

NSCC ASPIRE 2A Software List

Last Updated: 2025-10-23

ASPIRE2A uses Red Hat Enterprise Linux 8 (RHEL) as its operating system (OS). Cray environment will be loaded by default. If a module file doesn't have a default version specified, the latest version will be used as the default.

For detailed instructions on customization and local directory installation, refer to the baseline README and Makefile in the "/app/apps/makefiles" and "/app/libs/makefiles" directory.

Type "module list" to see currently loaded modules.

Type "module avail" to see the available modules on ASPIRE2A.

Applications

A

Module Name	Version	Default
abyss	2.3.2	
ambertools	22	
antlr	2.7.7	
aocc	4.1.0	
aocc	4.0.0	
aocc	3.2.0	✓
arm-forge	25.0.2	
arm-forge	24.0.4	✓
arm-forge	23.1.2	
arm-forge	21.1.3	
arm-forge	21.1.2	

B

Module Name	Version	Default
bazel	4.2.2	
bcftools	1.15.1	
beast	2.6.7	
beast	1.10.4	
bedtools	2.30.0	
berkeleygw	3.0.1-b73	
berkeleygw	3.0.1-b72-gcc10-mkl23	
berkeleygw	3.0.1-b2	
berkeleygw	3.0.1	
bolt	2.4.1-intel	
bowtie	2.4.5	
bowtie	1.1.2	
bwa	0.7.17	

C

Module Name	Version	Default
cdo	2.4.4	
cdo	2.0.5	
cmake	4.1.0	
cmake	3.31.3	✓
cmake	3.23.1	
cp2k	9.1	
cp2k	2022.1	
cuda	12.2.2	
cuda	12.2.1	
cuda	11.8.0	
cuda	11.7.0	
cuda	11.6.2	✓
cuda	11.2	
cuda	10.0	
cylc	8.4.2	
cylc	7.9.6	

D

Module Name	Version	Default
darshan	3.4.6	
dftb	23.1-intel	
dftb	23.1-icc24	
doxygen	1.9.6	

E

Module Name	Version	Default
eccodes	2.16.0	
emacs	26.3	

F

Module Name	Version	Default
fcm	2021.05.0	
ffmpeg	5.0.1	

G

Module Name	Version	Default
gatk	4.6.2.0	
gatk	4.2.6.1	
gcc	9.5.0-nsc	
gcc	8.5.0-nsc	
gcc	14.2-nsc	
gcc	12.3.0-nsc	
gcc	12.2.0-nsc	
gcc	12.1.0-nsc	
gcc	11.4.0-nsc	
gcc	11.3.0-nsc	
gcc	11.2.0-nsc	
gcc	10.3.0-nsc	
ghostscript	9.25	
go	1.24.4	
go	1.23.4	
go	1.21.1	

go	1.18.1	
grace	5.1.25	
grads	2.2.1	
graphviz	7.0.5	
gromacs	5.1.2	
gromacs	2025.2-gnu	
gromacs	2023.2-gpu	
gromacs	2023.2-gnu	
gromacs	2022.1-gpu	
gromacs	2022.1	
gromacs	2021.4-hpe	
gromacs	2021.4-cuda-hpe	
gromacs	2020.2-plumed.2.6.1	
gromacs	2018.8-plumed.2.6.4-gnu-gpu	
gromacs	2018.8-plumed.2.6.4	
gromacs	2018.2-gpu	
gromacs	2018.2-gnu-gpu	
gromacs	2018.2	

I

Module Name	Version	Default
intel	2025.1.3	
intel	2025.0.1	
intel	2024.2.1	
intel	2024.0	✓
intel	2023.1.0	
intel	2023.0.0	
intel	2022.1.0	
intel	2022.0.2	
intel-classic	2023.1.0	
intel-classic	2023.0.0	
intel-classic	2022.1.0	
intel-classic	2022.0.2	✓
intel-oneapi	2025.1.3	
intel-oneapi	2025.0.1	

intel-oneapi	2024.2.1	
intel-oneapi	2024.0	
intel-oneapi	2023.1.0	
intel-oneapi	2023.0.0	
intel-oneapi	2022.1.0	
intel-oneapi	2022.0.2	✓

J

Module Name	Version	Default
java	24.0.1-jdk	
java	19.0.2-jdk	
java	18.0.2.1-jdk	
java	18.0.1.1-jdk	
java	17.0.6-jdk	
java	17.0.3.1-jdk	
java	11.0.15-openjdk	
java	1.8.0_332-openjdk	
julia	1.7.2-hpe	
julia	1.7.2	
julia	1.11.5	
julia	1.11.1	

L

Module Name	Version	Default
lammps	29Sep2021_update3	
lammps	23Jun2022_update1-gpu	
lammps	23Jun2022_update1-b1	
lammps	23Jun2022_update1	
lammps	22Jul2025_icc24	
lammps	22Jul2025_icc22	
lammps	22Jul2025_gpu11	
linaro-forge	25.0.2	
linaro-forge	24.0.4	✓
linaro-forge	23.1.2	

M

Module Name	Version	Default
matlab	2024b_runtime	
matlab	2022bup4_runtime	
matlab	2018b_runtime	
matlab	2015b_runtime	
matlab	2013a_runtime	
meld	3.16.4	
miniforge3	25.3.1	
miniforge3	23.10	
mistral	mistral-2023.1.1	
mlip	2.1	
mrtrix	3.0.3	
mumax	3.10-gpu	
mvapich	4.0-icc24	
mvapich	4.0-gnu11	
mvapich	2.3.7-icc24	
mvapich	2.3.7-icc22	
mvapich	2.3.7-hpe	

N

Module Name	Version	Default
nasm	2.15.05	
ncbi-blast	2.13.0	
ncl	6.6.2	
nco	5.1.6	
nco	5.0.6	
ncview	2.1.7	
nedit	5.7	
nek5000	19.0	
nektar	5.2.0	
nextflow	25.04.6	
nextflow	24.10.5	
nextflow	22.04.0	✓
ninja	1.11.1	

nqstat	nqstat-v1	
nqstat	default	
numactl	2.0.14	
nvhpc	23.7	
nvhpc	22.5	
nvhpc	22.3	✓
nvhpc	22.11	
nvhpc-byo-compiler	22.3	
nvhpc-nompi	22.3	
nvidia	23.7	
nvidia	22.5	
nvidia	22.3	✓
nvidia	22.11	
nwchem	7.2.3-icc23	
nwchem	7.0.2-icc23	
nwchem	7.0.2	

O

Module Name	Version	Default
octave	7.1.0	
openfoam	2412	
openfoam	2406-ompi505	
openfoam	2406	
openfoam	2212	
openfoam	2206	
openfoam	2112-hpe	
openfoam	2112	✓
openfoam	1912	
openmpi	5.0.8-gcc11-cu12	
openmpi	5.0.8-gcc11	
openmpi	5.0.5-nv22.11	
openmpi	5.0.5-icc24.2.1	
openmpi	5.0.5-gcc11	
openmpi	4.1.7-icc24.2.1	
openmpi	4.1.7-gcc11	

openmpi	4.1.6-gcc11	
openmpi	4.1.2-hpe	✓

P

Module Name	Version	Default
parallel	20240522	
plumed	2.6.4	
plumed	2.6.1	
python	3.9.12	
python	3.8.13	
python	3.7.13	
python	3.13.3-gcc11	
python	3.12.1-gcc11	
python	3.11.7-gcc11	
python	3.11.5-gcc12	
python	3.11.3-gcc10	
python	3.10.9	
python	3.10.4	
python	2.7.18	
python	2.7.11	
pytorch	2.6.0-py3-cu11.8	
pytorch	2.6.0-py3	
pytorch	1.11.0-py3-gpu	
pytorch	1.11.0-py3	
pytorch	1.11.0-hpe-gpu	
pytorch	1.11.0-hpe	

Q

Module Name	Version	Default
qe	7.4-icx24-mkl	
qe	7.4-hpcx-nvhpc22.11-cuda11.8	
qe	7.1-gpu	
qe	7.0	

R

Module Name	Version	Default
r	4.2.0	
relion	3.1.3	
rose	2019.01.5	

S

Module Name	Version	Default
sambamba	0.8.2	
samtools	1.15.1	
siesta	4.1.5	
singularity	4.3.1	
singularity	4.2.2	
singularity	4.0.0	
singularity	3.11.4	
singularity	3.10.0	✓

T

Module Name	Version	Default
tensorflow	2.8.1-py3-gpu	
tensorflow	2.8.1-py3	
tensorflow	2.7.0-hpe-gpu	
tensorflow	2.7.0-hpe	
tensorflow	2.19-py3-gpu	
tensorflow	2.19-py3	
tensorflow	1.15.5-hpe-gpu	
tensorflow	1.15.5-hpe	

V

Module Name	Version	Default
velvet	1.2.10	
vmd	1.9.3	

W

Module Name	Version	Default
wps	3.9.1-b2	
wrf	4.4.1-b2	
wrf	4.2.2-hpe	
wrf	3.9.1-b2	

X

Module Name	Version	Default
xios	r2331	
xios	2.5	
xios	1.0.703	
xxdiff	4.0.1	

Software Libraries

A

Module Name	Version	Default
aocl	4.1.0-gcc13.1	
aocl	4.1.0-aocc4.1	
aocl	4.0.0-gcc11.2	
aocl	4.0.0-aocc4.0	
aocl	3.2.0-gcc11.2	
aocl	3.2.0-aocc3.2	
aocl	3.1.0-gcc11.1	
aocl	3.1.0-aocc3.2	
atlas	3.10.3-hpe	

B

Module Name	Version	Default
beagle-lib	3.1.2-gcc11-cuda11	
beagle-lib	3.1.2-gcc11	
blis	0.8.1-hpe	
boost	1.81.0	
boost	1.76.0-gnu11	

C

Module Name	Version	Default
cudnn	12-9.8.0.87	
cudnn	12-8.9.4.25	
cudnn	11.6-8.4.0.27	
cudnn	11.2-8.1.1.33	
cudnn	11-8.9.4.25	
cudnn	10.0-7.6.5.32	
cuquantum	23.03	

E

Module Name	Version	Default
eigen	3.4.0	
eigen	3.3.9	
elpa	2024.05.001-icc24	
elpa	2024.05.001-icc23	

F

Module Name	Version	Default
fftw	3.3.4-intel	
fftw	3.3.10-icc22-mpi4	
fftw	3.3.10-icc22-mpi	
fftw	3.3.10-gcc11-mpi4	
fftw	3.3.10-gcc11	
flex	2.6.4	

G

Module Name	Version	Default
g2clib	1.6.0	
gdal	3.10.2	
gdal	2.4.4	
gdal	2.2.4	
geos	3.10.1	
gmp	6.2.1	
grib_api	1.25.0	
gsl	2.7.1-hpe	
gsl	2.7.1-gcc11	

H

Module Name	Version	Default
hdf5	1.8.23-parallel-icc22-vmapi2	
hdf5	1.8.17-intel	
hdf5	1.12.2-parallel-icc22-cmpi	
hdf5	1.12.1-parallel-icc24-ompi4	
hdf5	1.12.1-parallel-icc23-cmpi	
hdf5	1.12.1-parallel-icc22-ompi4	
hdf5	1.12.1-parallel-icc22-cmpi	
hdf5	1.12.1-nvhpc	
hdf5	1.10.8-parallel-icc22-cmpi	
hdf5	1.10.5	
hdfeos5	1.16	

J

Module Name	Version	Default
jasper	2.0.14	
jasper	1.900.1	
jpeg	9c	

L

Module Name	Version	Default
lapack	3.11-intel	
lapack	3.11-cray	

M

Module Name	Version	Default
mkl	2025.1	
mkl	2025.0	
mkl	2024.2	
mkl	2024.0	✓
mkl	2023.1.0	
mkl	2023.0.0	
mkl	2022.1.0	
mkl	2022.0.2	

N

Module Name	Version	Default
nccl	12.2-2.26.2-1	
nccl	12.2-2.18.3-1	
nccl	11.6-2.12.10-1	
nccl	11.0-2.18.3-1	
nsi	2.28	

O

Module Name	Version	Default
oasis3-mct	2.8	
openblas	0.3.23	
openblas	0.3.21-icc22	
openjpeg	2.4.0	
openjpeg	1.5.2	

P

Module Name	Version	Default
pcre2	10.42	
petsc	3.16.5-hpe	
proj	8.1.1	
proj	4.9.3	

Q

Module Name	Version	Default
qt	5	

R

Module Name	Version	Default
readline	8.2	

S

Module Name	Version	Default
scalapack	2.2.0-icc24-cmpi	
scalapack	2.2.0-icc23-cmpi-mkl23	
scalapack	2.2.0-icc22-ompi4-mkl22	
scalapack	2.2.0-icc22-cmpi-openblas	
sndfile	1.2.0	
sparsehash	2.0.4-gcc11	
swig	4.1.1	
szip	2.1.1	

U

Module Name	Version	Default
udunits	2.2.26	

Cray Programming Environment**A**

Module Name	Version	Default
atp	3.14.10	✓

C

Module Name	Version	Default
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	✓
cray-pmi	6.1.1	✓

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

G

Module Name	Version	Default
gcc	8.1.0	
gcc	11.2.0	✓
gcc	10.3.0	
gdb4hpc	4.13.10	✓

L

Module Name	Version	Default
libfabric	1.11.0.4.125	✓

P

Module Name	Version	Default
papi	6.0.0.14	✓
perftools		
perftools-base	22.04.0	✓
perftools-lite		
perftools-lite-events		
perftools-lite-gpu		
perftools-lite-hbm		
perftools-lite-loops		
perftools-preload		
PrgEnv-aocc	8.3.3	✓
PrgEnv-cray	8.3.3	✓
PrgEnv-gnu	8.3.3	✓
PrgEnv-intel	8.3.3	✓
PrgEnv-nvhpc	8.3.3	✓
PrgEnv-nvidia	8.3.3	✓

V

Module Name	Version	Default
valgrind4hpc	2.12.7	✓

The table below outlines the software scheduled for updates in the upcoming quarter. Software not listed will be updated on a best-effort basis.

Q1	Q2	Q3	Q4
TensorFlow	GROMACS	LAMMPS	CP2K
OpenFOAM	Singularity	ncl	R
PyTorch	gatk	miniforge3	SAMtools
Python	julia	Arm-forge	BerkeleyGW
nextflow	OpenMPI	mvapich	cdo
nwchem	intel		matlab_runtime
QE	java		plumed
GCC	GO		hdf5
CUDA	MKL		AOCC
NCCL			Boost
cuDNN			