Package Programs List (Molecular Science)

Last update: Aug 6, 2025.

Compilers and Libraries

Most packages are installed under /apl.
Please check this page for Basic Biology software packages.

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)
	13.3.1	module: gcc-toolset/13 (gcc-toolset-13)
	14.2.1	module: gcc-toolset/14 (gcc-toolset-14)
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]	3.6.8*	(/usr/bin/python3)
	2.7.18*	(/usr/bin/python2)
	3.11.11	(/usr/bin/python3.11)
	3.9.20	(/usr/bin/python3.9)
	3.12.9	miniforge3 env (/apl/conda/20250310; source conda_init.sh or conda_init.csh to load env)
	3.10.13 (base) 3.12.2 (gpuenv)	miniforge3 env (/apl/conda/20240305; source conda_init.sh or conda_init.csh to load env)

name	version	note
	3.10.9	miniforge3 env (/apl/conda/20230214; source conda_init.sh or conda_init.csh to load env)
NVIDIA HPC SDK	25.3	module: nvhpc/25.3, nvhpc/25.3-byo, nvhpc/25.3-nompi
	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]	2025.2.0, 2025.1.1, 2025.1.0, 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)
Intel MKL	2025.2.0, 2025.1.0, 2025.0.0.1, 2025.0, 2024.2, 2024.1, 2024.0, 2023.2.0, 2023.1.0, 2023.0.0, 2022.2.1, 2022.0.2	module: mkl/(version) 2025.0.0.1 => (major 2025, minor 0, update 0, patch 1; 2025.0.1 is the correct name?)
Intel MPI	2021.16, 2021.15, 2021.14.1, 2021.14, 2021.13, 2021.12, 2021.11, 2021.10.0, 2021.9, 2021.8, 2021.7.1, 2021.5.1	module: intelmpi/(version)
CUDA	12.8 Update 1*	module: cuda/12.8u1
	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	5.0.6, 5.0.5, 5.0.1 4.1.8, 4.1.6, 4.1.5 3.1.6	module: openmpi/(version) (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	4.0, 3.0, 2.3.7	module: mvapich/(version) (modules for GCC and AOCC available)
Julia	1.11.3, 1.10.0, 1.8.5 1.10.8 (LTS), 1.6.7 (LTS)	module: julia/(version)
Apptainer/Singularity	1.3.6	(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		
	version	**install date**	**note**
ABCluster	Software for cluster structure optimization and conformation search		
	3.0	○ (2023-Nov-28)	
ABINIT-MP	A software for fast Fragment-Molecular-Orbital (FMO) calculations.		
	v2r8	○ (2025-Jan-7)	
	v2r4	○ (2023-Feb-21)	
	v1r22	○ (2023-Feb-21)	
ADF(*9)		(not available)	
AlphaFold (version3) (version2)	AI program for predictions of protein structure.		
	3.0.0 (Jan 16, 2025)	△ (2025-Jan-16)	GPU is required for inference. AlphaFold3 model parameters must be requested and downloaded by users themselves.
	3.0.0 (Nov 26, 2024)	△ (2024-Nov-26)	
	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	Package of molecular simulation programs.		
	24-update3 + AmberTools25	○ (2025-May-19)☆	
	24-update3	○ (2025-Mar-6)☆	There is a note on "module" command. Please check notes of installation details. (AmberTools24-update8)
	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	Automated docking tools		
	4.2.6	○ (2023-Nov-24)	
AutoDock-GPU	GPU-enabled version of AutoDock		
	1.5.3	○ (2023-Nov-24)☆	
	Improved version of AutoDock		
	1.2.7	○ (2025-Jul-7)	

AutoDock Vina **name**	**description**		
	version	**install date**	**note**
	1.2.5	○ (2023-Nov-24)	
CENSO	Program for evaluating structure ensembles at DFT level.		
	2.1.3	○ (2025-May-1)	anmr from ENSO 2.0.2 was added manually.
	1.2.0	○ (2024-May-22)	(precomipled binary) anmr and nmrplot.py from ENSO 2.0.2 were added manually.
ColabFold	Software to predict protein 3D structure from sequence information		
	1.5.5	○ (2023-Apr-6)	
CP2K	A quantum chemistry and solid state physics software package.		
	2024.3	○ (2024-Oct-24)	
	2024.2	○ (2024-Aug-22)	
	2023.1	○ (2023-Apr-6)	
	9.1	○ (2023-Jan-X)	
CREST	A program for the automated exploration of the low-energy molecular chemical space.		
	3.0.1	○ (2024-May-21)	
CRYSTAL	General-purpose programs for the study of crystalline solids.		
	23-1.0.1	○ (2024-Jul-19)	(*21)
	17-1.0.2	○ (2023-Jan-X)	
Dalton	Quantum chemistry software capable of calculating various molecular properties		
	2020.1	○ (2024-Nov-8)	
DFTB+	Fast and efficient versatile quantum mechanical simulation software package		
	23.1	○ (2023-Jul-19)☆ MPI / OpenMP	MPI and OpenMP versions available
DIRAC(*22)	Computes molecular properties using relativistic quantum chemical methods (named after P. A. M. Dirac).		
	23.0	○ (2023-May-8)	
	19.0	○ (2023-Jan-27)	
GAMESS	General atomic and molecular electronic structure system.		
	2024-R2(Jul15)	○ (2024-Oct-31)	(NBO 7.0.10 enabled)
	2023-R2(Sep30)	○ (2023-Dec-7)	(NBO 7.0.10 enabled)
	2022-R2(Sep30)	○ (2023-Jan-X)	(NBO 7.0.7 enabled)
	2021-R1(Jun30)	○ (2023-Jan-X)	(NBO 7.0.7 enabled)
Gaussian	Ab initio molecular orbital calculations.		
	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	Molecular dynamics and modeling software for bimolecular systems such as proteins, lipids, glycans, and their complexes.		
	2.1.4	○ (2025-Jan-10)☆ CPU / GPU	
	2.1.2	○ (2024-Jan-16)☆ CPU / GPU	
	2.0.3	○ (2023-Jan-X)☆ CPU / GPU	
	Fast, Free and Flexible MD		

name	description		
	version	**install date**	**note**
GROMACS	2025.2	○ (2025-May-27)☆ CPU / GPU	NNP enabled (libtorch 2.7.0)
	2024.5	○ (2025-Jan-27)☆ CPU / GPU	
	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	Automated Exploration of Reaction Pathways.		
	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	Large-scale Atomic/Molecular Massively Parallel Simulator.		
	22Jul2025	○ (2025-Aug-6)☆ CPU(GCC,Intel) / GPU	
	29Aug2024 Update 4	○ (2025-Jul-29)☆ CPU(GCC,Intel) / GPU	
	29Aug2024 Update 3	○ (2025-Jul-15)☆ CPU(GCC,Intel) / GPU	
	29Aug2024 Update 2	○ (2025-Apr-18)☆ CPU(GCC,Intel) / GPU	
	29Aug2024 Update 1	○ (2025-Feb-21)☆ CPU(GCC,Intel) / GPU	

name	description		
	version	**install date**	**note**
	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
	29Sep21 Update 3	○ (2023-Apr-18)☆ CPU / GPU	Intel MPI
	29Sep21	○ (2023-Jan-X)☆ CPU / GPU	(netcdf off)
LigandMPNN	Software for designing sequences that bind to small ligands		
		△ (2024-Mar-27)☆	latest code on Mar 27, 2024
Molpro	Complete system of ab initio programs.		
	2025.1.0	△ (2025-Mar-14)	
	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	Scalable molecular dynamics program.		
	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	Discovery tool for chemical insights from complex wavefunctions.		
	7.0.10	△ (2023-Feb-14)	
	7.0.7	△ (2023-Jan-X)	

name	description		
	version	**install date**	**note**
NTChem(*17)	Comprehensive new software of ab initio quantum chemistry made in Riken-RCCS from scratch.		
	2013.13.0.0	○ (2023-Apr-28)	
NWChem	Computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems		
	7.2.3	○ (2025-Feb-27) CPU / GPU	
	7.2.2	○ (2024-Mar-5)☆ CPU / GPU	
	7.0.2	○ (2023-Mar-6)	
	6.8	○ (2023-Mar-6)	for ReactionPlus
OmegaFold	A Protein Structure Prediction Software		
	1.1.0	○ (2024-Jun-12)☆	
OpenBabel	Chemical toolbox designed to speak the many languages of chemical data		
	3.1.1	○ (2025-Mar-10)	
OpenMM	A high-performance toolkit for molecular simulation.		
	8.2.0	○ (2025-Mar-6)	
	8.1.0	○ (2023-Dec-5)	
OpenMolcas	Quantum chemistry software. (Open source version of Molcas)		
	24.10	○ (2024-Nov-18)	
	23.06	○ (2023-Jul-25)	
	22.10	○ (2023-Mar-6)	
	21.10	○ (2023-Mar-6)	
ORCA	An ab initio quantum chemistry program package		
	6.1.0	○ (2025-Jun-18)	(registration required)
	6.0.1	○ (2024-Nov-6)	
	5.0.4	○ (2023-Mar-20)	
	5.0.3	○ (2022-Feb-22)	
	4.2.1	○ (2020-Jan-8)	
Parallel CONFLEX(*9)			
ProteinMPNN	Software for amino acid sequence prediction from a given main chain structure		
		△ (2023-Oct-26)☆	latest code on Oct 25, 2023
PSI4	Open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties.		
	1.9.1	○ (2024-Mar-5)	
	1.7	○ (2023-Jan-30)	
Quantum ESPRESSO	Integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale.		
	7.4.1	○ (2024-Feb-12)☆ CPU / GPU	
	7.4	○ (2024-Feb-6)☆ CPU / GPU	
	7.3	○ (2024-Feb-6)☆ CPU / GPU	
	7.2	○ (2023-Apr-11)☆ CPU / GPU	

name	description		
	version	**install date**	**note**
	6.8	○ (2023-Jan-26)☆ CPU / GPU	
ReactionPlus	Program to obtain the transition state and reaction path along the user's expected reaction mechanism.		
	1.0	○ (2018-Jan-22)	
RFdiffusion	AI-based Main Chain Structure Generation Software		
		△ (2023-Oct-26)☆	latest code on Oct 25, 2023
RFDiffusion AA	Software for modeling and design of various biomolecules		
		△ (2024-Mar-27)☆	latest code on Mar 27, 2024
SIESTA	Efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids		
	5.2.2	○ (2025-Feb-19)	
	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	One of the fastest programs for standard quantum chemical applications.		
	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	Program for Extended Tight Binding calculation		
	6.7.1	○ (2025/3/5)	
	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.

Alternatively, you can use these GUI applications on desktop of Open OnDemand (regardless of your computer's OS) using a web browser. (Please check this page to start using Open OnDemand.)

name	description		
	version	**command name / path**	**install date**
GaussView	Viewer for Gaussian 09 / 16.		
	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	GUI program for Molpro		
	1.0.1	/apl/imolpro/1.0.1/bin/imolpro-*	○ (2024-Mar-8)
	GUI program for Molcas/OpenMolcas		

name	description		
	version	**command name / path**	**install date**
luscus	0.8.6	/apl/luscus/0.8.6/bin/luscus	○ (2023-Oct-4)
Molden	Visualization program of molecular and structure.		
	7.2.1	/apl/molden/7.2.1/bin/molden	○ (2023-Feb-6)
VMD	Molecular graphics viewer		
	1.9.4 alpha (2022/4/27)	/apl/vmd/1.9.4a57/bin/vmd	○ (2023-Jan-X)
XCrySDen	A crystalline and molecular structure visualisation program		
	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

(*4) We cannot install. (Licensed users can install into their directories.)
(*5) English guide for GRRM17 is available at https://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 fees.
(*17) You have to cite some papers when you publish papers with NTChem results. Please read official 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