Software List

List of software centrally available via the modules tool at the INCD Cirrus HPC and HTC clusters as of **August 2022**. Full list changes and to request the installation of additional software contact the INCD support **helpdesk**.

Intel Compilers available

Users can also install software on their own for further information see the section on **User Software Installation**. Execution of user defined software environments (operating system and libraries) using Linux containers in the HPC and HTC clusters with **uDocker** and **Singularity** is also supported.

INCD-Lisbon HPC and HTC cluster (Cirrus-A)

AlmaLinux 8

```
[jpina@cirrus01 ~]$ module avail

---------------------------------------------------------------------------------------------------------- /cvmfs/sw.el8/modules/hpc/main
----------------------------------------------------------------------------------------------------------------
   R/4.4.3        (D)    gcc-11.3    gcc-8.5            julia/1.9.4     julia/1.11.4         (D)    matlab-runtime/9.0.1
python/3.7     python/3.11 (D)    spack/0.19.1       udocker/1.3.16
   aoc-4.0.0             gcc-13.2    intel/oneapi/2023    julia/1.10.5    matlab-runtime/R2016a       matlab-
runtime/24.1  (D)    python/3.8     qgis/3.40.5        spack/0.21.1 (D)    udocker/1.3.17 (D)
   bazelisk/1.22.0       gcc-14.1    julia/1.6.7          julia/1.11.0    matlab-runtime/R2024a       opam
python/3.10    qgis/3.44.2 (D)    spark/3.1.1

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/cvmfs/sw.el8/modules/hpc/aoc40
----------------------------------------------------------------------------------------------------------------
   aoc40/R/4.2.2          aoc40/gromacs/2023     aoc40/libs/blas/3.11.0     aoc40/libs/gsl/2.7
aoc40/libs/jemalloc/5.3.0     aoc40/libs/libpng/1.6.39     aoc40/libs/openblas/0.3.21     aoc40/openmpi/4.1.4
   aoc40/gamess/2023-R2     aoc40/libs/aocl/4.0     aoc40/libs/fftw/3.3.10     aoc40/libs/hdf5/1.14.0
```

aoc40/libs/lapack/3.11.0 aoc40/libs/nlopt/2.7.1 aoc40/mvapich2/2.3.7

/cvmfs/sw.el8/modules/hpc/gcc85

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gcc85/R/4.2.2 gcc85/libs/gsl/2.7 gcc85/libs/lapack/3.11.0 gcc85/libs/openblas/0.3.21 gcc85/netcdf-cxx/4.2 gcc85/openfoam-org/11 gcc85/plumed/2.9.0
gcc85/libs/blas/3.11.0 gcc85/libs/hdf5/1.14.0 gcc85/libs/libpng/1.6.39 gcc85/mvapich2/2.3.7 gcc85/netcdf-cxx4/4.3.1 gcc85/openfoam/2306 gcc85/spin/6.5.1
gcc85/libs/fftw/3.3.10 gcc85/libs/jemalloc/5.3.0 gcc85/libs/nlopt/2.7.1 gcc85/netcdf-c/4.9.0 gcc85/netcdf-fortran/4.6.0 gcc85/openmpi/4.1.4

/cvmfs/sw.el8/modules/hpc/gcc11

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gcc11/R/4.2.2 gcc11/gromacs/2022.5 gcc11/libs/boost/1.80.0 gcc11/libs/jemalloc/5.3.0 gcc11/libs/openblas/0.3.21 gcc11/netcdf-cxx4/4.3.1 gcc11/openfoam-org/10 (D) gcc11/paraview/5.10.1 gcc11/slim/4.2.2
gcc11/cp2k/2023.1 gcc11/gromacs/2023 (D) gcc11/libs/fftw/3.3.10 gcc11/libs/lapack/3.11.0 gcc11/mvapich2/2.3.7 gcc11/netcdf-fortran/4.6.0 gcc11/openfoam/2012 gcc11/pfft/1.0.8 gcc11/slim/5.0 (D)
gcc11/gromacs/2020.4 gcc11/keras/2.10.0 gcc11/libs/gsl/2.7 gcc11/libs/libpng/1.6.39 gcc11/netcdf-c/4.9.0 gcc11/ngspice/37 gcc11/openfoam/2206 (D) gcc11/plumed/2.8.0
gcc11/gromacs/2021.4 gcc11/libs/blas/3.11.0 gcc11/libs/hdf5/1.14.0 gcc11/libs/nlopt/2.7.1 gcc11/netcdf-cxx/4.2 gcc11/openfoam-org/2.4.0 gcc11/openmpi/4.1.4 gcc11/plumed/2.9.0 (D)

/cvmfs/sw.el8/modules/hpc/gcc13

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gcc13/arpack/3.9.1 gcc13/brams/6.0.0 gcc13/foam-extend/4.1 gcc13/libs/hdf5/1.14.3 gcc13/netcdf-c/4.9.2 gcc13/openfoam/2206 gcc13/openmpi/4.1.6 gcc13/spooles/2.2 gcc13/xbeach/1.24.6057
gcc13/blas/3.12.0 gcc13/calculix/2.20 gcc13/gromacs/2020.4 gcc13/mooring gcc13/netcdf-fortran/4.6.1 gcc13/openfoam/2306 gcc13/petsc/3.22 gcc13/vtk/9.4.1 gcc13/xbeach/1.24.6088M (D)
gcc13/boost/1.86.0 gcc13/eigen3/3.4.0 gcc13/lapack/3.12.0 gcc13/mvapich2/2.3.7 gcc13/openblas/0.3.28 gcc13/openfoam/2406 (D) gcc13/precice/3.1.2 gcc13/xbeach/1.23.5960

--- /cvmfs/sw.el8/modules/hpc/intel

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gmxMMPBSA/1.6.3 intel/libs/blas/3.11.0 intel/libs/hdf5/1.14.0 intel/libs/lapack/3.11.0

intel/mvapich2/2.3.7 intel/netcdf-cxx4/4.3.1 intel/openfoam-org/11 intel/openmpi/4.1.4
intel/castep/24.1 intel/libs/fftw/3.3.10 intel/libs/hdf5/1.14.3 (D) intel/libs/libpng/1.6.39 intel/netcdf-c/4.9.2 intel/netcdf-fortran/4.6.1 intel/openfoam/2306 intel/openmpi/4.1.6 (D)
intel/gamess/2023-R2 intel/libs/gsl/2.7 intel/libs/jemalloc/5.3.0 intel/libs/nlopt/2.7.1 intel/netcdf-cxx/4.2 intel/nwchem/nwchem-7.2.2 intel/openfoam/2506 (D)

---------- /cvmfs/sw.el8/modules/gpu ----------
cuda/10.2 cuda/11.2 cuda/11.8 cuda/12.1 cuda/12.6 (D) nvhpc-byo-compiler/23.1 nvhpc-nompi/23.1 nvhpc/23.1 tensorflow/2.14.0 tensorflow/2.18.0 tensorflow/2.19.0 (D)

---------- /cvmfs/sw.el8/modules/bio ----------
R/4.2.2 bcftools/1.8 bowtie2/2.5.1 (D) fastqc/0.11.9 grenepipe/0.14.0 igv/2.12.3 orca/6.0.1 raxml/8.2.12 star/2.7.6a trinity/2.14.0
R/4.4.3 beagle/5.4 bwa/0.7.17 fastqc/0.12.1 (D) grenepipe/0.15.0 (D) iqtree2/2.1.2 orca/shared/5.0.4 salmon/1.10.3 star/2.7.10b (D) vcftools/0.1.14
admixture/1.3.0 bismark/0.23.0 chimera/1.18 figtree/0.12.1 hisat2/2.2.1 iqtree2/2.2.2 (D) orca/static/5.0.4 samtools/1.8 stringtie/3.0.0 vcftools/0.1.16 (D)
alphafold/2.3.2 bismark/0.24.1 (D) chromopainter/0.0.4 figtree/1.4.3 (D) hmmer/3.3.2 jellyfish/2.3.1 picard/3.1.1 samtools/1.17 (D) suitesparse/7.8.2 vina-gpu/2.1
alphapulldown/2.0.1 blast-plus/2.12.0 cutadapt/4.4 finestructure/4.1.1 hmmer/3.4 (D) kallisto/0.50.1 plink/1.07 sickle/1.33 transdecoder/5.5.0
autodock-gpu-develop/11.3.0 blast-plus/2.14.1 (D) eigensoft/8.0.0 freebayes/1.3.6 htslib/1.8 mrbayes/3.2.7a plink2/2.00a4.3 sratoolkit/3.0.0 transdecoder/5.7.1 (D)
autodock-vina/1.2.3 bowtie2/2.4.2 evigene/23.7.15 gatk/4.5.0.0 htslib/1.17 (D) openbabel/3.0.0 popoolation2/1.201 stAIcalc trimgalore/0.6.10

---------- /cvmfs/sw.el8/modules/LIP ----------
gcc11/geant/4.10.7.3 gcc11/topas/3.9 gcc85/gdcm/2.8.9 gcc85/geant/4.10.7.3 gcc85/root/6.24.06 gcc85/root/6.28.10 gcc85/root/6.30.04 (D) madgraph/2.9.14

- If software required not listed please ask INCD support

Access and Middleware

Besides conventional login using SSH, the cirrus-A computing resources can be accessed via middleware using the Unified Middleware Distribution through the EGI and IBERGRID distributed computing infrastructures.

INCD-D HPC and HTC cluster (Cirrus-D)

Almalinux 8

```
[jpina@cirrus01 ~]$ module avail


------------------------------------------------------------------------------- /cvmfs/sw.el7/modules/hpc
-------------------------------------------------------------------------------
   DATK                        gcc-6.3                     gcc83/gromacs/2021.2            intel/openfoam/1906
python-2.7.11
   aoc22/libs/openblas/0.3.10  gcc-7.3                     gcc83/iqtree2/2.1.3
intel/openfoam/2012         python-3.5.1
   aoc22/openmpi/4.0.3         gcc-7.4                     gcc83/libs/gsl/2.6              intel/openfoam/2112
(D)    python-3.5.4
   aocc/2.2.0                  gcc-7.5                     gcc83/mvapich2/2.3.5            intel/openmpi/4.0.3
python/3.7.2
   aocl/2.2                    gcc-8.3                     gcc83/nlopt/2.6.2               intel/openmpi/4.1.1    (D)
python/3.9.12               (D)
   aster-13.1.0                gcc55/openmpi/4.0.3         gcc83/openmpi/4.0.3
intel/swan/41.31            r-3.2.5
   autodock/4.2.6              gcc63/fftw/3.3.9            gcc83/openmpi/4.1.1    (D)    kallisto-0.43.0
r-3.5.2
   beast/1.10.4                gcc63/libs/blas/3.9.0       gcc83/prover9/2009-11A
libs/32/jemalloc/5.3.0      r-3.6.3
   blat-36.2                   gcc63/libs/gsl/2.6          git/2.9.5                       libs/blas/3.9.0            r-4.0.2
   boost-1.55                  gcc63/libs/lapack/3.9.0     gromacs-4.6.7                   libs/gsl/2.6               sbcl-
1.3.4
   bowtie2-2.3.0               gcc63/libs/libpng/1.6.37    hdf4/4.2.15                     libs/jemalloc/5.3.0
sicer-1.1
   clang/7.0.0                 gcc63/libs/openblas/0.3.10  hdf5-1.8.16                     libs/lapack/3.9.0
star-2.5.2b
   clang/ngspice/30            gcc63/mpich-3.2             hdf5/1.12.0                     libs/libpng/1.6.37
tensorflow/2.4.1
   clang/openmpi/4.0.3         gcc63/mvapich2/2.3.5        homer-4.8
```

libs/openblas/0.3.10 tensorflow/2.7.0 (D)
cmake/3.5.2 gcc63/netcdf-fortran/4.4.4 hwloc/2.1.0 macs-1.4.2 trimmomatic-0.33
cmake/3.11.2 gcc63/netcdf-fortran/4.5.2 (D) intel/2019 matlab/R2018a udocker/1.1.3
cmake/3.17.3 gcc63/netcdf/4.6.1 intel/2020 matlab/R2018b udocker/1.1.4
cmake/3.20.3 (D) gcc63/netcdf/4.7.4 (D) intel/gromacs/2021.5 matlab/R2019b (D) udocker/1.1.7
conn-R2018b gcc63/ngspice/34 intel/hdf4/4.2.15 mpich-3.2 udocker/alphafold/2.1.1
cuda gcc63/openmpi/1.10.7 intel/hdf5/1.12.0 mvapich2/2.3.5 udocker/tensorflow/cpu/2.4.1
cuda-10.2 gcc63/openmpi/2.1.0 intel/libs/libpng/1.6.37 netcdf-fortran/4.5.2 udocker/tensorflow/gpu/2.4.1
cuda-11.2 gcc63/openmpi/4.0.3 intel/libs/openblas/0.3.10 netcdf/4.7.4 view3dscene/3.18.0
elsa/1.0.2 gcc63/openmpi/4.1.1 (D) intel/mvapich2/2.3.5 nlopt/2.6.2 (D) vim/8.2
fastqc-0.11.5 gcc63/r-3.4.2 intel/netcdf-fortran/4.5.2 openmpi/1.10.7 weblogo-2.8.2
fftw/3.3.4 gcc63/schism/5.4.0 intel/netcdf/4.7.4 openmpi/2.1.0 wine/4.2
fftw/3.3.5 (D) gcc63/xbeach/1.23.5527 intel/oneapi/2021.3 openmpi/4.0.3 ww3/6.07.1
freewrl/4.4.0 gcc74/gromacs/2019.4 intel/oneapi/2022.1 (D) openmpi/4.1.1 (D)
gcc-4.8 gcc74/openmpi/4.0.3 intel/openfoam/5.0 parallel/20180622
gcc-5.5 gcc74/plumed/2.5.3 intel/openfoam/8.0 plumed/2.2.1

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