

NSCC ASPIRE 2A Software List

Last Updated: 2 September 2022

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
<p>A</p> <p>abyss/2.3.2 ambertools/22 anaconda2/2019.10 anaconda3/2021.11 aocc/3.2.0 arm-forge/21.1.2</p> <p>B</p> <p>bazel/4.2.2 bcftools/1.15.1 beast/1.10.4 beast/2.6.7 bedtools/2.30.0 berkeleygw/3.0.1 bowtie/2.4.5 bwa/0.7.17</p> <p>C</p> <p>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</p> <p>E</p> <p>eccodes/2.16.0</p> <p>F</p> <p>fcm/2021.05.0 ffmpeg/5.0.1</p> <p>G</p> <p>gatk/4.2.6.1 gcc/8.5.0-nsccl gcc/11.2.0-nsccl gcc/11.3.0-nsccl gcc/12.1.0-nsccl go/1.18.1 grace/5.1.25 gromacs/2021.4-cuda-hpe</p>	<p>A</p> <p>aocl/3.1.0-aocc3.2 aocl/3.1.0-gcc11.1 atlas/3.10.3-hpe</p> <p>B</p> <p>beagle-lib/3.1.2-gcc11 beagle-lib/3.1.2-gcc11-cuda11 blis/0.8.1-hpe</p> <p>C</p> <p>cudnn/10.0-7.6.5.32 cudnn/11.2-8.1.1.33 cudnn/11.6-8.4.0.27</p> <p>E</p> <p>eigen/3.3.9 eigen/3.4.0</p> <p>F</p> <p>fftw/3.3.10-gcc11</p> <p>G</p> <p>g2clib/1.6.0 gdal/2.2.4 gdal/2.4.4 geos/3.10.1 grib_api/1.25.0 gsl/2.7.1-gcc11 gsl/2.7.1-hpe</p> <p>H</p> <p>hdf5/1.10.5 hdfeos5/1.16</p> <p>J</p> <p>jasper/1.900.1 jasper/2.0.14 jpeg/9c</p> <p>M</p> <p>mkl/2022.0.2</p> <p>N</p>	<p>A</p> <p>atp/3.14.10</p> <p>C</p> <p>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 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</p>

<p>gromacs/2021.4-hpe gromacs/2022.1 gromacs/2022.1-gpu</p> <p>I intel/2022.0.2 intel-classic/2022.0.2 intel-oneapi/2022.0.2</p> <p>J java/1.8.0_332-openjdk java/11.0.15-openjdk java/17.0.3.1-jdk java/18.0.1.1-jdk julia/1.7.2</p> <p>L lammps/23June2022 lammps/29Sep2021</p> <p>M miniconda3/py38_4.8.3 miniconda3/py39_4.11.0 mrtrix/3.0.3 mumax/3.10-gpu mvapich/2.3.7-hpe</p> <p>N namd/2.14 nasm/2.15.05 ncbi-blast/2.13.0 ncl/6.6.2 nco/5.0.6 ncview/2.1.7 nek5000/19.0 nektar/5.2.0 nextflow/22.04.0 numactl/2.0.14 nvhpc/22.3 nvhpc/22.5 nvhpc-byo-compiler/22.3 nvhpc-nompi/22.3 nvidia/22.3 nvidia/22.5 nwchem/7.0.2</p> <p>O octave/7.1.0 openfoam/2112 openmpi/4.1.2-hpe</p> <p>P python/2.7.18 python/3.7.13 python/3.8.13 python/3.9.12 python/3.10.4 pytorch/1.11.0-py3 pytorch/1.11.0-py3-gpu</p>	<p>nccl/11.6-2.12.10-1</p> <p>O oasis3-mct/2.8 openjpeg/1.5.2 openjpeg/2.4.0</p> <p>P petsc/3.16.5-hpe proj/4.9.3 proj/8.1.1</p> <p>S sparsehash/2.0.4-gcc11 szip/2.1.1</p> <p>U udunits/2.2.26</p>	<p>cray-pmi-lib/6.0.17 cray-python/3.9.7.1 cray-R/4.1.2.0 cray-stat/4.11.9</p> <p>G gcc/10.3.0 gcc/11.2.0 gcc/8.1.0 gdb4hpc/4.13.10</p> <p>L libfabric/1.11.0.4.125</p> <p>P papi/6.0.0.14 perftools perftools-base/22.04.0</p> <p>V valgrind4hpc/2.12.7</p>
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<p>Q qe/7.0</p> <p>R r/4.2.0 relion/3.1.3 rose/2019.01.5</p> <p>S sambamba/0.8.2 samtools/1.15.1 siesta/4.1.5 singularity/3.10.0</p> <p>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</p> <p>V velvet/1.2.10</p> <p>W wrf/4.2.2-hpe wrf/4.4</p> <p>X xios/1.0.703 xios/2.5 xios/r2331 xxdiff/4.0.1</p>		
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