Package Programs List (Molecular Science)

Last update: Jan 10, 2025.

Compilers and Libraries

Most packages are installed under /apl.

name	version	note
GCC	8.5.0*	(system default package)
	9.2.1	module: gcc-toolset/9 (gcc-toolset-9)
	10.3.1	module: gcc-toolset/10 (gcc-toolset-10)
	11.2.1	module: gcc-toolset/11 (gcc-toolset-11)
	12.2.1	module: gcc-toolset/12 (gcc-toolset-12)
	13.1.1	module: gcc-toolset/13 (gcc-toolset-13)
AOCC	5.0.0	module: aocc/5.0.0
	4.2.0	module: aocc/4.2.0
	4.1.0	module: aocc/4.1.0
	4.0.0*	module: aocc/4.0.0
	3.2.0	module: aocc/3.2.0
AOCL	5.0.0	module: aocl/5.0.0-aocc5.0 (built with AOCC), aocl/5.0.0-gcc13.2 (built with GCC)
	4.2.0	module: aocl/4.2.0-aocc4.2 (built with AOCC), aocl/4.2.0-gcc13.1 (built with GCC)
	4.1.0	module: aocl/4.1.0-aocc4.1 (built with AOCC), aocl/4.1.0-gcc13.1 (built with GCC)
	4.0	module: aocl/4.0-aocc4.0 (built with AOCC), aocl/4.0-gcc11.2 (built with GCC)
	3.2.0	module: aocl/3.2.0-aocc3.2 (built with AOCC), aocl/3.2.0-gcc11.2 (built with GCC)
Python [1]	3.9.18	
	3.6.8*	(/usr/bin/python3)
	2.7.18*	(/usr/bin/python2)
	3.10.13 (base) 3.12.2 (gpuenv)	miniforge3 env (/apl/conda/20240305; source conda_init.sh or conda_init.csh to load env)
	3.10.9	miniforge3 env (/apl/conda/20230214; source conda_init.sh or conda_init.csh to load env)
NVIDIA HPC SDK	24.9	module: nvhpc/24.9, nvhpc/24.9-byo, nvhpc/24.9-nompi
	24.3	module: nvhpc/24.3, nvhpc/24.3-byo, nvhpc/24.3-nompi
	23.9	module: nvhpc/23.9, nvhpc/23.9-byo, nvhpc/23.9-nompi
	23.5	module: nvhpc/23.5, nvhpc/23.5-byo, nvhpc/23.5-nompi
	22.11	module: nvhpc/22.11, nvhpc/22.11-byo, nvhpc/22.11-nompi
Intel oneAPI Compiler Runtime [2]	2025.0.4, 2025.0, 2024.2.1, 2024.2, 2024.1.0, 2024.0.2, 2024.0, 2023.2.0, 2023.1.0, 2023.0.0, 2022.2.1, 2022.0.2	module: compiler-rt/(version)
	2025.0.0.1	module: mkl/2025.0.0.1
	2025.0	module: mkl/2025.0

name	version	note
Intel MKL	2024.2	module: mkl/2024.2
	2024.1	module: mkl/2024.1
	2024.0	module: mkl/2024.0
	2023.2.0	module: mkl/2023.2.0
	2023.1.0	module: mkl/2023.1.0
	2023.0.0	module: mkl/2023.0.0
	2022.2.1	module: mkl/2022.2.1
	2022.0.2	module: mkl/2022.0.2
Intel MPI	2021.14.1	module: intelmpi/2021.14.1
	2021.14	module: intelmpi/2021.14
	2021.13	module: intelmpi/2021.13
	2021.12	module: intelmpi/2021.12
	2021.11	module: intelmpi/2021.11
	2021.10.0	module: intelmpi/2021.10.0
	2021.9	module: intelmpi/2021.9
	2021.8	module: intelmpi/2021.8
	2021.7.1	module: intelmpi/2021.7.1
	2021.5.1	module: intelmpi/2021.5.1
CUDA	12.6 Update 2	module: cuda/12.6u2
	12.4 Update 1	module: cuda/12.4u1
	12.2 Update 2	module: cuda/12.2u2
	12.1 Update 1	module: cuda/12.1u1
	12.0*	module: cuda/12.0
	11.6	module: cuda/11.6
	11.2	module: cuda/11.2
Open MPI	5.0.5	module: openmpi/5.0.5 (modules for each compiler available)
	5.0.1	module: openmpi/5.0.1 (modules for each compiler available)
	4.1.6	module: openmpi/4.1.6 (modules for each compiler available)
	4.1.5	module: openmpi/4.1.5 (modules for each compiler available)
	3.1.6	module: openmpi/3.1.6 (modules for each compiler available)
HPC-X	2.16 (Open MPI 4.1.5)	module: openmpi/4.1.5-hpcx2.16 (modules for each compiler available)
	2.13.1 (Open MPI 4.1.5)	module: openmpi/4.1.5-hpcx (modules for each compiler available)
	2.11 (Open MPI 4.1.4)	module: openmpi/4.1.4-hpcx (modules for each compiler available)
MVAPICH	3.0	module: mvapich/3.0 (modules for GCC and AOCC available)
	2.3.7	module: mvapich/2.3.7 (modules for each compiler available)
Julia	1.10.0	module: julia/1.10.0
	1.8.5	module: julia/1.8.5
	1.6.7 (LTS)	module: julia/1.6.7
Apptainer/Singularity	1.3.1	(singularity is an alias of apptainer)

*: default version

[1]: you can install packages to your home directory by using "pip3 install (package name) --user" command. Installing miniforge might be another good choice. However, the initialization of conda environment might take long time (only upon first time; this is due to the fundamental mechanism of lustre filesystem). If you need only a few packages, you should install them to your home directory via "pip3".
[2]: Compilers (such as ifort, ifx) are not installed in /apl. In case you need Intel compilers, please install Intel oneAPI Base Toolkit or HPC Toolkit into your directory.

Application Software

The list of installed software is shown below. (Blacked out package names indicate that they have not yet been installed but will be installed.) For the manual/documentations, please visit the official website. Packages are installed under /apl directory which are accessible from both of frontend and computation nodes. See this page for detailed information about installation.

name	description
ABINIT-MP	A software for fast Fragment-Molecular-Orbital (FMO) calculations.
AlphaFold	AI program for predictions of protein structure.
AMBER	Package of molecular simulation programs.
CENSO	Program for evaluating structure ensembles at DFT level.
CP2K	A quantum chemistry and solid state physics software package.
CREST	A program for the automated exploration of the low-energy molecular chemical space.
CRYSTAL	General-purpose programs for the study of crystalline solids.
DFTB+	Fast and efficient versatile quantum mechanical simulation software package
DIRAC(*22)	Computes molecular properties using relativistic quantum chemical methods (named after P. A. M. Dirac).
GAMESS	General atomic and molecular electronic structure system.
Gaussian	Ab initio molecular orbital calculations.
GENESIS	Molecular dynamics and modeling software for bimolecular systems such as proteins, lipids, glycans, and their complexes.
GROMACS	Fast, Free and Flexible MD
GRRM	Automated Exploration of Reaction Pathways.
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator.
OpenMolcas	Quantum chemistry software.
Molpro	Complete system of ab initio programs.
NAMD	Scalable molecular dynamics program.
NBO	Discovery tool for chemical insights from complex wavefunctions.
NTChem(*17)	Comprehensive new software of ab initio quantum chemistry made in Riken-RCCS from scratch.
NWChem	Computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems
ORCA	An ab initio quantum chemistry program package
PSI4	Open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties.
Quantum ESPRESSO	Integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale.
Reaction Plus	Program to obtain the transition state and reaction path along the user’s expected reaction mechanism.
SIESTA	Efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids
TURBOMOLE	One of the fastest programs for standard quantum chemical applications.
GaussView	Viewer for Gaussian 09 / 16.
Molden	Visualization program of molecular and structure.
VMD	Molecular graphics viewer

name	version	install date	note
ABCluster	3.0	○ (2023-Nov-28)	
ABINIT-MP	v2r8	○ (2025-Jan-7)	
	v2r4	○ (2023-Feb-21)	
	v1r22	○ (2023-Feb-21)	
ADF(*9)		(not available)	
AlphaFold	3.0.0	△ (2024-Nov-26)	GPU is required for inference. AlphaFold3 model parameters must be requested and downloaded by the user themselves.
	2.3.2	△ (2024-Feb-8)☆	
	2.3.1	△ (2023-Feb-6)☆	
	2.2.0	△ (2022-Mar-14)☆	
	2.1.1	△ (2021-Nov-8)☆	
	2.1.0	△ (X-X-X)☆	
	2.0.0 (2021/8/19)	△ (2021-Aug-23)☆	
	2.0.0 (2021/7/20)	△ (2021-Jul-26)☆	
Amber	24-update1	○ (2024-Jun-11)☆	(AmberTools24-update2)
	22-update4	○ (2023-Aug-25)☆	(Ambertools23-update4)
	22-update1	○ (2023-Jan-X)☆	(AmberTools22-update4)
	20-update13	○ (2023-Jan-X)☆	(built with configure)
AutoDock	4.2.6	○ (2023-Nov-24)	
AutoDock-GPU	1.5.3	○ (2023-Nov-24)☆	
AutoDock Vina	1.2.5	○ (2023-Nov-24)	
CENSO	1.2.0	○ (2024-May-22)	(precomipled binary) anmr and nmrplot.py from ENSO 2.0.2 are added manually.
ColabFold	1.5.5	○ (2023-Apr-6)	
CP2K	2024.3	○ (2024-Oct-24)	
	2024.2	○ (2024-Aug-22)	
	2023.1	○ (2023-Apr-6)	
	9.1	○ (2023-Jan-X)	
CREST	3.0.1	○ (2024-May-21)	
CRYSTAL	23-1.0.1	○ (2024-Jul-19)	(*21)
	17-1.0.2	○ (2023-Jan-X)	
Dalton	2020.1	○ (2024-Nov-8)	
DFTB+	23.1	○ (2023-Jul-19)☆ MPI / OpenMP	MPI and OpenMP versions available
DIRAC	23.0	○ (2023-May-8)	
	19.0	○ (2023-Jan-27)	
	2024-R2(Jul15)	○ (2024-Oct-31)	(NBO 7.0.10 enabled)
	2023-R2(Sep30)	○ (2023-Dec-7)	(NBO 7.0.10 enabled)

GAMESS name	version	install date	note
	2022-R2(Sep30)	○ (2023-Jan-X)	(NBO 7.0.7 enabled)
	2021-R1(Jun30)	○ (2023-Jan-X)	(NBO 7.0.7 enabled)
Gaussian	16.C.02	○ (2022-Mar-14)	(NBO 7.0.10 enabled)
	16.C.01	○ (2019-Aug-2)	(NBO 7.0.10 enabled)
	16.B.01	○ (2018-Mar-12)	
	09.E.01	○ (2015-Dec-24)	
GENESIS	2.1.4	○ (2025-Jan-10)☆ CPU / GPU	
	2.1.2	○ (2024-Jan-16)☆ CPU / GPU	
	2.0.3	○ (2023-Jan-X)☆ CPU / GPU	
GROMACS	2024.4	○ (2024-Nov-5)☆ CPU / GPU	
	2024.2	○ (2024-May-16)☆ CPU / GPU	
	2023.5	○ (2024-May-7)☆ CPU / GPU	
	2023.4	○ (2024-Jan-26)☆ CPU / GPU	
	2023.2	○ (2023-Aug-9)☆ CPU / GPU	
	2022.6	○ (2023-Jul-12)☆ CPU / GPU	
	2022.4	○ (2023-Jan-X)☆ CPU / GPU	
	2021.7	○ (2023-Apr-14)☆ CPU / GPU	
	2021.6	○ (2023-Jan-X)☆ CPU / GPU	
	2021.4	○ (2023-Jan-X)☆ CPU / GPU	
GRRM	23	○ (2024-Jan-11)	Application is required for use. (multinode parallel available)
	17(*5)	○ (2021-Jan-27)	(multinode parallel available)
	14	○ (2015-Jul-29)	
LAMMPS	29Aug2024	○ (2024-Sep-6)☆ CPU(GCC,Intel) / GPU	
	2Aug23	○ (2023-Oct-16)☆ CPU(GCC,Intel) / GPU	Intel MPI
	23Jun22 Update 2	○ (2023-Jan-X)☆ CPU / GPU	(netcdf off)
		○ (2023-Apr-18)☆ CPU / GPU	Intel MPI

name	version	install date	note
	29Sep21 Update 3	○ (2023-Apr-18)☆ CPU / GPU	Intel MPI
	29Sep21	○ (2023-Jan-X)☆ CPU / GPU	(netcdf off)
LigandMPNN		△ (2024-Mar-27)☆	latest code on Mar 27, 2024
Molpro(*2)	2024.3.0	△ (2024-Nov-15)	
	2024.2.0	△ (2024-Sep-9)	
	2024.1.0	△ (2024-Mar-11)	
	2023.2.0	△ (2023-Oct-11)	
	2023.1.0	△ (2023-Sep-19)	
	2022.3.0	△ (2023-Jan-X)	(HPC-X)
		△ (2023-May-18)	(MVAPICH)
	2022.2.2	△ (2023-Jan-X)	
	2021.3.1	△ (2023-May-10)	
	2015.1-44	△ (2023-Jan-X)	
NAMD	3.0.1	○ (2024-Oct-31)☆ MPI / SMP / SMP+CUDA	
	3.0	○ (2024-Jul-5)☆ MPI / SMP / SMP+CUDA	
	3.0b7	○ (2024-May-23)☆ MPI / SMP / SMP+CUDA	
	3.0b6	○ (2024-Mar-6)☆ MPI / SMP / SMP+CUDA	
	3.0b2	○ (2023-Apr-10)☆	(GPU version only)
	2.14	○ (2023-Jan-X)☆ CPU / GPU	
NBO	7.0.10	△ (2023-Feb-14)	
	7.0.7	△ (2023-Jan-X)	
NTChem	2013.13.0.0	○ (2023-Apr-28)	
NWChem	7.2.2	○ (2024-Mar-5)☆ CPU / GPU	
	7.0.2	○ (2023-Mar-6)	
	6.8	○ (2023-Mar-6)	for ReactionPlus
OmegaFold	1.1.0	○ (2024-Jun-12)☆	
OpenMM	8.1.0	○ (2023-Dec-5)	
OpenMolcas	24.10	○ (2024-Nov-18)	
	23.06	○ (2023-Jul-25)	
	22.10	○ (2023-Mar-6)	
	21.10	○ (2023-Mar-6)	
ORCA	6.0.1	○ (2024-Nov-6)	(registration required)
	5.0.4	○ (2023-Mar-20)	
	5.0.3	○ (2022-Feb-22)	

name	version	install date	note
	4.2.1	○ (2020-Jan-8)	
Parallel CONFLEX(*9)			
ProteinMPNN		△ (2023-Oct-26)☆	latest code on Oct 25, 2023
PSI4	1.9.1	○ (2024-Mar-5)	
	1.7	○ (2023-Jan-30)	
Quantum ESPRESSO	7.3	○ (2024-Feb-6)☆ CPU / GPU	
	7.2	○ (2023-Apr-11)☆ CPU / GPU	
	6.8	○ (2023-Jan-26)☆ CPU / GPU	
ReactionPlus	1.0	○ (2018-Jan-22)	
RFdiffusion		△ (2023-Oct-26)☆	latest code on Oct 25, 2023
RFDiffusion AA		△ (2024-Mar-27)☆	latest code on Mar 27, 2024
SIESTA	5.0.1	○ (2024-Jul-29) OpenMPI / IntelMPI	Open MPI and Intel MPI versions avail
	5.0.0	○ (2024-May-29) OpenMPI / IntelMPI	Open MPI and Intel MPI versions avail
	4.1.5	○ (2023-Jan-X) MPI / OpenMP	MPI and OpenMP versions available
TURBOMOLE(*3)	7.9	○ (2024-Dec-12)☆	
	7.8.1	○ (2024-Nov-12)☆	
	7.8	○ (2023-Dec-18)☆	
	7.7	○ (2023-Jul-18)☆	
	7.6	○ (2021-Dec-23)	
VASP(*4)		(not available)	
xTB	6.7.0	○ (2024/5/7)	
	6.5.1	○ (2024/5/22)	

Following GUI applications are available (X11 forwarding necessary). On Windows, you can use X11 forwarding easily with MobaXterm (WSLg, Xming, VcXsrv may also work). On mac, install and start XQuartz, and then connect via ssh with "-XY" option.

name	version	command name / path	install date
GaussView	6.1.1	gview6	△ (2019-Oct-29)
	6.0.16	/apl/gaussian/16b01/gv/gview.sh	△ (2017-Feb-2)
	5.0.9	gview5	△ (2013-Mar-13)
iMolpro	1.0.1	/apl/imolpro/1.0.1/bin/imolpro-*	○ (2024-Mar-8)
Luscus	0.8.6	/apl/luscus/0.8.6/bin/luscus	○ (2023-Oct-4)
Molden	7.2.1	/apl/molden/7.2.1/bin/molden	○ (2023-Feb-6)
VMD	1.9.4 alpha (2022/4/27)	/apl/vmd/1.9.4a57/bin/vmd	○ (2023-Jan-X)

name	version	command name / path	install date
XCrySDen	1.6.2	exec "module load xcrysden/1.6.2" and then xcrysden	○ (2024-Aug-23)

○: module available
△: module not available/not necessary
☆: GPU version available

Note

(*2) molpro license will be expired on Sep 15, 2025. The license will be renewed every year.
(*3) Only non-commercial users in Japan can use this. The license will be expired in Feb, 2026. The license will be renewed every year.
(*4) We cannot install. (Licensed users can install into their directories.)
(*5) English guide for GRRM17 is available athttps://afir.sci.hokudai.ac.jp/documents/manual/54. Japanese guide for this center (for GRRM14) is also available.
(*9) We cannot install ADF and Parallel CONFLEX due to their very high license fee.

(*17) You have to cite some papers when you publish papers with NTChem results. Please readofficial page and documentation(japanese) of NTChem.
(*21) To use CRYSTAL, license agreement is required for each user and version. CRYSTAL17 users also need to sign a new license agreement to use CRYSTAL23. Once the agreement is arrived at RCCS, you will be able to use CRYSTAL23 or/and CRYSTAL17. (CRYSTAL23 license agreement) (CRYSTAL17 license agreement)
(*22) References listed in this page must be cited when you publish results obtained with DIRAC.

Attachment	Size
CRYSTAL17 license agreement	255.58 KB
CRYSTAL23 license agreement	314 KB