

## Package Programs List (Molecular Science)

Last update: Apr 8, 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) |
|            | 3.10.9                            | miniforge3 env (/apl/conda/20230214; source conda_init.sh or conda_init.csh to load env) |
|            | 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                                     |

| name                                  | version                                                                                                                    | note                                                                                                               |
|---------------------------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|
| NVIDIA HPC SDK                        | 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]     | 2025.1.0, 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                             | 2025.1.0, 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 => (major 2025, minor 0, update 0, patch 1; 2025.0.1 is the correct name?) |
| Intel MPI                             | 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                                                                                                  |
| Open MPI                              | 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) (modules for each compiler available)                                                    |
|                                       | 2.16 (Open MPI 4.1.5)                                                                                                      | module: openmpi/4.1.5-hpcx2.16 (modules for each compiler available)                                               |
| HPC-X                                 | 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<br>1.10.8 (LTS), 1.6.7 (LTS)                                                                         | module: julia/(version)                                                                                            |
| <a href="#">Apptainer/Singularity</a> | 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                                                        |
|---------------------------|--------------------------------------------------------------------|
| <a href="#">ABINIT-MP</a> | A software for fast Fragment-Molecular-Orbital (FMO) calculations. |

| name                    | description                                                                                                                                       |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| 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 <sup>(*22)</sup>  | 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 <sup>(*17)</sup> | 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                  |
| OpenBabel               | Chemical toolbox designed to speak the many languages of chemical data                                                                            |
| 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 <sup>(*9)</sup> |                         | (not available) |                                                                                                                        |
|                     | 3.0.0<br>(Jan 16, 2025) | △ (2025-Jan-16) | AlphaFold3 model parameters must be requested and downloaded by the user themselves.<br>GPU is required for inference. |
|                     | 3.0.0<br>(Nov 26, 2024) | △ (2024-Nov-26) |                                                                                                                        |
|                     |                         |                 |                                                                                                                        |

| name          | version              | install date                                                 | note                                                                                                                           |
|---------------|----------------------|--------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| AlphaFold     | 2.3.2                | △ (2024-Feb-8) <sup>☆</sup>                                  |                                                                                                                                |
|               | 2.3.1                | △ (2023-Feb-6) <sup>☆</sup>                                  |                                                                                                                                |
|               | 2.2.0                | △ (2022-Mar-14) <sup>☆</sup>                                 |                                                                                                                                |
|               | 2.1.1                | △ (2021-Nov-8) <sup>☆</sup>                                  |                                                                                                                                |
|               | 2.1.0                | △ (X-X-X) <sup>☆</sup>                                       |                                                                                                                                |
|               | 2.0.0<br>(2021/8/19) | △ (2021-Aug-23) <sup>☆</sup>                                 |                                                                                                                                |
|               | 2.0.0<br>(2021/7/20) | △ (2021-Jul-26) <sup>☆</sup>                                 |                                                                                                                                |
| Amber         | 24-update3           | ○ (2025-Mar-6) <sup>☆</sup>                                  | There is a note on "module" command.<br>Please check notes of <a href="#">installation details</a> .<br>(AmberTools24-update8) |
|               | 24-update1           | ○ (2024-Jun-11) <sup>☆</sup>                                 | (AmberTools24-update2)                                                                                                         |
|               | 22-update4           | ○ (2023-Aug-25) <sup>☆</sup>                                 | (AmberTools23-update4)                                                                                                         |
|               | 22-update1           | ○ (2023-Jan-X) <sup>☆</sup>                                  | (AmberTools22-update4)                                                                                                         |
|               | 20-update13          | ○ (2023-Jan-X) <sup>☆</sup>                                  | (built with configure)                                                                                                         |
| AutoDock      | 4.2.6                | ○ (2023-Nov-24)                                              |                                                                                                                                |
| AutoDock-GPU  | 1.5.3                | ○ (2023-Nov-24) <sup>☆</sup>                                 |                                                                                                                                |
| AutoDock Vina | 1.2.5                | ○ (2023-Nov-24)                                              |                                                                                                                                |
| CENSO         | 1.2.0                | ○ (2024-May-22)                                              | (precompiled binary)<br>anmr and nmrplot.py from ENSO 2.0.2<br>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) <sup>☆</sup><br><a href="#">MPI / OpenMP</a> | MPI and OpenMP versions available                                                                                              |
| DIRAC         | 23.0                 | ○ (2023-May-8)                                               |                                                                                                                                |
|               | 19.0                 | ○ (2023-Jan-27)                                              |                                                                                                                                |
| GAMESS        | 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      | 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)                                              |                                                                                                                                |

| name    | version                                  | install date                                         | note                                                               |
|---------|------------------------------------------|------------------------------------------------------|--------------------------------------------------------------------|
| GENESIS | 2.1.4                                    | ○ (2025-Jan-10) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2.1.2                                    | ○ (2024-Jan-16) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2.0.3                                    | ○ (2023-Jan-X) <sup>☆</sup><br>CPU / GPU             |                                                                    |
| GROMACS | 2024.5                                   | ○ (2025-Jan-27) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2024.4                                   | ○ (2024-Nov-5) <sup>☆</sup><br>CPU / GPU             |                                                                    |
|         | 2024.2                                   | ○ (2024-May-16) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2023.5                                   | ○ (2024-May-7) <sup>☆</sup><br>CPU / GPU             |                                                                    |
|         | 2023.4                                   | ○ (2024-Jan-26) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2023.2                                   | ○ (2023-Aug-9) <sup>☆</sup><br>CPU / GPU             |                                                                    |
|         | 2022.6                                   | ○ (2023-Jul-12) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2022.4                                   | ○ (2023-Jan-X) <sup>☆</sup><br>CPU / GPU             |                                                                    |
|         | 2021.7                                   | ○ (2023-Apr-14) <sup>☆</sup><br>CPU / GPU            |                                                                    |
|         | 2021.6                                   | ○ (2023-Jan-X) <sup>☆</sup><br>CPU / GPU             |                                                                    |
| 2021.4  | ○ (2023-Jan-X) <sup>☆</sup><br>CPU / GPU |                                                      |                                                                    |
| GRRM    | 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  | 29Aug2024 Update 1                       | ○ (2025-Feb-21) <sup>☆</sup><br>CPU(GCC,Intel) / GPU |                                                                    |
|         | 29Aug2024                                | ○ (2024-Sep-6) <sup>☆</sup><br>CPU(GCC,Intel) / GPU  |                                                                    |
|         | 2Aug23                                   | ○ (2023-Oct-16) <sup>☆</sup><br>CPU(GCC,Intel) / GPU | Intel MPI                                                          |
|         | 23Jun22 Update 2                         | ○ (2023-Jan-X) <sup>☆</sup><br>CPU / GPU             | (netcdf off)                                                       |
|         |                                          | ○ (2023-Apr-18) <sup>☆</sup><br>CPU / GPU            | Intel MPI                                                          |

| name                   | version                          | install date                                                         | note                        |
|------------------------|----------------------------------|----------------------------------------------------------------------|-----------------------------|
|                        | 29Sep21<br>Update 3              | ○ (2023-Apr-18) <sup>☆</sup><br><a href="#">CPU / GPU</a>            | Intel MPI                   |
|                        | 29Sep21                          | ○ (2023-Jan-X) <sup>☆</sup><br><a href="#">CPU / GPU</a>             | (netcdf off)                |
| LigandMPNN             |                                  | △ (2024-Mar-27) <sup>☆</sup>                                         | latest code on Mar 27, 2024 |
| Molpro <sup>(*2)</sup> | 2025.1.0                         | △ ( <a href="#">2025-Mar-14</a> )                                    |                             |
|                        | 2024.3.0                         | △ ( <a href="#">2024-Nov-15</a> )                                    |                             |
|                        | 2024.2.0                         | △ ( <a href="#">2024-Sep-9</a> )                                     |                             |
|                        | 2024.1.0                         | △ ( <a href="#">2024-Mar-11</a> )                                    |                             |
|                        | 2023.2.0                         | △ ( <a href="#">2023-Oct-11</a> )                                    |                             |
|                        | 2023.1.0                         | △ ( <a href="#">2023-Sep-19</a> )                                    |                             |
|                        | 2022.3.0                         | △ ( <a href="#">2023-Jan-X</a> )                                     | (HPC-X)                     |
|                        |                                  | △ ( <a href="#">2023-May-18</a> )                                    | (MVAPICH)                   |
|                        | 2022.2.2                         | △ ( <a href="#">2023-Jan-X</a> )                                     |                             |
|                        | 2021.3.1                         | △ ( <a href="#">2023-May-10</a> )                                    |                             |
| 2015.1-44              | △ ( <a href="#">2023-Jan-X</a> ) |                                                                      |                             |
| NAMD                   | 3.0.1                            | ○ (2024-Oct-31) <sup>☆</sup><br><a href="#">MPI / SMP / SMP+CUDA</a> |                             |
|                        | 3.0                              | ○ (2024-Jul-5) <sup>☆</sup><br><a href="#">MPI / SMP / SMP+CUDA</a>  |                             |
|                        | 3.0b7                            | ○ (2024-May-23) <sup>☆</sup><br><a href="#">MPI / SMP / SMP+CUDA</a> |                             |
|                        | 3.0b6                            | ○ (2024-Mar-6) <sup>☆</sup><br><a href="#">MPI / SMP / SMP+CUDA</a>  |                             |
|                        | 3.0b2                            | ○ ( <a href="#">2023-Apr-10</a> ) <sup>☆</sup>                       | (GPU version only)          |
|                        | 2.14                             | ○ (2023-Jan-X) <sup>☆</sup><br><a href="#">CPU / GPU</a>             |                             |
| NBO                    | 7.0.10                           | △ (2023-Feb-14)                                                      |                             |
|                        | 7.0.7                            | △ (2023-Jan-X)                                                       |                             |
| NTChem                 | 2013.13.0.0                      | ○ (2023-Apr-28)                                                      |                             |
| NWChem                 | 7.2.3                            | ○ (2025-Feb-27)<br><a href="#">CPU / GPU</a>                         |                             |
|                        | 7.2.2                            | ○ (2024-Mar-5) <sup>☆</sup><br><a href="#">CPU / GPU</a>             |                             |
|                        | 7.0.2                            | ○ ( <a href="#">2023-Mar-6</a> )                                     |                             |
|                        | 6.8                              | ○ ( <a href="#">2023-Mar-6</a> )                                     | for ReactionPlus            |
| OmegaFold              | 1.1.0                            | ○ (2024-Jun-12) <sup>☆</sup>                                         |                             |
| OpenBabel              | 3.1.1                            | ○ (2025-Mar-10)                                                      |                             |
| OpenMM                 | 8.2.0                            | ○ (2025-Mar-6)                                                       |                             |
|                        | 8.1.0                            | ○ (2023-Dec-5)                                                       |                             |
|                        | 24.10                            | ○ ( <a href="#">2024-Nov-18</a> )                                    |                             |

| name                             | version | install date                              | note                                  |
|----------------------------------|---------|-------------------------------------------|---------------------------------------|
| OpenMolcas                       | 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)                           |                                       |
|                                  | 4.2.1   | ○ (2020-Jan-8)                            |                                       |
| Parallel CONPLEX <sup>(*9)</sup> |         |                                           |                                       |
| ProteinMPNN                      |         | △ (2023-Oct-26) <sup>☆</sup>              | latest code on Oct 25, 2023           |
| PSI4                             | 1.9.1   | ○ (2024-Mar-5)                            |                                       |
|                                  | 1.7     | ○ (2023-Jan-30)                           |                                       |
| Quantum ESPRESSO                 | 7.4.1   | ○ (2024-Feb-12) <sup>☆</sup><br>CPU / GPU |                                       |
|                                  | 7.4     | ○ (2024-Feb-6) <sup>☆</sup><br>CPU / GPU  |                                       |
|                                  | 7.3     | ○ (2024-Feb-6) <sup>☆</sup><br>CPU / GPU  |                                       |
|                                  | 7.2     | ○ (2023-Apr-11) <sup>☆</sup><br>CPU / GPU |                                       |
|                                  | 6.8     | ○ (2023-Jan-26) <sup>☆</sup><br>CPU / GPU |                                       |
| ReactionPlus                     | 1.0     | ○ (2018-Jan-22)                           |                                       |
| RFdiffusion                      |         | △ (2023-Oct-26) <sup>☆</sup>              | latest code on Oct 25, 2023           |
| RFDiffusion AA                   |         | △ (2024-Mar-27) <sup>☆</sup>              | latest code on Mar 27, 2024           |
| SIESTA                           | 5.2.2   | ○ (2025-Feb-19)                           |                                       |
|                                  | 5.0.1   | ○ (2024-Jul-29)<br>OpenMPI / IntelMPI     | Open MPI and Intel MPI versions avail |
|                                  | 5.0.0   | ○ (2024-May-29)<br>OpenMPI / IntelMPI     | Open MPI and Intel MPI versions avail |
|                                  | 4.1.5   | ○ (2023-Jan-X)<br>MPI / OpenMP            | MPI and OpenMP versions available     |
| TURBOMOLE <sup>(*3)</sup>        | 7.9     | ○ (2024-Dec-12) <sup>☆</sup>              |                                       |
|                                  | 7.8.1   | ○ (2024-Nov-12) <sup>☆</sup>              |                                       |
|                                  | 7.8     | ○ (2023-Dec-18) <sup>☆</sup>              |                                       |
|                                  | 7.7     | ○ (2023-Jul-18) <sup>☆</sup>              |                                       |
|                                  | 7.6     | ○ (2021-Dec-23)                           |                                       |
| VASP <sup>(*4)</sup>             |         | (not available)                           |                                       |
|                                  | 6.7.1   | ○ (2025/3/5)                              |                                       |

| name <sub>xTB</sub> | version | install date  | note |
|---------------------|---------|---------------|------|
|                     | 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<br>(2022/4/27) | /apl/vmd/1.9.4a57/bin/vmd                            | ○ (2023-Jan-X)  |
| XCrySDen  | 1.6.2                      | exec "module load xcrysdn/1.6.2" and then<br>xcrysdn | ○ (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 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 fee.

(\*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      |
|---------------------------------------------|-----------|
| <a href="#">CRYSTAL17 license agreement</a> | 255.58 KB |
| <a href="#">CRYSTAL23 license agreement</a> | 314 KB    |