Package Programs List (Molecular Science)

Last update: Oct 30, 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	25.9, 25.7, 25.3 24.9, 24.3 23.9, 23.5 22.11	module: nvhpc/(version), nvhpc/(version)-byo, nvhpc/(version)-nompi
Intel oneAPI Compiler Runtime [2]	2025.3.0, 2025.2.1, 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	2025.4, 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	2021.17, 2021.16.1, 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	13.0 Update 2	module: cuda/13.0u2
	12.9 Update 1	module: cuda/12.9u1
	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	5.0.8, 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	4.1, 4.0, 3.0, 2.3.7	module: mvapich/(version) (modules for GCC, AOCC, and Intel 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.

Please cick links in "install date" column to see installation details.

name	description		
	version	**install date**	**job sample path & note**
ABCluster	Software for cluster structure optimization and conformation search		
	3.0	○ (2023-Nov-28)	/apl/abcluster/3.0/samples
ABINIT-MP	A software for fast Fragment-Molecular-Orbital (FMO) calculations.		
	v2r8	○ (2025-Jan-7)	/apl/ABINIT-MP/v2r8/samples
	v2r4	○ (2023-Feb-21)	/apl/ABINIT-MP/v2r4/samples
	v1r22	○ (2023-Feb-21)	/apl/ABINIT-MP/v1r22/samples
ADF(*9)		(not available)	
AlphaFold (version3) (version2)	AI program for predictions of protein structure.		
	3.0.0 (Jan 16, 2025)	△ (2025-Jan-16)	/apl/alphafold/samples/3.0.0-20250116 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)	/apl/alphafold/samples/3.0.0-20241126 (same notice as above)
	2.3.2	△ (2024-Feb-8)☆	/apl/alphafold/samples/2.3.2
	2.3.1	△ (2023-Feb-6)☆	/apl/alphafold/samples/2.3.1
	2.2.0	△ (2022-Mar-14)☆	/apl/alphafold/samples/2.2.0
	2.1.1	△ (2021-Nov-8)☆	/apl/alphafold/samples/2.1.1
	2.1.0	△ (X-X-X)☆	-
	2.0.0 (2021/8/19)	△ (2021-Aug-23)☆	-
	2.0.0 (2021/7/20)	△ (2021-Jul-26)☆	/apl/alphafold/samples/2.0.0-20210720
Amber	Package of molecular simulation programs.		
	24-update3 + AmberTools25	○ (2025-May-19)☆	/apl/amber/24u3+at25/samples
	24-update3	○ (2025-Mar-6)☆	/apl/amber/24u3/samples There is a note on "module" command. Please check notes of installation details. (AmberTools24-update8)
	24-update1	○ (2024-Jun-11)☆	/apl/amber/24u1/samples (AmberTools24-update2)
	22-update4	○ (2023-Aug-25)☆	/apl/amber/22u4/samples (Ambertools23-update4)
	22-update1	○ (2023-Jan-X)☆	/apl/amber/22u1/samples (AmberTools22-update4)

name	description		
	version	install date	job sample path & note
	20-update13	○ (2023-Jan-X)☆	/apl/amber/20u13/samples (built with configure)
AutoDock	Automated docking tools		
	4.2.6	○ (2023-Nov-24)	/apl/autodock/4.2.6/samples
AutoDock-GPU	GPU-enabled version of AutoDock		
	1.5.3	○ (2023-Nov-24)☆	/apl/autodock-gpu/1.5.3/samples
AutoDock Vina	Improved version of AutoDock		
	1.2.7	○ (2025-Jul-7)	/apl/autodock-vina/1.2.7/samples
	1.2.5	○ (2023-Nov-24)	/apl/autodock-vina/1.2.5/samples
CENSO	Program for evaluating structure ensembles at DFT level.		
	2.1.4	○ (2025-Sep-10)	/apl/censo/2.1.4/samples anmr from ENSO 2.0.2 was added manually.
	2.1.3	○ (2025-May-1)	/apl/censo/2.1.3/samples anmr from ENSO 2.0.2 was added manually.
	1.2.0	○ (2024-May-22)	/apl/censo/1.2.0/samples (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)	/apl/colabfold/1.5.5/samples
CP2K	A quantum chemistry and solid state physics software package.		
	2024.3	○ (2024-Oct-24)	/apl/cp2k/2024.3/samples
	2024.2	○ (2024-Aug-22)	/apl/cp2k/2024.2/samples
	2023.1	○ (2023-Apr-6)	/apl/cp2k/2023.1/samples
	9.1	○ (2023-Jan-X)	/apl/cp2k/9.1/samples
CREST	A program for the automated exploration of the low-energy molecular chemical space.		
	3.0.1	○ (2024-May-21)	/apl/crest/3.0.1/samples
CRYSTAL	General-purpose programs for the study of crystalline solids.		
	23-1.0.1	○ (2024-Jul-19)	/apl/crystal/23-1.0.1/samples (*21)
	17-1.0.2	○ (2023-Jan-X)	/apl/crystal/17-1.0.2/samples (*21)
Dalton	Quantum chemistry software capable of calculating various molecular properties		
	2020.1	○ (2024-Nov-8)	/apl/dalton/2020.1/samples
DFTB+	Fast and efficient versatile quantum mechanical simulation software package		
	23.1	○ (2023-Jul-19)☆ MPI / OpenMP	/apl/dftb+/23.1/mpi/samples /apl/dftb+/23.1/nompi/samples 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)	/apl/dirac/23.0/samples
	19.0	○ (2023-Jan-27)	/apl/dirac/19.0/samples
	General atomic and molecular electronic structure system.		

name	description		
	version	install date	job sample path & note
GAMESS	2024-R2(Jul15)	○ (2024-Oct-31)	/apl/gamess/2024R2/samples (NBO 7.0.10 enabled)
	2023-R2(Sep30)	○ (2023-Dec-7)	/apl/gamess/2023R2/samples (NBO 7.0.10 enabled)
	2022-R2(Sep30)	○ (2023-Jan-X)	/apl/gamess/2022R2/samples (NBO 7.0.7 enabled)
	2021-R1(Jun30)	○ (2023-Jan-X)	/apl/gamess/2021R1/samples (NBO 7.0.7 enabled)
Gaussian	Ab initio molecular orbital calculations.		
	16.C.02	○ (2022-Mar-14)	(g16sub is available) /apl/gaussian/16c02/samples (NBO 7.0.10 enabled)
	16.C.01	○ (2019-Aug-2)	(g16sub is available) /apl/gaussian/16c01/samples (NBO 7.0.10 enabled)
	16.B.01	○ (2018-Mar-12)	(g16sub is available) /apl/gaussian/16b01/samples
	09.E.01	○ (2015-Dec-24)	(g09sub is available) /apl/gaussian/09e01/samples
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	/apl/genesis/2.1.4/samples /apl/genesis/2.1.4-CUDA/samples
	2.1.2	○ (2024-Jan-16)☆ CPU / GPU	/apl/genesis/2.1.2/samples /apl/genesis/2.1.2-CUDA/samples
	2.0.3	○ (2023-Jan-X)☆ CPU / GPU	/apl/genesis/2.0.3/samples /apl/genesis/2.0.3-CUDA/samples
GROMACS	Fast, Free and Flexible MD		
	2025.2	○ (2025-May-27)☆ CPU / GPU	/apl/gromacs/2025.2/samples /apl/gromacs/2025.2-CUDA/samples NNP enabled (libtorch 2.7.0)
	2024.6	○ (2025-Aug-25)☆ CPU / GPU	/apl/gromacs/2024.6/samples /apl/gromacs/2024.6-CUDA/samples
	2024.5	○ (2025-Jan-27)☆ CPU / GPU	/apl/gromacs/2024.5/samples /apl/gromacs/2024.5-CUDA/samples
	2024.4	○ (2024-Nov-5)☆ CPU / GPU	/apl/gromacs/2024.4/samples /apl/gromacs/2024.4-CUDA/samples
	2024.2	○ (2024-May-16)☆ CPU / GPU	/apl/gromacs/2024.2/samples /apl/gromacs/2024.2-CUDA/samples
	2023.5	○ (2024-May-7)☆ CPU / GPU	/apl/gromacs/2023.5/samples /apl/gromacs/2023.5-CUDA/samples
	2023.4	○ (2024-Jan-26)☆ CPU / GPU	/apl/gromacs/2023.4/samples /apl/gromacs/2023.4-CUDA/samples
	2023.2	○ (2023-Aug-9)☆ CPU / GPU	/apl/gromacs/2023.2/samples /apl/gromacs/2023.2-CUDA/samples

name	description		
	version	install date	job sample path & note
	2022.6	○ (2023-Jul-12)☆ CPU / GPU	/apl/gromacs/2022.6/samples /apl/gromacs/2022.6-CUDA/samples
	2022.4	○ (2023-Jan-X)☆ CPU / GPU	/apl/gromacs/2022.4/samples /apl/gromacs/2022.4-CUDA/samples
	2021.7	○ (2023-Apr-14)☆ CPU / GPU	/apl/gromacs/2021.7/samples /apl/gromacs/2021.7-CUDA/samples
	2021.6	○ (2023-Jan-X)☆ CPU / GPU	/apl/gromacs/2021.6/samples /apl/gromacs/2021.6-CUDA/samples
	2021.4	○ (2023-Jan-X)☆ CPU / GPU	/apl/gromacs/2021.4/samples /apl/gromacs/2021.4-CUDA/samples
GRRM	Automated Exploration of Reaction Pathways.		
	23	○ (2024-Jan-11)	/apl/GRRM/23/samples Application is required for use. (multinode parallel available)
	17(*5)	○ (2021-Jan-27)	/apl/GRRM/17/samples (multinode parallel available)
	14	○ (2015-Jul-29)	/apl/GRRM/14/samples
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator.		
	22Jul2025 Update 1	○ (2025-Sep-4)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2025-Jul22-u1/samples /apl/lammps/2025-Jul22-u1-intel/samples /apl/lammps/2025-Jul22-u1-CUDA/samples
	22Jul2025	○ (2025-Aug-6)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2025-Jul22/samples /apl/lammps/2025-Jul22-intel/samples /apl/lammps/2025-Jul22-CUDA/samples
	29Aug2024 Update 4	○ (2025-Jul-29)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2024-Aug29-u4/samples /apl/lammps/2024-Aug29-u4-intel/samples /apl/lammps/2024-Aug29-u4-CUDA/samples
	29Aug2024 Update 3	○ (2025-Jul-15)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2024-Aug29-u3/samples /apl/lammps/2024-Aug29-u3-intel/samples /apl/lammps/2024-Aug29-u3-CUDA/samples
	29Aug2024 Update 2	○ (2025-Apr-18)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2024-Aug29-u2/samples /apl/lammps/2024-Aug29-u2-intel/samples /apl/lammps/2024-Aug29-u2-CUDA/samples
	29Aug2024 Update 1	○ (2025-Feb-21)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2024-Aug29-u1/samples /apl/lammps/2024-Aug29-u1-intel/samples /apl/lammps/2024-Aug29-u1-CUDA/samples
	29Aug2024	○ (2024-Sep-6)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2024-Aug29/samples /apl/lammps/2024-Aug29-intel/samples /apl/lammps/2024-Aug29-CUDA/samples
	2Aug23	○ (2023-Oct-16)☆ CPU(GCC,Intel) / GPU	/apl/lammps/2023-Aug2/samples /apl/lammps/2023-Aug2-intel/samples /apl/lammps/2023-Aug2-CUDA/samples Intel MPI
	23Jun22 Update	○ (2023-Jan-X)☆ CPU / GPU	/apl/lammps/2022-Jun23/samples /apl/lammps/2022-Jun23-CUDA/samples (netcdf off)

name	description		
	version	install date	job sample path & note
		○ (2023-Apr-18)☆ CPU / GPU	/apl/lammps/2022-Jun23-impi/samples /apl/lammps/2022-Jun23-impi-CUDA/samples Intel MPI
	29Sep21 Update 3	○ (2023-Apr-18)☆ CPU / GPU	/apl/lammps/2021-Sep29-impi/samples /apl/lammps/2021-Sep29-impi-CUDA/samples Intel MPI
	29Sep21	○ (2023-Jan-X)☆ CPU / GPU	/apl/lammps/2021-Sep29/samples /apl/lammps/2021-Sep29-CUDA/samples (netcdf off)
LigandMPNN	Software for designing sequences that bind to small ligands		
		△ (2024-Mar-27)☆	/apl/LigandMPNN/20240327/samples latest code on Mar 27, 2024
Molpro	Complete system of ab initio programs.		
	2025.3.0	△ (2025-Sep-29)	/apl/molpro/2025.3.0/samples
	2025.1.0	△ (2025-Mar-14)	/apl/molpro/2025.1.0/samples
	2024.3.0	△ (2024-Nov-15)	/apl/molpro/2024.3.0/samples
	2024.2.0	△ (2024-Sep-9)	/apl/molpro/2024.2.0/samples
	2024.1.0	△ (2024-Mar-11)	/apl/molpro/2024.1.0/samples
	2023.2.0	△ (2023-Oct-11)	/apl/molpro/2023.2.0/samples
	2023.1.0	△ (2023-Sep-19)	/apl/molpro/2023.1.0/samples
	2022.3.0	△ (2023-Jan-X)	/apl/molpro/2022.3.0/samples (HPC-X)
		△ (2023-May-18)	/apl/molpro/2022.3.0-mva/samples (MVAPICH)
	2022.2.2	△ (2023-Jan-X)	/apl/molpro/2022.2.2/samples
	2021.3.1	△ (2023-May-10)	/apl/molpro/2021.3.1/samples
	2015.1-44	△ (2023-Jan-X)	/apl/molpro/2015.1.44/samples
NAMD	Scalable molecular dynamics program.		
	3.0.1	○ (2024-Oct-31)☆ MPI / SMP / SMP+CUDA	/apl/namd/3.0.1-mpi/samples /apl/namd/3.0.1-smp/samples /apl/namd/3.0.1-smp-cuda/samples
	3.0	○ (2024-Jul-5)☆ MPI / SMP / SMP+CUDA	/apl/namd/3.0-mpi/samples /apl/namd/3.0-smp/samples /apl/namd/3.0-smp-cuda/samples
	3.0b7	○ (2024-May-23)☆ MPI / SMP / SMP+CUDA	/apl/namd/3.0b7-mpi/samples /apl/namd/3.0b7-smp/samples /apl/namd/3.0b7-smp-cuda/samples
	3.0b6	○ (2024-Mar-6)☆ MPI / SMP / SMP+CUDA	/apl/namd/3.0b6-mpi/samples /apl/namd/3.0b6-smp/samples /apl/namd/3.0b6-smp-cuda/samples
	3.0b2	○ (2023-Apr-10)☆	/apl/namd/3.0b2-CUDA/samples (GPU version only)
	2.14	○ (2023-Jan-X)☆ CPU / GPU	/apl/namd/2.14/samples /apl/namd/2.14-CUDA/samples
	Discovery tool for chemical insights from complex wavefunctions.		

name	description		
NBO	**version**	**install date**	**job sample path & note**
	7.0.10	△ (2023-Feb-14)	-
	7.0.7	△ (2023-Jan-X)	-
NTChem(*17)	Comprehensive new software of ab initio quantum chemistry made in Riken-RCCS from scratch.		
	2013.13.0.0	○ (2023-Apr-28)	/apl/ntchem/2013.13.0.0/samples
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	/apl/nwchem/7.2.3/samples /apl/nwchem/7.2.3-intel/samples
	7.2.2	○ (2024-Mar-5)☆ CPU / GPU	/apl/nwchem/7.2.2/samples /apl/nwchem/7.2.2-CUDA/samples
	7.0.2	○ (2023-Mar-6)	/apl/nwchem/7.0.2/samples
	6.8	○ (2023-Mar-6)	- for ReactionPlus
OmegaFold	A Protein Structure Prediction Software		
	1.1.0	○ (2024-Jun-12)☆	/apl/omegafold/1.1.0/samples
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)	/apl/openmm/8.2.0/samples
	8.1.0	○ (2023-Dec-5)	/apl/openmm/8.1.0/samples
OpenMolcas	Quantum chemistry software. (Open source version of Molcas)		
	24.10	○ (2024-Nov-18)	/apl/openmolcas/v24.10/samples
	23.06	○ (2023-Jul-25)	/apl/openmolcas/v23.06/samples
	22.10	○ (2023-Mar-6)	/apl/openmolcas/v22.10/samples
	21.10	○ (2023-Mar-6)	/apl/openmolcas/v21.10/samples
ORCA (registration required)	An ab initio quantum chemistry program package		
	6.1.0	○ (2025-Jun-18)	(osub is available) /apl/orca/6.1.0/samples
	6.0.1	○ (2024-Nov-6)	(osub is available) /apl/orca/6.0.1/samples
	5.0.4	○ (2023-Mar-20)	(osub is available) /apl/orca/5.0.4/samples
	5.0.3	○ (2022-Feb-22)	(osub is available) /apl/orca/5.0.3/samples
	4.2.1	○ (2020-Jan-8)	(osub is available) /apl/orca/4.2.1/samples
Parallel CONFLEX(*9)			-
ProteinMPNN	Software for amino acid sequence prediction from a given main chain structure		
		△ (2023-Oct-26)☆	/apl/ProteinMPNN/20231025/samples 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)	/apl/psi4/1.9.1/samples
	1.7	○ (2023-Jan-30)	/apl/psi4/1.7/samples
	Integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale.		
	7.5	○ (2025-Sep-8)☆ CPU / GPU	/apl/qe/7.5/samples /apl/qe/7.5-gpu/samples

name	description		
	version	**install date**	**job sample path & note**
Quantum ESPRESSO	7.4.1	○ (2025-Feb-12)☆ CPU / GPU	/apl/qe/7.4.1/samples /apl/qe/7.4.1-gpu/samples
	7.4	○ (2024-Feb-6)☆ CPU / GPU	/apl/qe/7.4/samples /apl/qe/7.4-gpu/samples
	7.3	○ (2024-Feb-6)☆ CPU / GPU	/apl/qe/7.3/samples /apl/qe/7.3-gpu/samples
	7.2	○ (2023-Apr-11)☆ CPU / GPU	/apl/qe/7.2/samples /apl/qe/7.2-gpu/samples
	6.8	○ (2023-Jan-26)☆ CPU / GPU	/apl/qe/6.8/samples /apl/qe/6.8-gpu/samples
ReactionPlus	Program to obtain the transition state and reaction path along the user's expected reaction mechanism.		
	1.0	○ (2018-Jan-22)	/apl/reactionplus/1.0/samples
RFdiffusion	AI-based Main Chain Structure Generation Software		
		△ (2023-Oct-26)☆	/apl/RFdiffusion/20231025/samples latest code on Oct 25, 2023
RFDiffusion AA	Software for modeling and design of various biomolecules		
		△ (2024-Mar-27)☆	/apl/RFDiffusionAA/20240327/samples latest code on Mar 27, 2024
Rosetta	Comprehensive Software Suite for Macromolecular Structure Modeling		
	3.15	○ (2025-Oct-30)	/apl/rosetta/3.15/samples
SIESTA	Efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids		
	5.4.1	○ (2025-Oct-6)	/apl/siesta/5.4.1/samples
	5.2.2	○ (2025-Feb-19)	/apl/siesta/5.2.2/samples
	5.0.1	○ (2024-Jul-29) OpenMPI / IntelMPI	/apl/siesta/5.0.1/samples /apl/siesta/5.0.1-impi/samples Open MPI and Intel MPI versions avail
	5.0.0	○ (2024-May-29) OpenMPI / IntelMPI	/apl/siesta/5.0.0/samples /apl/siesta/5.0.0-impi/samples Open MPI and Intel MPI versions avail
	4.1.5	○ (2023-Jan-X) MPI / OpenMP	/apl/siesta/4.1.5-mpi/samples /apl/siesta/4.1.5-omp/samples MPI and OpenMP versions available
TURBOMOLE	One of the fastest programs for standard quantum chemical applications.		
	7.9	○ (2024-Dec-12)☆	/apl/turbomole/7.9/samples
	7.8.1	○ (2024-Nov-12)☆	/apl/turbomole/7.8.1/samples
	7.8	○ (2023-Dec-18)☆	/apl/turbomole/7.8/samples
	7.7	○ (2023-Jul-18)☆	/apl/turbomole/7.7/samples
	7.6	○ (2021-Dec-23)	/apl/turbomole/7.6/samples
VASP(*4)		(not available)	-
	Program for Extended Tight Binding calculation		
	6.7.1	○ (2025/3/5)	/apl/xtb/6.7.1/samples

name xTB	description		
	version	install date	job sample path & note
	6.7.0	○ (2024/5/7)	/apl/xtb/6.7.0/samples
	6.5.1	○ (2024/5/22)	/apl/xtb/6.5.1/samples

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 (Note: can't detect molpro on Open OnDemand Desktop environment)		
	2025.2.0	/apl/imolpro/2025.2.0/bin/imolpro-*	○ (2025-Oct-30)
	1.0.1	/apl/imolpro/1.0.1/bin/imolpro-*	○ (2024-Mar-8)
Luscus	GUI program for Molcas/OpenMolcas		
	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