

Installation Details of Applications/Libraries

[Caution] Please confirm the software license whether you can use it outside your laboratory.

Apollo 2000/6500 Gen10 Plus (ccap; 2023/2~)

CPU: AMD EPYC 7763, GPU: NVIDIA A100 NVLink 80 GB; OS: Rocky Linux 8

- [AlphaFold 3.0.0](#)
- [AlphaFold 2.3.2](#)
- [AlphaFold 2.3.1](#)
- [AMBER24-up1 \(AmberTools24-up2\)](#)
- [Amber22-up4 \(AmberTools23-up4\)](#)
- [AMBER22-up1 \(AmberTools22-up4\)](#)
- [AMBER20-up13](#)
- [AutoDock-GPU v1.5.3](#)
- [ColabFold 1.5.5 \(local DB\)](#)
- [CP2K 2024.3](#)
- [CP2K 2024.2](#)
- [CP2K 2023.1](#)
- [CP2K 9.1](#)
- [CREST 3.0.1](#)
- [Dalton 2020.1](#)
- [DFTB+ 23.1 \(MPI / OpenMP\)](#)
- [DIRAC 23.0](#)
- [DIRAC 19.0](#)
- [FFmpeg 6.1](#)
- [GAMESS 2024R2](#)
- [GAMESS 2023R2](#)
- [GAMESS 2022R2](#)
- [GAMESS 2021R1](#)
- [GENESIS 2.1.2 \(CPU / GPU\)](#)
- [GENESIS 2.0.3 \(CPU / GPU\)](#)
- [Gromacs 2024.4 \(CPU / GPU\)](#)
- [Gromacs 2024.2 \(CPU / GPU\)](#)
- [Gromacs 2023.5 \(CPU / GPU\)](#)
- [Gromacs 2023.4 \(CPU / GPU\)](#)
- [Gromacs 2023.2 \(CPU / GPU\)](#)
- [Gromacs 2022.6 \(CPU / GPU\)](#)
- [Gromacs 2022.4 \(CPU / GPU\)](#)
- [Gromacs 2021.7 \(CPU / GPU\)](#)
- [Gromacs 2021.6 \(CPU / GPU\)](#)
- [Gromacs 2021.4 \(CPU / GPU\)](#)
- [Gromacs 2016.6 \(CPU\)](#)
- [iMolpro 1.0.1](#)
- [LAMMPS 29Aug2024 \(GCC / Intel / GPU\)](#)
- [LAMMPS 2Aug23 \(GCC / Intel / GPU\)](#)
- [LAMMPS-23Jun22 Update 2 \(CPU / GPU\)](#)
 - [Intel MPI version \(CPU / GPU\)](#)
- [LAMMPS-29Sep21 \(CPU / GPU\)](#)
 - [Update 3: Intel MPI version \(CPU / GPU\)](#)
- [Luscius 0.8.6](#)
- [Molpro 2024.3.0](#)
- [Molpro 2024.2.0](#)
- [Molpro 2024.1.0](#)
- [Molpro 2023.2.0](#)
- [Molpro 2023.1.0](#)
- [Molpro 2022.3.0 \(Open MPI / MVAPICH\)](#)
- [Molpro 2022.2.2](#)
- [Molpro 2021.3.1](#)
- [Molpro 2015.1.44](#)
- [NAMD 3.0.1 \(MPI / SMP / SMP+CUDA\)](#)
- [NAMD 3.0 \(MPI / SMP / SMP+CUDA\)](#)
- [NAMD 3.0b7 \(MPI / SMP / SMP+CUDA\)](#)

- [NAMD 3.0b6 \(MPI / SMP / SMP+CUDA\)](#)
- [NAMD 3.0b2 \(GPU\)](#)
- [NAMD 2.14 \(CPU / GPU\)](#)
- [NWChem 7.2.2 \(CPU / GPU\)](#)
- [NWChem 7.0.2](#)
- [NWChem 6.8 \(for reactionplus\)](#)
- [OpenMolcas v24.10](#)
- [OpenMolcas v23.06](#)
- [OpenMolcas v22.10](#)
- [OpenMolcas v21.10](#)
- [Open MPI 4.1.6](#)
- [Open MPI 3.1.6 \(GCC\)](#)
- [ProteinMPNN \(2023/10/25\)](#)
- [PSI4-1.9.1](#)
- [PSI4-1.7](#)
- [Quantum Espresso 7.3 \(CPU / GPU\)](#)
- [Quantum Espresso 7.2 \(CPU / GPU\)](#)
- [Quantum Espresso 6.8 \(CPU / GPU\)](#)
- [Rfdiffusion \(2023/10/25\)](#)
- [Siesta 5.0.1 \(OpenMPI / IntelMPI\)](#)
- [Siesta 5.0.0 \(OpenMPI / IntelMPI\)](#)
- [Siesta 4.1.5 \(MPI / OpenMP\)](#)
- [xtb 6.7.0](#)
- [xtb 6.5.1](#)

LX 406Rh-2/110Rh-1/108Th-4G (cclx; ~2022/9)

- [ABINIT-8.8.3](#)
- [AlphaFold2 \(2021/7/20\)](#)
- [AlphaFold2 \(2021/8/19\)](#)
- [AlphaFold-2.1.1 \(2021/11/6\)](#)
- [Amber22](#)
- [Amber20-up12](#)
- [Amber20-up9](#)
- [Amber20-up0](#)
- [Amber18-bf16](#)
- [Amber18-bf12](#)
- [Amber18-bf11-volta](#)
- [Amber18-bf1](#)
- [Amber16-bf15](#)
- [Anaconda3-2020.02 \(May 13, 2020\)](#)
- [Anaconda3-2019.03 \(Jul. 3, 2019\)](#)
- [Anaconda2-2019.03 \(Jul. 4, 2019\)](#)
- [CP2K-9.1](#)
- [CP2K-8.2.0](#)
- [CP2K-7.1.0 \(intel / gnu\)](#)
- [CP2K-6.1.0 \(intel / gnu\)](#)
- [DIRAC-19.0](#)
- [DIRAC-18.0](#)
- [FFmpeg-4.4](#)
- [GAMESS-2021Jun30 \(2021 R1\)](#)
- [GAMESS-2020Jun30](#)
- [GAMESS-2019Sep30](#)
- [GAMESS-2018Sep30](#)
- [GAMESS-2018Feb14](#)
- [GAMESS-2017Nov11](#)
- [GENESIS-1.7.0 \(CPU / GPU\)](#)
- [GENESIS-1.6.0 \(CPU / GPU\)](#)
- [GENESIS-1.4.0 \(CPU / GPU\)](#)
- [GENESIS-1.3.0 \(CPU / GPU\)](#)
- [GENESIS-1.1.6 \(CPU / GPU\)](#)
- [Gromacs-2021.4 \(CPU\(gnu\) / GPU\(gnu\) / CPU\(intel\) / GPU\(intel\)\)](#)
- [Gromacs-2021.2 \(CPU\(gnu\) / GPU\(gnu\) / CPU\(intel\) / GPU\(intel\)\)](#)
- [Gromacs-2020.7 \(CPU\(intel\) / GPU\(intel\) / CPU\(gcc\) / GPU\(gcc\)\)](#)
- [Gromacs-2020.6 \(CPU\(intel\) / GPU\(intel\) / CPU\(gcc\) / GPU\(gcc\)\)](#)

- Gromacs-2020.4 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2020.2 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2019.6 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2019.4 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2019.2 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2018.8 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2018.7 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2018.6 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2018.3 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2018.1 (CPU(intel) / CPU(gcc))
- Gromacs-2016.6 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-2016.5 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Gromacs-5.1.5 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- LAMMPS-29Sep21 (CPU / CPU+GPU)
- LAMMPS-29Oct20 (CPU / CPU+GPU)
- LAMMPS-7Aug19 (CPU / CPU+GPU)
- LAMMPS-22Aug18
- LAMMPS-16Mar18 (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc))
- Luscus-0.8.6
- Molpro2022.2.2
- Molpro2021.3.1
- Molpro2021.1.0
- Molpro2020.1.2 (gcc / intel)
- Molpro2019.2.3
- Molpro2019.1.2
- Molpro2018.2
- Molpro2015.1-pl44
- Molpro2015.1-pl33
- Molpro2015.1-pl27
- NAMD-2.13 (CPU / CPU+GPU)
- NBO-7.0.7
- NBO-7.0.2
- NWChem-7.0.2
- NWChem-6.8
- OpenMolcas v21.10
- OpenMolcas v20.10
- OpenMolcas (June 4, 2019)
- OpenMPI-4.0.2 (gcc, intel)
- OpenMPI-4.0.0 (gcc, intel)
- OpenMPI-3.1.0 (gcc, intel)
- OpenMPI-2.1.3 (gcc, intel)
- PSI4-1.5
- Python 3.9.9 (miniforge3)
- Quantum Espresso 6.8 (CPU / GPU)
- Quantum Espresso 6.7 (CPU / GPU)
- Quantum ESPRESSO 6.5
- Quantum ESPRESSO 6.3
- Quantum ESPRESSO 5.4
- Siesta-4.1.5 (MPI / OpenMP)
- Siesta-4.0.2
- VMD-1.9.3

Primergy RX300/CX2550 (ccpg)

- ABINIT-7.8.2
- Amber16-bf3
- Amber14-bf11
- Amber14-bf10
- Amber14-bf0
- Amber12-bf21
- Amber12-bf7
- AutoDock-4.2.6
- GAMESS-2017Apr20
- GAMESS-2014Dec05
- GAMESS-2013May01

- GAMESS-2012May01
- GENESIS-1.1.5 (CPU / GPU)
- GENESIS-1.1.1 (CPU / GPU)
- GENESIS-1.1.0 (CPU / GPU)
- Gromacs-2016.3 (CPU / GPU)
- Gromacs-2016.1 (CPU / GPU)
- Gromacs-5.1.4 (CPU / GPU)
- Gromacs-5.1.2 (CPU / GPU)
- Gromacs-5.0.6
- Gromacs-5.0.4
- Gromacs-5.0
- Gromacs-4.6.6
- Gromacs-4.6.5
- Gromacs-4.6.1
- Gromacs-4.5.5
- Molcas-8.2
- Molcas-8.0sp1
- Molcas-8.0
- Molpro2015.1-pl19
- Molpro2015.1-pl5
- Molpro2015.1-pl0
- Molpro2012.1-pl37
- Molpro2012.1-pl25
- Molpro2012.1-pl15
- NAMD-2.11
- NAMD-2.9
- PSI-4.0b5
- Quantum ESPRESSO-6.1
- Quantum ESPRESSO-5.1.1
- SIESTA-3.1
- SMASH-2.2.0
- SMASH-2.1.0
- SMASH-2.0.0
- SMASH-1.1.0

UV2000 (ccuv)

- Amber16-bf3
- Amber14-bf10
- Amber14-bf0
- Amber12-bf21
- Amber12-bf7
- GAMESS-2017Apr20
- GAMESS-2014Dec05
- GAMESS-2013May01
- GAMESS-2012May01
- GENESIS-1.1.5
- GENESIS-1.1.1
- GENESIS-1.1.0
- Gromacs-5.1.4
- Gromacs-5.1.2
- Gromacs-5.0.6
- Gromacs-5.0.4
- Gromacs-5.0
- Gromacs-4.6.6
- Gromacs-4.6.5
- Gromacs-4.5.5
- Molcas-8.2
- Molcas-8.0sp1
- Molcas-8.0
- Molpro2015.1-pl19
- Molpro2015.1-pl5
- Molpro2015.1-pl0
- Molpro2012.1-pl37
- Molpro2012.1-pl25

- Molpro2012.1-pl15
- PSI-4.0b5
- SMASH-2.2.0
- SMASH-2.1.0
- SMASH-2.0.0
- SMASH-1.1.0