CADES Software list

Software list on cades open	Type* (C/L /A)	Current versions	Versions to keep	Versions to disable	Notes
abaqus	A	2019 (default)	2019	N/A	
aflow	A	1.0 (default)	1.0	N/A	
amber	A	16 (default); 18	16; 18	N/A	Move default version from 16 to 18
AMS	L	2018	2018	N/A	
anaconda2	A	5.1.0 (default)	5.1.0	N/A	
anaconda3	A	5.1.0 (default)	5.1.0	N/A	
ArmForge	A	18.0 (default)	18.0	N/A	
ATLAS	L	3.10.3 (default)	3.10.3	N/A	
autoconf	A	2.69 (default)	2.69	N/A	
automake	A	1.15 (default)	1.15	N/A	
bioconda	A	09-18	09-18	N/A	special build upon user request
blas	L	3.8.0 (default)	3.8.0	N/A	
blast	L	2.10	2.10	N/A	
boost	L	1.61.0; 1.64.0; 1.67.0 (default); 1.67.0-pe3; 1.69.0; 1.70.0	1.67.0; 1.67.0-pe3; 1.69.0; 1.70.0	1.61.0; 1.64.0	move default version to 1.70.0
bzip2	L	1.0.6 (default)	1.0.6	N/A	
caffe	L	1.0	1.0	N/A	
cctools	A	6.2.7 (default)	6.2.7	N/A	
cdo	A	1.8.2 (default)	1.8.2	N/A	
cmake	C	3.8.2; 3.11.0 (default); 3.11.4; 3.12.0	3.11.0; 3.11.4; 3.12.0	3.8.2	move default version to 3.12.0
conda-forge	A	09-18	09-18	N/A	special build upon user request
cp2k	A	5.1 (default); 6.1; 6.1-parallel; 7.0-cuda	6.1; 6.1-parallel; 7.0-cuda	5.1	move default version to 6.1
cuda	A	8.0(default); 9.0; 9.2; 10.1; 11.0	9.2; 10.1; 11.0	8.0; 9.0	move default version to 11.0
cudnn	L	7.1.4	7.1.4	N/A	
curl	A	7.61.1	7.61.1	N/A	
darshan	A	3.1.4	3.1.4	N/A	
dftbplus	A	19.1; 19.1-mpi	19.1; 19.1-mpi	N/A	
dgal	L	3.0.1 (default)	3.0.1	N/A	
dl_poly	A	4.09; 4.09_hpc	4.09; 4.09_hpc	4.09	special build upon user request
DOCK	A	6.9	6.9	N/A	
eden	A	clm	clm	N/A	
eigen3	L	3.3.7	3.3.7	N/A	
exodus	L	5.14 (default)	5.14	N/A	
EMSOFT	A	4.0-apr16-18 (default)	4.0-apr16-18	N/A	
ferret	A	7.2 (default)	7.2	N/A	
fftw	L	3.3.5 (default)	3.3.5	N/A	
gamess	A	092018	092018	N/A	

gcc	C	4.9.3; 4.9.4; 5.3.0; 6.2.0; 6.3.0 (default) 7.2.0; 8.1.0; 8.3.0; 9.2.0	6.3.0; 7.2.0; 8.1.0; 8.3.0; 9.2.0	4.9.3; 4.9.4; 5.3.0; 6.2.0	
git	A	2.11.0 (default)	2.11.0	N/A	
glibc	L	2.25; 2.27		2.25; 2.27	special build upon user request; No need to keep them for Redhat OS
gnuplot	A	5.0.6 (default)	5.0.6	N/A	
go	A	1.13	1.13	N/A	
gromacs	A	2016.3 (default); 2016.3-AVX2; 2018.2; 2018.3; 2019.4-pe3; 2019.5-pe3; 2019-GPU; 5.1.2	2018.2; 2018.3; 2019.4-pe3; 2019.5-pe3; 2019-GPU	5.1.2; 2016.3; 2016.3-AVX2;	
gtk+	A	2.24.31 (default)	2.24.31	N/A	
hdf5	L	1.8.17 (default); 1.8.21; 1.10.1; 1.10.2; 1.10.3; 1.10.3-intel19; 1.10.4; 1.12.0	1.10.3; 1.10.3-intel19; 1.10.4; 1.12.0	1.8.17; 1.8.21; 1.10.1; 1.10.2	move default version to 1.12.0
hdf5_parallel	L	1.8.17 (default); 1.8.21; 1.10.3; 1.10.6	1.8.17; 1.8.21; 1.10.3; 1.10.6	N/A	move default version to 1.10.6
hwloc	L	2.0.1; 2.0.4	2.0.1; 2.0.4	N/A	
hypre	L	2.11.1 (default)	2.11.1	N/A	
idl	A	8.6 (default)	8.6	N/A	
ilamb	A	2.1; latest (default)	latest	2.1	
intel	C	14.0.2; 16.0.1; 17.0.0; 17.0.1; 18.0.0 (default); 19.0.1; 19.0.3; 2021.1	18.0.0; 19.0.1; 19.0.3; 2021.1	14.0.2; 16.0.1; 17.0.0; 17.0.1	move default version to 12021.1
java	A	15.0.1; 1.8.0_131 (default)	1.8.0_131	15.0.1	
keras	L	2.0.2	2.0.2	N/A	
lammps	A	07Aug19; 22Aug18; 31Mar17; 31Mar17-kokkos	07Aug19; 22Aug18	31Mar17; 31Mar17-kokkos	move default version to 07Aug19
lapack	L	3.7.1 (default); 3.8.0	3.7.1 (default); 3.8.0	N/A	
libxml2	L	2/2.9.9	2/2.9.9	N/A	
magma	A	2.4.0; 2.5.1	2.4.0; 2.5.1	N/A	
matlab	A	R2017a (default)	R2017a	N/A	
mcstas	A	2.5	2.5	N/A	
mesa	A	17.1.1	17.1.1	N/A	
metis	A	5.1.0 (default); 17.1.1	17.1.1	5.1.0	move default version to 17.1.1
mkl	L	2016 (default); 2017; 2018.1.163	2017; 2018.1.163	2016	move default version to 2018.1.163
mpich	L	3.2 (default); 3.3.2	3.2; 3.3.2	N/A	
nag	C	6.0, 6.2, 7.0	7.0	6.0, 6.2	
namd	A	2.11, 2.11-cuda, 2.11-cuda9.2, 2.12, 2.13	2.12, 2.13	2.11, 2.11-cuda, 2.11-cuda9.2	have the existing versions build with cuda
ncl	A	6.3.0	6.3.0	N/A	
ncview	A	2.1.7	2.1.7	N/A	
netcdf	L	4.3.3.1, 4.6.1, 4.7.4	4.6.1, 4.7.4	4.3.3.1	
netcdf-hdf5parallel	L	4.3.3.1, 4.7.4	4.7.4	4.3.3.1	
nextflow	A	0.27.6	remove	remove	Not being used
nwchem	A	6.6_MPI_PR, 6.6_p3, 6.8, 7.0.0	7.0.0, 6.8	6.6_MPI_PR, 6.6_p3	
openBlas	L	0.2.19, 0.2.20	0.2.20	0.2.19	
openDIEL	A	V3-AM	remove	remove	not being used
OpenFOAM	A	5.0, 7.0, dev	dev, 7.0	5.0	
openjdk	C	11.0.2	11.0.2	N/A	

openmpi	L	1.6.5, 1.10.1, 1.10.2, 1.10.3, 2.1.1, 2.1.2, 3.0.0, 3.0.0-gcc-6.3.0, 3.1.1, 3.1.1-or-slurm, 3.1.5, 3.1.5-intel19, 4.0.0, 4.0.1, 4.1.0	3.1.1, 4.0.0, 4.1.0	1.6.5, 1.10.1, 1.10.2, 1.10.3, 2.1.1, 2.1.2, 3.0.0, 3.0.0-gcc-6.3.0, 3.1.1-or-slurm, 3.1.5, 3.1.5-intel19, 4.0.1	build with slurm bindings
orca	A	4.2.0	4.2.0	N/A	
p4vasp	A	0.3.30	0.3.30	N/A	
parallel	A	20201122	20201122	N/A	install latest
paraview	A	5.4.0, 5.5.0, 5.5.2, 5.8.0	5.5.2, 5.8.0	N/A	
pegasus	A	4.8.2	remove	remove	defunct
perl	C	5.30.1	remove	remove	use system perl
phonopy	A	1.14.2, 2.1.1	2.1.1	1.14.2	
plumed	A	2, 2.6-pe3	2.6-pe3	2	
pnetcdf	L	1.9.0	1.9.0	N/A	
postgresql	A	9.3.5	9.3.5	N/A	
protobuf	L	3.6.1	3.6.1	N/A	
python2	C	2.7.12, 2.7.13	remove	remove	no support for python2
python3	C	3.6.6, 3.7.0, 3.9.4	3.7.0, 3.9.4	3.6.6	
QE	A	6.0, 6.1, 6.3, 6.3-qmcpack, 6.5, 6.5-modify	6.3, 6.5	6.0, 6.1	merge modify and qmcpack to 6.5
qmcpack	A	3.6.0	3.6.0	N/A	
qt	L	5.6.1, 5.9.6, 5.11.1	5.11.1	5.6.1, 5.9.6	
R	C	3.5.0, 3.5.0-pe3, 3.6.0	3.5.0-pe3, 3.6.0	3.5.0	
rdock	A	2013.1	2013.1	N/A	
rstudio	C	1.1.456	remove	remove	defunct
rust	C	1.28	1.28	N/A	perhaps install system-level
sassena	A	1.4.2	1.4.2	N/A	
scalapack	L	2.0.2	2.0.2	N/A	install latest
schrodinger	A	2018-1	2018-1	N/A	install latest
scorep	A	4.0	4.0	N/A	
silo	A	4.9.1, 4.10.2	4.10.2	4.9.1	
singularity	A	3.2.1, 3.6.3	3.6.3	3.2.1	install latest
SPEC2006	A	1.2	1.2	N/A	
swift	A	1.4	1.4	N/A	
swig	L	3.0.12	3.0.12	N/A	
szip	A	2.1	2.1	N/A	
Tecplot	A	2020	2020	N/A	
tensorflow	A	0.11-cpu, 0.11-cpu-conda, 0.11-gpu, 1.10.0-conda-cpu, 1.10.0-conda-gpu, 1.12.0-conda-gpu, 2.2-conda-gpu	2.2-conda-gpu	0.11-cpu, 0.11-cpu-conda, 0.11-gpu, 1.10.0-conda-cpu, 1.10.0-conda-gpu, 1.12.0-conda-gpu	install 2.2-conda-cpu
texlive	C	2020	2020	N/A	
theano	A	0.9-conda	remove	0.9-conda	defunct
trilinos	A	12.12.1	12.12.1	N/A	
triqs	A	2.1.0	2.1.0	N/A	
valgrind	L	3.14.0	3.14.0	N/A	install latest
vasp	A	5.4.4, 5.4.4-vannier, 5.4.4-pe3	5.4.4-pe3	5.4.4	install 6.2
vinampi	A	v2	v2	N/A	install latest
visit	A	2.10.3, 2.13.1, 2.13.2, 2.13.3, 2.13.3-server	2.13.2, 2.13.3	2.10.3, 2.13.1	keep only the server version
vmd	A	1.9.3	1.9.3	N/A	
votca	A	1.4.1	1.4.1	N/A	

VTK	A	8.2.0	8.2.0	N/A	
wannier90	A	1.2-pe3, 3.0.0-pe3, 3.1.0-pe3	3.0.0-pe3, p.1.0-pe3	1.2-pe3	
wxpython	L	3.0.2.0	3.0.2.0	N/A	
xalt	A	0.7.5, 0.7.6	0.7.6	0.7.5	maybe install latest
zeromq	A	4.2.3	4.2.3	N/A	
zlib	L	1.2.8, 1.2.11, 1.2.11-pe3	1.2.11, 1.2.11-pe3	1.2.8	maybe install latest

*A = Application; C=Compiler ; L=Library