1

U
udunits/2.2.26

Q qe/7.0 qe/7.1-gpu R r/4.2.0 relion/3.1.3 rose/2019.01.5 S sambamba/0.8.2 samtools/1.15.1 siesta/4.1.5 singularity/3.10.0 T tensorflow/1.15.5-hpe tensorflow/1.15.5-hpe-gpu tensorflow/2.7.0-hpe tensorflow/2.7.0-hpe-gpu tensorflow/2.8.1-py3 tensorflow/2.8.1-py3-gpu V velvet/1.2.10 vmd/1.9.3 W wps/3.9.1-b2 wrf/3.9.1-b2 wrf/4.2.2-hpe wrf/4.4.1-b2 X xios/1.0.703 xios/2.5 xios/r2331 xxdiff/4.0.1		