## Package Programs List (Molecular Science)

Last update: Aug 29, 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)<br>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 | 25.7, 25.3<br>24.9, 24.3<br>23.9, 23.5<br>22.11 | module: nvhpc/(version), nvhpc/(version)-byo, nvhpc/(version)-nompi |
| Intel oneAPI Compiler Runtime [2] | 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 | 2025.2.0, 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)<br><br>2025.0.0.1 =><br>(major 2025, minor 0, update 0, patch 1; 2025.0.1 is the correct name?) |
| Intel MPI | 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 | 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<br>4.1.8, 4.1.6, 4.1.5<br>3.1.6 | module: openmpi/(version)<br>(modules for each compiler available) |
| HPC-X | 2.16 (Open MPI 4.1.5) | module: openmpi/4.1.5-hpcx2.16<br>(modules for each compiler available) |
| | 2.13.1 (Open MPI 4.1.5) | module: openmpi/4.1.5-hpcx<br>(modules for each compiler available) |
| | 2.11 (Open MPI 4.1.4) | module: openmpi/4.1.4-hpcx<br>(modules for each compiler available) |
| MVAPICH | 4.0, 3.0, 2.3.7 | module: mvapich/(version)<br>(modules for GCC and AOCC available) |
| Julia | 1.11.3, 1.10.0, 1.8.5<br>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)☆ | |
| AutoDock Vina | Improved version of AutoDock | | |
| | 1.2.7 | ○ (2025-Jul-7) | |
| | 1.2.5 | ○ (2023-Nov-24) | |
| | Program for evaluating structure ensembles at DFT level. | | |
| | 2.1.3 | ○ (2025-May-1) | anmr from ENSO 2.0.2 was added manually. |

| name | description | | |
|---|---|---|---|
| CENSO | **version** | **install date** | **note** |
| | 1.2.0 | ○ (2024-May-22) | (precomipled binary)<br>anmr and nmrplot.py from ENSO 2.0.2<br>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)☆<br>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)☆<br>CPU / GPU | |
| | 2.1.2 | ○ (2024-Jan-16)☆<br>CPU / GPU | |
| | 2.0.3 | ○ (2023-Jan-X)☆<br>CPU / GPU | |
| | Fast, Free and Flexible MD | | |
| | 2025.2 | ○ (2025-May-27)☆<br>CPU / GPU | NNP enabled (libtorch 2.7.0) |
| | 2024.6 | ○ (2025-Aug-25)☆<br>CPU / GPU | |

| name | description | | |
|---|---|---|---|
| | **version** | **install date** | **note** |
| GROMACS | 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.<br>(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 | |
| | 29Aug2024 | ○ (2024-Sep-6)☆ CPU(GCC,Intel) / GPU | |

| name | description | | |
|---|---|---|---|
| | **version** | **install date** | **note** |
| | 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) | |
| NTChem(*17) | Comprehensive new software of ab initio quantum chemistry made in Riken-RCCS from scratch. | | |
| | 2013.13.0.0 | ○ (2023-Apr-28) | |

| name | description | | |
|---|---|---|---|
| | **version** | **install date** | **note** |
| 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 | |
| | 6.8 | ○ (2023-Jan-26)☆ CPU / GPU | |

| name | description | | |
|---|---|---|---|
| | **version** | **install date** | **note** |
| 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) |
| Luscus | GUI program for Molcas/OpenMolcas | | |
| | 0.8.6 | /apl/luscus/0.8.6/bin/luscus | ○ (2023-Oct-4) |
| | Visualization program of molecular and structure. | | |

| name | description | | |
|---|---|---|---|
| Molden | **version** | **command name / path** | **install date** |
| | 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 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 fees.
(*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 |