Available software

A current list of the software available on LUIS Computing Cluster is below. This list changes frequently as new software is added. You can request the installation or updating of a particular program or library by contacting cluster support. If you wish to use the LUIS Custer software environment on your own system **within the Leibniz University network**, please see accessing CVMFS.

Here are a few things to know about the available software

- Docker is not available on compute cluster but Singularity is installed on all compute nodes. Docker containers can be converted to Singularity as discussed here
- Some of the software packages listed below are not immediately usable because they require you to have a license. Contact cluster support If you need to be granted an access to them
- All software are accessed by loading a **module**. See section on how to use the Lmod module system

To display a list of hidden modules, after logging into the cluster, on the command line, enter:
`module --show-hidden spider`

Skylake(AVX512)

Installed software as of Wed, 23 Oct 2024 07:35:08 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	6.14-2, 2016, 2017-hotfix-1819, 2017, 2018, 2019-hotfix-1939, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341	Desc Finite Element Analysis software for modeling, visualization and best-in-class implicit and explicit dynamics FEA.
AMPL-MP		3.1.0	Desc An open-source library for mathematical programming.
ANSYS	ANSYS / CFX	15.0, 16.0, 16.2, 17.2, 18.0, 18.2, 19.0, 19.2, 19.3, 2019.2, 2019.3, 2020.1, 2020.2, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ANSYSEM		17.2, 18.0, 18.1, 18.2, 19.0, 19.1, 20.2, 2022.2, 2023.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ARIA		2.3.1-Python-2.7.11	Desc ARIA (Ambiguous Restraints for Iterative Assignment) is a software for automated NOE assignment and NMR structure calculation
ASE		3.16.0-Python-2.7.11, 3.16.2-Python-3.6.6, 3.21.1	Desc ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language. From version 3.20.1 we also include the ase-ext package, it contains optional reimplementations in C of functions in ASE. ASE uses it automatically when installed.
ATK		2.20.0	Desc ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications.
ATSAS		2.7.2-5.el6.x86_64	Desc ATSAS is a program suite for small-angle scattering data analysis from biological macromolecules. - Homepage: http://www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html
Advisor		2016_update3, 2019_update3, 2023.2.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain - Homepage: https://software.intel.com/intel-advisor-xe

Modules	Documentation	Versions	Description
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		18-AmberTools-18-patchlevel-9-5-CUDA, 22.0-AmberTools-22.3-CUDA-11.4.1	Desc Amber (originally Assisted Model Building with Energy Refinement) is software for performing molecular dynamics and structure prediction.
Armadillo		11.4.3	Desc Armadillo is an open-source C+ + linear algebra library (matrix maths) aiming towards a good balance between speed and ease of use. Integer, floating point and complex numbers are supported, as well as a subset of trigonometric and statistics functions.
BLIS		0.8.1, 0.9.0	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
BWA		0.7.17	Desc Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome.
Bazel		0.5.2, 0.7.0, 0.16.1, 0.18.0, 0.26.1, 0.29.1, 2.0.0, 3.4.1, 3.7.2, 4.2.2, 6.3.1	Desc Bazel is a build tool that builds code quickly and reliably. It is used to build the majority of Google's software.
Biopython		1.78	Desc Biopython is a set of freely available tools for biological computation written in Python by an international team of developers. It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics.
Bonnie+ +		Bonnie+ 1.97	Desc Bonnie+ +-1.97: Enhanced performance Test of Filesystem I/O
Boost		1.47.0, 1.58.0-Python-2.7.11, 1.59.0-Python-2.7.11, 1.60.0-Python-2.7.11, 1.60.0, 1.61.0-Python-2.7.11, 1.61.0, 1.63.0-Python-3.5.2, 1.66.0, 1.67.0, 1.68.0-Python-2.7.15, 1.71.0, 1.74.0, 1.77.0, 1.81.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Boost.Python		1.67.0-Python-2.7.15	Desc Boost.Python is a C+ + library which enables seamless interoperability between C+ + and the Python programming language.
Brunsli		0.1	Desc Brunsli is a lossless JPEG repacking library.
CFITSIO		3.38, 3.45, 4.2.0	Desc CFITSIO is a library of C and Fortran subroutines for reading and writing data files in FITS (Flexible Image Transport System) data format.
CGAL		4.8-Python-2.7.11, 4.8.1-Python-3.5.2, 4.8.1, 4.11.1-Python-2.7.15, 4.14.1-Python-3.7.4, 4.14.3, 5.2	Desc The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C+ + library.
CGNS		3.3.1	Desc The CGNS system is designed to facilitate the exchange of data between sites and applications, and to help stabilize the archiving of aerodynamic data.
CMake		2.8.4, 3.4.1, 3.4.3, 3.5.2, 3.6.1, 3.7.1, 3.9.6, 3.11.4, 3.12.1, 3.15.3, 3.16.4, 3.18.4, 3.20.1, 3.21.1, 3.22.1, 3.24.3, 3.27.6	Desc CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.
CNS		1.3-haddock-2.2, 1.3-haddock-2.4, 1.21-aria2.3	Desc Crystallography & NMR System (CNS) has been designed to provide a flexible multi-level hierachical approach for the most commonly used algorithms in macromolecular structure determination
COMSOL	COMSOL	5.1, 5.2, 5.4, 5.5, 5.6, 6.0, 6.1, 6.2	Desc COMSOL Multiphysics is a finite element analysis, solver and simulation software/FEA software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. - Homepage: https://www.comsol.com/
CPMD	CPMD	4.1, 4.3-omp, 4.3	Desc CPMD The CPMD code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.
CREST		2.11.2, 2.12	Desc CREST is an utility/driver program for the xtb program. Originally it was designed as conformer sampling program, hence the abbreviation Conformer–Rotamer Ensemble Sampling Tool, but now offers also some utility functions for calculations with the GFNn–xTB methods. Generally the program functions as an IO based OMP scheduler (i.e., calculations are performed by the xtb program) and tool for the creation and analysation of structure ensembles.
CRYSTAL14		1.0.4	Desc Crystal is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations
CUDA		7.5.18, 8.0.44, 9.2.88, 10.1.105, 10.1.243, 11.1.1, 11.4.1, 11.7.0, 12.0.0, 12.3.0, 12.3.2, 12.4.0	Desc CUDA (formerly Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. CUDA gives developers access to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs.
CheMPS2		1.8.11	Desc CheMPS2 is a scientific library which contains a spin-adapted implementation of the density matrix renormalization group (DMRG) for ab initio quantum chemistry.
Clang		9.0.1, 16.0.4	Desc C, C+ +, Objective-C compiler, based on LLVM. Does not include C+ + standard library – use libstdc+ + from GCC.

Modules	Documentation	Versions	Description
CoordgenLibs		3.0.0	Desc Schrodinger-developed 2D Coordinate Generation
Cython		0.24-Python-2.7.11, 0.24-Python-3.4.3, 0.29.22	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
DMTCP		2.6.0	Desc DMTCP is a tool to transparently checkpoint the state of multiple simultaneous applications, including multi-threaded and distributed applications. It operates directly on the user binary executable, without any Linux kernel modules or other kernel modifications.
DendroPy		4.5.2	Desc A Python library for phylogenetics and phylogenetic computing: reading, writing, simulation, processing and manipulation of phylogenetic trees (phylogenies) and characters.
Doxygen		1.8.11	Desc Doxygen is a documentation system for C+ +, C, Java, Objective-C, Python, IDL (Corba and Microsoft flavors), Fortran, VHDL, PHP, C#, and to some extent D.
ELPA		2021.05.001	Desc Eigenvalue SoLvers for Petaflop-Applications .
EPA-ng		0.3.8	Desc EPA-ng - Fast, parallel, highly accurate Maximum Likelihood Phylogenetic Placement of genetic sequences on a user-supplied reference tree and alignment
EasyBuild-custom		1.0	Desc EasyBuild is a software build and installation framework - Homepage: http://hpcugent.github.com/easybuild/
Eigen		3.2.9, 3.3.4, 3.3.7, 3.3.8, 3.3.9, 3.4.0	Desc Eigen is a C+ + template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
FDS		6.4.0, 6.5.2, 6.6.0, 6.7.3, 6.7.4	Desc Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires.
FEKO	FEKO	2017.2_hw, 2017.2.5_hw, 2018_hw, 2019_hw, 2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering
FFTW		3.3.4-PFFT-20150905, 3.3.4, 3.3.6, 3.3.8, 3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FFTW.MPI		3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FLANN		1.8.4-Python-2.7.15	Desc FLANN is a library for performing fast approximate nearest neighbor searches in high dimensional spaces.
Fiona		1.8.13-Python-3.7.4, 1.8.20	Desc Fiona is designed to be simple and dependable. It focuses on reading and writing data in standard Python IO style and relies upon familiar Python types and protocols such as files, dictionaries, mappings, and iterators instead of classes specific to OGR. Fiona can read and write real-world data using multi-layered GIS formats and zipped virtual file systems and integrates readily with other Python GIS packages such as pyproj, Rtree, and Shapely.
FlexiBLAS		3.0.4, 3.2.1, 3.3.1	Desc FlexiBLAS is a wrapper library that enables the exchange of the BLAS and LAPACK implementation used by a program without recompiling or relinking it.
Flux		2019	Desc Altair Flux captures the complexity of electromagnetic and thermal phenomena to predict the behavior of future products with precision.
FriBidi		1.0.5, 1.0.10, 1.0.12, 1.0.13	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		24.5.4, 24.5.6_nhus, 24.7.4_nhus, 24.7.4, 26.1.0_nhus, 26.1.0, 30.3.0, 45.7.0, 46.5.0	Desc The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. - Homepage: https://www.gams.com/
GCC		4.9.2, 4.9.3-2.25, 5.4.0-2.26, 6.3.0-2.27, 6.4.0-2.28, 7.3.0-2.30, 8.2.0-2.31.1, 8.3.0, 9.3.0, 10.2.0, 10.3.0, 11.2.0, 12.2.0, 13.2.0	Desc The GNU Compiler Collection includes front ends for C, C+ +, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc+ +, libgcj,...).
GDB		9.1-Python-3.7.4	Desc The GNU Project Debugger
GEOS		3.6.1-Python-2.7.12	Desc GEOS (Geometry Engine - Open Source) is a C+ + port of the Java Topology Suite (JTS)
GMP		6.1.0, 6.1.1, 6.1.2, 6.2.0, 6.2.1, 6.3.0	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers.
GNUGo		3.8	Desc GNU Go is a free program that plays the game of Go
GPAW		1.4.0-Python-2.7.11, 1.4.0-Python-3.6.6	Desc GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.
GROMACS		5.1.2-hybrid, 2018.4-CUDA-9.2.88, 2018.4, 2019, 2023.5-CUDA-12.0.0	Desc GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. This is a GPU enabled build, containing both MPI and threadMPI binaries. It also contains the gmxapi extension for the single precision MPI build.
GSL		1.16, 2.1, 2.5, 2.6, 2.7	Desc The GNU Scientific Library (GSL) is a numerical library for C and C+ + programmers. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting.

Modules	Documentation	Versions	Description
GST-plugins-base		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing.
GStreamer		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing.
GTK+		2.24.30	Desc The GTK+ 2 package contains libraries used for creating graphical user interfaces for applications.
GTK3		3.24.35	Desc GTK+ is the primary library used to construct user interfaces in GNOME. It provides all the user interface controls, or widgets, used in a common graphical application. Its object-oriented API allows you to construct user interfaces without dealing with the low-level details of drawing and device interaction.
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g09.D01, g09.E01, g16.A03, g16.B01	Desc Gaussian provides state-of-the-art capabilities for electronic structure modeling.
GitPython		2.1.11-Python-3.6.6	Desc GitPython is a python library used to interact with Git repositories
Go		1.16.6	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
GraphicsMagick		1.3.23	Desc GraphicsMagick is the swiss army knife of image processing.
Graphviz		2.50.0	Desc Graphviz is open source graph visualization software. Graph visualization is a way of representing structural information as diagrams of abstract graphs and networks. It has important applications in networking, bioinformatics, software engineering, database and web design, machine learning, and in visual interfaces for other technical domains.
Guile		1.8.8	Desc Guile is a programming language, designed to help programmers create flexible applications that can be extended by users or other programmers with plug-ins, modules, or scripts.
Gurobi		6.5.0, 7.0.2, 7.5.2, 8.1.0, 9.0.1, 9.1.2, 9.5.0, 11.0.0	Desc The Gurobi Optimizer is a state-of-the-art solver for mathematical programming. The solvers in the Gurobi Optimizer were designed from the ground up to exploit modern architectures and multi-core processors, using the most advanced implementations of the latest algorithms.
HADDOCK		2.2-Python-2.7.11, 2.4-Python-2.7.16	Desc HADDOCK (High Ambiguity Driven biomolecular DOCKing) is an information-driven flexible docking approach for the modelling of biomolecular complexes
HDF		4.2.15	Desc HDF (also known as HDF4) is a library and multi-object file format for storing and managing data between machines.
HDF5		1.8.16-serial, 1.8.16, 1.8.17, 1.10.2, 1.10.5, 1.10.7, 1.12.1, 1.14.0	Desc HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.
HDFView		2.14-Java-1.8.0_152-centos7	Desc HDFView is a visual tool for browsing and editing HDF4 and HDF5 files.
HH-suite		3.3.0	Desc The HH-suite is an open-source software package for sensitive protein sequence searching based on the pairwise alignment of hidden Markov models (HMMs).
HMMER		3.2.1, 3.3.2	Desc HMMER is used for searching sequence databases for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs). Compared to BLAST, FASTA, and other sequence alignment and database search tools based on older scoring methodology, HMMER aims to be significantly more accurate and more able to detect remote homologs because of the strength of its underlying mathematical models. In the past, this strength came at significant computational expense, but in the new HMMER3 project, HMMER is now essentially as fast as BLAST.
Hadoop-cluster		1.0	Desc Framework for deploying Hadoop clusters on traditional HPC - Homepage: http://luis.uni-hannover.de
Highway		1.0.3	Desc Highway is a C+ + library for SIMD (Single Instruction, Multiple Data), i.e. applying the same operation to 'lanes'.
ICU		61.1, 64.2, 67.1, 69.1, 72.1	Desc ICU is a mature, widely used set of C/C+ + and Java libraries providing Unicode and Globalization support for software applications.
IPython		3.2.3-Python-2.7.11, 7.2.0-Python-3.6.6, 7.9.0-Python-3.7.4, 7.18.1-Python-3.7.4, 7.25.0	Desc IPython provides a rich architecture for interactive computing with: Powerful interactive shells (terminal and Qt-based). A browser-based notebook with support for code, text, mathematical expressions, inline plots and other rich media. Support for interactive data visualization and use of GUI toolkits. Flexible, embeddable interpreters to load into your own projects. Easy to use, high performance tools for parallel computing.
ImageMagick		7.0.8-11, 7.0.9-5, 7.0.10-35, 7.1.0-4, 7.1.0-53	Desc ImageMagick is a software suite to create, edit, compose, or convert bitmap images

Modules	Documentation	Versions	Description
Imath		3.1.6	Desc Imath is a C+ + and python library of 2D and 3D vector, matrix, and math operations for computer graphics
Inspector		2016_update3, 2019_update3, 2023.2.0	Desc Intel Inspector XE is an easy to use memory error checker and thread checker for serial and parallel applications - Homepage: http://software.intel.com/en-us/intel-inspector-xe
Ipopt		3.14.4	Desc IPOPT (Interior Point Optimizer, pronounced Eye-Pea-Opt) is an open source software package for large-scale nonlinear optimization.
Java		1.8.0_45, 1.8.0_72, 1.8.0_92, 1.8.0_144, 1.8.0_152, 11.0.2, 11.0.16, 11.0.18	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.
Julia		1.6.1-linux-x86_64, 1.7.0-linux-x86_64, 1.7.2-linux-x86_64, 1.10.2-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter in the cluster	2.2.8-Python-3.7.4, 3.1.14	Desc JupyterLab is the next-generation user interface for Project Jupyter offering all the familiar building blocks of the classic Jupyter Notebook (notebook, terminal, text editor, file browser, rich outputs, etc.) in a flexible and powerful user interface. JupyterLab will eventually replace the classic Jupyter Notebook.
Kalign		3.3.1	Desc Kalign is a fast multiple sequence alignment program for biological sequences.
Keras		2.2.4-Python-3.7.4, 2.3.1-Python-3.7.4, 2.4.0-Python-3.7.4	Desc Keras is a minimalist, highly modular neural networks library, written in Python and capable of running on top of either TensorFlow or Theano.
LAME		3.100	Desc LAME is a high quality MPEG Audio Layer III (MP3) encoder licensed under the LGPL.
LAMMPS		3Mar2020-Python-3.7.4-kokkos, 23Jun2022-kokkos	Desc LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.
LAPACK		3.5.0	Desc LAPACK is written in Fortran90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems.
LERC		4.0.0	Desc LERC is an open-source image or raster format which supports rapid encoding and decoding for any pixel type (not just RGB or Byte). Users set the maximum compression error per pixel while encoding, so the precision of the original input image is preserved (within user defined error bounds).
Lua		5.4.2, 5.4.3, 5.4.4	Desc Lua is a powerful, fast, lightweight, embeddable scripting language. Lua combines simple procedural syntax with powerful data description constructs based on associative arrays and extensible semantics. Lua is dynamically typed, runs by interpreting bytecode for a register-based virtual machine, and has automatic memory management with incremental garbage collection, making it ideal for configuration, scripting, and rapid prototyping.
Lumerical		2020-2.4, 2021-2.3, 2022-1, 2023-1, 2024-1.02	Desc Ansys Lumerical photonic multiphysics and circuit simulation suites. Design components and analyze electrical, thermal and optical effects at the physical level. Simulate and optimize the performance of photonic integrated circuits
MATLAB	MATLAB	2015a, 2016b, 2017a, 2017b, 2018a, 2018b, 2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b	Desc MATLAB is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C+ +, and Fortran. - Homepage: http://www.mathworks.com/products/matlab
METIS		5.1.0, 5.1.0-32bitIDX	Desc METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms implemented in METIS are based on the multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning schemes.
MPC		1.3.1	Desc Gnu Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It extends the principles of the IEEE-754 standard for fixed precision real floating point numbers to complex numbers, providing well-defined semantics for every operation. At the same time, speed of operation at high precision is a major design goal.
MPFR		3.1.4, 4.0.1, 4.0.2, 4.1.0, 4.2.0, 4.2.1	Desc The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.
MUMPS		5.2.1-metis, 5.3.5-metis, 5.4.1-metis, 5.6.1-metis	Desc A parallel sparse direct solver
Mako		1.0.4-Python-2.7.12, 1.0.7-Python-2.7.15, 1.1.0, 1.1.3, 1.1.4, 1.2.4	Desc A super-fast templating language that borrows the best ideas from the existing templating languages
Maple		17, 18, 2015.0, 2017, 2020.1, 2021.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface. - Homepage: http://www.maplesoft.com/products/maple/

Modules	Documentation	Versions	Description
Mathematica		10.4.1, 11.3.0, 12.1.1, 12.3.0, 13.0.0, 13.2.1	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields. - Homepage: http://www.wolfram.com/mathematica
Mesa		20.2.1	Desc Mesa is an open-source implementation of the OpenGL specification - a system for rendering interactive 3D graphics.
Meson		0.51.2-Python-3.7.4, 0.53.2-Python-3.8.2, 0.55.3, 0.58.0, 0.58.2, 0.64.0, 1.2.3	Desc Meson is a cross-platform build system designed to be both as fast and as user friendly as possible.
Mesquite		2.3.0	Desc Mesh-Quality Improvement Library
Miniconda2		4.5.1, 4.5.12, 4.7.10	Desc Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.
Miniconda3	Conda	4.10.3, 22.11.1-1, 23.5.2-0	Desc Miniconda is a free minimal installer for conda. It is a small, bootstrap version of Anaconda that includes only conda, Python, the packages they depend on, and a small number of other useful packages.
Modeller		9.19-Python-2.7.11	Desc MODELLER is used for homology or comparative modeling of protein three-dimensional structures (1,2). The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.
Molden		5.0, 5.6, 5.7, 5.9, 5.9.4	Desc Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK, GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac
Mothur		1.40.3-Python-2.7.11, 1.40.5-Python-2.7.11, 1.41.3-Python-2.7.15, 1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.
NAMD		2.12-mpi, 2.13-mpi	Desc NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
NCCL		2.3.7, 2.4.8, 2.8.3-CUDA-11.1.1, 2.10.3-CUDA-11.4.1, 2.16.2-CUDA-12.0.0, 2.20.5-CUDA-12.4.0	Desc The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.
NFFT	NFFT	3.1.3, 3.3.0, 3.3.1, 3.5.0	Desc The NFFT (nonequispaced fast Fourier transform or nonuniform fast Fourier transform) is a C subroutine library for computing the nonequispaced discrete Fourier transform (NDFT) and its generalisations in one or more dimensions, of arbitrary input size, and of complex data.
NVHPC		23.1-CUDA-12.0.0	Desc C, C+ + and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
Ninja		1.8.2, 1.9.0, 1.10.0, 1.10.1, 1.10.2, 1.11.1	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1, 5.0.4	Desc ORCA is a flexible, efficient and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated ab initio methods. It can also treat environmental and relativistic effects.
Octave		3.8.2, 4.0.0, 4.4.1, 5.1.0, 9.1.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations.
Octopus		5.0.0-mpi, 5.0.0, 7.3-mpi, 7.3, 9.1-mpi, 11.4, 13.0	Desc Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory (DFT), in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation.
OpenBLAS		0.2.15-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.1, 0.2.19-LAPACK-3.7.0, 0.2.20, 0.3.1, 0.3.5, 0.3.7, 0.3.9, 0.3.12, 0.3.18, 0.3.21, 0.3.24	Desc OpenBLAS is an optimized BLAS library based on GotoBLAS2 1.13 BSD version.
OpenBabel		3.1.1-Python-3.7.4	Desc Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.
OpenCV		2.4.12, 3.1.0, 4.0.1-Python-2.7.15, 4.2.0-Python-3.7.4, 4.5.1-contrib	Desc OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products.
OpenEXR		2.5.5, 3.1.5	Desc OpenEXR is a high dynamic-range (HDR) image file format developed by Industrial Light & Magic for use in computer imaging applications
OpenFAST		2.3.0, 2.4.0, 3.1.0	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.

Modules	Documentation	Versions	Description
OpenFOAM		v1612+, v1906, v1912, v2012, v2106, v2112, v2206, v2212, 2.3.0, 2.3.1, 3.0.0, 4.0, 4.1, 6, 7, 8, 9, 10	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.
OpenFOAM-Extend		3.2, 4.0	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.
OpenMPI		1.10.2, 1.10.3, 2.0.2, 2.1.1, 3.1.1, 3.1.3, 3.1.4, 4.0.3, 4.0.5, 4.1.1, 4.1.4, 4.1.6	Desc The Open MPI Project is an open source MPI-3 implementation.
OpenPGM		5.2.122	Desc OpenPGM is an open source implementation of the Pragmatic General Multicast (PGM) specification in RFC 3208 available at www.ietf.org. PGM is a reliable and scalable multicast protocol that enables receivers to detect loss, request retransmission of lost data, or notify an application of unrecoverable loss. PGM is a receiver-reliable protocol, which means the receiver is responsible for ensuring all data is received, absolving the sender of reception responsibility.
OpenSSL		1.0.1s, 1.0.2g, 1.0.2h, 1.1, 1.1.1d	Desc The OpenSSL Project is a collaborative effort to develop a robust, commercial-grade, full-featured, and Open Source toolchain implementing the Secure Sockets Layer (SSL v2/v3) and Transport Layer Security (TLS v1) protocols as well as a full-strength general purpose cryptography library.
PCL		1.9.1-Python-2.7.15, 1.12.1-Python-3.8.6	Desc The Point Cloud Library (PCL) is a standalone, large scale, open project for 2D/3D image and point cloud processing.
PFFT		1.0.8-alpha	Desc PFFT is a software library for computing massively parallel, fast Fourier transformations on distributed memory architectures. PFFT can be understood as a generalization of FFTW-MPI to multidimensional data decomposition.
PGI		16.5-GCC-5.4.0-2.26	Desc C, C+ + and Fortran compilers from The Portland Group - PGI
PICRUSt2		2.5.0-Python-3.9.6	Desc PICRUSt2 (Phylogenetic Investigation of Communities by Reconstruction of Unobserved States) is a software for predicting functional abundances based only on marker gene sequences. Check out the pre-print here.
PLUMED		2.5.3-Python-3.7.4, 2.7.3	Desc PLUMED is an open source library for free energy calculations in molecular systems which works together with some of the most popular molecular dynamics engines. Free energy calculations can be performed as a function of many order parameters with a particular focus on biological problems, using state of the art methods such as metadynamics, umbrella sampling and Jarzynski-equation based steered MD. The software, written in C+ +, can be easily interfaced with both fortran and C/C+ + codes.
PMIx		3.1.5	Desc Process Management for Exascale Environments PMI Exascale (PMIx) represents an attempt to provide an extended version of the PMI standard specifically designed to support clusters up to and including exascale sizes. The overall objective of the project is not to branch the existing pseudo-standard definitions - in fact, PMIx fully supports both of the existing PMI-1 and PMI-2 APIs - but rather to (a) augment and extend those APIs to eliminate some current restrictions that impact scalability, and (b) provide a reference implementation of the PMI-server that demonstrates the desired level of scalability.
POV-Ray		3.7.0.8	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. POV-Ray is a high-quality, Free Software tool for creating stunning three-dimensional graphics. The source code is available for those wanting to do their own ports.
POVRay		3.6.1	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms.
PSI4		1.7	Desc PSI4 is an open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties. We can routinely perform computations with more than 2500 basis functions running serially or in parallel.
PSolver		1.8.3	Desc Interpolating scaling function Poisson Solver Library
Pandoc		3.1.8	Desc If you need to convert files from one markup format into another, pandoc is your swiss-army knife
ParMETIS		4.0.3	Desc ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. ParMETIS extends the functionality provided by METIS and includes routines that are especially suited for parallel AMR computations and large scale numerical simulations. The algorithms implemented in ParMETIS are based on the parallel multilevel k-way graph-partitioning, adaptive repartitioning, and parallel multi-constrained partitioning schemes.
ParMGridGen		1.0	Desc ParMGridGen is an MPI-based parallel library that is based on the serial package MGridGen, that implements (serial) algorithms for obtaining a sequence of successive coarse grids that are well-suited for geometric multigrid methods.

Modules	Documentation	Versions	Description
ParaView		4.4.0-mpi, 4.4.0, 5.1.2-mpi, 5.2.0-mpi, 5.4.1-mpi, 5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi, 5.11.1	Desc ParaView is a scientific parallel visualizer.
Perl		5.22.1-bare, 5.22.1, 5.28.0, 5.28.1, 5.30.0, 5.30.2, 5.32.0-minimal, 5.32.0, 5.32.1-minimal, 5.32.1, 5.34.0, 5.36.0-minimal, 5.36.0, 5.38.0	Desc Larry Wall's Practical Extraction and Report Language This is a minimal build without any modules. Should only be used for build dependencies.
Perl-bundle-CPAN		5.38.0	Desc A set of common packages from CPAN
Pies		1.3	Desc GNU Pies stands for the Program Invocation and Execution Supervisor.
Pillow		3.4.2-Python-3.5.1, 5.3.0-Python-3.6.6, 6.2.1, 8.0.1, 8.3.2, 9.4.0, 10.2.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
Pillow-SIMD		9.5.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
PnetCDF		1.12.3	Desc Parallel netCDF: A Parallel I/O Library for NetCDF File Access
ProFit		3.1, 3.3	Desc ProFit is the protein least squares fitting program
Pth		2.0.7	Desc GNU Pth - The GNU Portable Threads
PyQt5		5.11.3-Python-3.6.6, 5.13.1-Python-3.7.4, 5.15.1	Desc PyQt5 is a set of Python bindings for v5 of the Qt application framework from The Qt Company. This bundle includes PyQtWebEngine, a set of Python bindings for The Qt Company’s Qt WebEngine framework.
PyTorch		1.2.0-Python-3.6.6, 1.6.0-Python-3.7.4, 1.9.0, 1.10.0, 1.13.1-CUDA-12.0.0, 1.13.1	Desc Tensors and Dynamic neural networks in Python with strong GPU acceleration. PyTorch is a deep learning framework that puts Python first.
PyTorch-bundle		2022.1	Desc PyTorch Geometric (PyG) is a geometric deep learning extension library for PyTorch.
PyZMQ		15.2.0-Python-2.7.11-zmq4	Desc Python bindings for ZeroMQ
Python		2.7.11, 2.7.12, 2.7.15-bare, 2.7.15, 2.7.16, 2.7.18-bare, 2.7.18, 3.4.3, 3.5.1, 3.5.2, 3.6.1, 3.6.4, 3.6.6, 3.7.0, 3.7.2, 3.7.4, 3.8.2, 3.8.6, 3.9.5-bare, 3.9.5, 3.9.6-bare, 3.9.6, 3.10.8-bare, 3.10.8, 3.11.5	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Python-bundle-PyPI		2023.10	Desc Bundle of Python packages from PyPI
Qt		4.8.7	Desc Qt is a comprehensive cross-platform C+ + application framework.
Qt5		5.6.0, 5.7.0, 5.10.1, 5.13.1, 5.14.2, 5.15.2, 5.15.7	Desc Qt is a comprehensive cross-platform C+ + application framework.
QuTiP		4.3.1-Python-3.6.6	Desc QuTiP is open-source software for simulating the dynamics of open quantum systems.
R	Conda, Jupyter in the cluster	3.3.1, 3.4.1-X11-20160819, 3.5.1, 3.6.1, 4.0.3, 4.1.0, 4.1.2, 4.2.2	Desc R is a free software environment for statistical computing and graphics.
ROOT		v5.34.36-Python-2.7.11, 6.14.06-Python-2.7.15	Desc The ROOT system provides a set of OO frameworks with all the functionality needed to handle and analyze large amounts of data in a very efficient way.
Rust		1.52.1, 1.54.0, 1.65.0, 1.73.0	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAS		9.4	Desc SAS is a software suite for advanced analytics, multivariate analyses, business intelligence, data management, and predictive analytics.
SCIPOptSuite		8.0.1, 8.0.4-Gurobi-9.5.0, 8.0.4, 9.0.1	Desc SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access of detailed information down to the guts of the solver.
SCOTCH		6.0.4, 6.0.6, 6.0.9, 6.1.0, 6.1.2-no-thread, 6.1.2, 7.0.2, 7.0.3	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.
SEPP		4.5.1	Desc SATe-enabled Phylogenetic Placement - addresses the problem of phylogenetic placement of short reads into reference alignments and trees.
SUMO		1.9.2-Python-3.7.4, 1.16.0-Python-3.9.6	Desc “Simulation of Urban MObility” (SUMO) is an open source, highly portable, microscopic and continuous traffic simulation package designed to handle large networks. It allows for intermodal simulation including pedestrians and comes with a large set of tools for scenario creation.
ScaFaCoS		1.0.1	Desc ScaFaCoS is a library of scalable fast coulomb solvers.
ScaLAPACK		2.0.2-OpenBLAS-0.2.15-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.1, 2.0.2-OpenBLAS-0.2.19-LAPACK-3.7.0, 2.0.2-OpenBLAS-0.2.20, 2.0.2-OpenBLAS-0.3.1, 2.0.2-OpenBLAS-0.3.5, 2.0.2, 2.1.0-fb, 2.1.0, 2.2.0-fb	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.

Modules	Documentation	Versions	Description
Schrodinger		2015-3_Linux-x86_64	Desc Schrödinger aims to provide integrated software solutions and services that truly meet its customers' needs. We want to empower researchers around the world to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials. - Homepage: http://www.schrodinger.com/
SciPy-bundle		2019.03, 2019.10-Python-3.7.4, 2020.03-Python-3.8.2, 2020.11, 2021.10, 2023.02, 2023.11	Desc Bundle of Python packages for scientific software
Shapely		1.7.0-Python-3.7.4, 1.8a1	Desc Shapely is a BSD-licensed Python package for manipulation and analysis of planar geometric objects. It is based on the widely deployed GEOS (the engine of PostGIS) and JTS (from which GEOS is ported) libraries.
Siesta		4.1.5	Desc SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
Singularity		2.3.1, 2.4.2, 2.6.1, 3.5.3	Desc Singularity is a portable application stack packaging and runtime utility.
Sphinx		1.8.1-Python-3.6.6	Desc Sphinx is a tool that makes it easy to create intelligent and beautiful documentation. It was originally created for the new Python documentation, and it has excellent facilities for the documentation of Python projects, but C/C+ + is already supported as well, and it is planned to add special support for other languages as well.
Spyder		3.3.6-Python-3.6.6, 4.1.5-Python-3.7.4, 5.1.5	Desc Spyder is an interactive Python development environment providing MATLAB-like features in a simple and light-weighted software.
Subversion		1.12.0, 1.14.1	Desc Subversion is an open source version control system.
SuiteSparse		4.4.5-METIS-5.1.0, 4.5.3-METIS-5.1.0, 5.1.2-METIS-5.1.0, 5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0, 5.13.0-METIS-5.1.0	Desc SuiteSparse is a collection of libraries manipulate sparse matrices.
Tcl		8.6.4, 8.6.5, 8.6.6, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13	Desc Tcl (Tool Command Language) is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more.
Tecplot360ex		2021.1	Desc Quickly plot and animate your CFD results exactly the way you want. Analyze complex solutions, arrange multiple layouts, and communicate your results with professional images and animations.
TensorFlow		1.2.0-Python-3.5.1, 1.4.0-Python-3.5.1, 1.12.0-Python-2.7.15, 1.12.0-Python-3.6.6, 1.15.2-Python-3.7.4, 2.1.0-Python-3.7.4, 2.2.0-Python-3.7.4, 2.3.1-Python-3.7.4, 2.4.1, 2.5.0, 2.8.4-CUDA-11.4.1	Desc An open-source software library for Machine Intelligence
TensorRT		4.0.1.6-Python-2.7.15	Desc NVIDIA TensorRT is a platform for high-performance deep learning inference
Theano		1.0.4-Python-3.7.4	Desc Theano is a Python library that allows you to define, optimize, and evaluate mathematical expressions involving multi-dimensional arrays efficiently.
Tk		8.6.4-no-X11, 8.6.5, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12	Desc Tk is an open source, cross-platform widget toolchain that provides a library of basic elements for building a graphical user interface (GUI) in many different programming languages.
Tkinter		3.7.2	Desc Tkinter module, built with the Python buildsystem
TurboVNC		2.1.2, 2.2.1	Desc TurboVNC is a derivative of VNC (Virtual Network Computing) that is tuned to provide peak performance for 3D and video workloads.
UCX		1.11.2	Desc Unified Communication X An open-source production grade communication framework for data centric and high-performance applications
VMD		1.9.3-Python-2.7.11, 1.9.3-Python-2.7.15, 1.9.4a51	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.
VSEARCH		2.8.0, 2.9.1, 2.22.1	Desc VSEARCH supports de novo and reference based chimera detection, clustering, full-length and prefix dereplication, rereplication, reverse complementation, masking, all-vs-all pairwise global alignment, exact and global alignment searching, shuffling, subsampling and sorting. It also supports FASTQ file analysis, filtering, conversion and merging of paired-end reads.
VTK		5.4.2, 6.3.0-Python-2.7.11, 7.0.0-Python-2.7.11, 8.1.1-Python-2.7.15, 9.0.1, 9.1.0	Desc The Visualization Toolkit (VTK) is an open-source, freely available software system for 3D computer graphics, image processing and visualization. VTK consists of a C+ + class library and several interpreted interface layers including Tcl/Tk, Java, and Python. VTK supports a wide variety of visualization algorithms including: scalar, vector, tensor, texture, and volumetric methods; and advanced modeling techniques such as: implicit modeling, polygon reduction, mesh smoothing, cutting, contouring, and Delaunay triangulation.
VTune		2016_update3, 2019_update3, 2022.3.0, 2023.2.0	Desc Intel VTune Amplifier XE is the premier performance profiler for C, C+ +, C#, Fortran, Assembly and Java. - Homepage: http://software.intel.com/en-us/intel-vtune-amplifier-xe

Modules	Documentation	Versions	Description
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools
VirtualGL		2.5.2, 2.6.2, 2.6.4	Desc VirtualGL is an open source toolkit that gives any Linux or Unix remote display software the ability to run OpenGL applications with full hardware acceleration.
Voro+ +		Voro+ 0.4.6	Desc Voro+ + is a software library for carrying out three-dimensional computations of the Voronoi tessellation. A distinguishing feature of the Voro+ + library is that it carries out cell-based calculations, computing the Voronoi cell for each particle individually. It is particularly well-suited for applications that rely on cell-based statistics, where features of Voronoi cells (eg. volume, centroid, number of faces) can be used to analyze a system of particles.
WPS		4.4-dmpar	Desc WRF Preprocessing System (WPS) for WRF. The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
WRF		4.4.1-dmpar	Desc The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
X11		20200222	Desc The X Window System (X11) is a windowing system for bitmap displays
Xvfb		1.20.8	Desc Xvfb is an X server that can run on machines with no display hardware and no physical input devices. It emulates a dumb framebuffer using virtual memory.
YACS		0.1.8	Desc YACS was created as a lightweight library to define and manage system configurations, such as those commonly found in software designed for scientific experimentation. These “configurations” typically cover concepts like hyperparameters used in training a machine learning model or configurable model hyperparameters, such as the depth of a convolutional neural network.
Z3		4.12.2, 4.13.0	Desc Z3 is a theorem prover from Microsoft Research.
ZeroMQ		4.1.4, 4.2.5, 4.3.2, 4.3.3	Desc ZeroMQ looks like an embeddable networking library but acts like a concurrency framework. It gives you sockets that carry atomic messages across various transports like in-process, inter-process, TCP, and multicast. You can connect sockets N-to-N with patterns like fanout, pub-sub, task distribution, and request-reply. It's fast enough to be the fabric for clustered products. Its asynchronous I/O model gives you scalable multicore applications, built as asynchronous message-processing tasks. It has a score of language APIs and runs on most operating systems.
arpack-ng		3.3.0, 3.5.0, 3.7.0, 3.8.0, 3.9.1	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
at-spi2-atk		2.34.1, 2.38.0	Desc AT-SPI 2 toolkit bridge
at-spi2-core		2.34.0, 2.38.0, 2.46.0	Desc Assistive Technology Service Provider Interface.
cURL		7.47.0, 7.49.1, 7.55.1, 7.60.0, 7.66.0, 7.69.1, 7.72.0, 7.76.0, 7.78.0, 7.86.0, 8.3.0	Desc libcurl is a free and easy-to-use client-side URL transfer library, supporting DICT, FILE, FTP, FTPS, Gopher, HTTP, HTTPS, IMAP, IMAPS, LDAP, LDAPS, POP3, POP3S, RTMP, RTSP, SCP, SFTP, SMTP, SMTPS, Telnet and TFTP. libcurl supports SSL certificates, HTTP POST, HTTP PUT, FTP uploading, HTTP form based upload, proxies, cookies, user+password authentication (Basic, Digest, NTLM, Negotiate, Kerberos), file transfer resume, http proxy tunneling and more.
cairo		1.14.6	Desc Cairo is a 2D graphics library with support for multiple output devices. Currently supported output targets include the X Window System (via both Xlib and XCB), Quartz, Win32, image buffers, PostScript, PDF, and SVG file output. Experimental backends include OpenGL, BeOS, OS/2, and DirectFB
ccpnmr		2.4.2-Python-2.7.11	Desc CcpNmr Analysis is a graphics-based interactive NMR spectrum visualisation, resonance assignment and data analysis program
cffi		1.15.1	Desc C Foreign Function Interface for Python. Interact with almost any C code from Python, based on C-like declarations that you can often copy-paste from header files or documentation.
cryptography		41.0.5	Desc cryptography is a package designed to expose cryptographic primitives and recipes to Python developers.
cuDNN		7.1.4.18, 7.6.4.38, 8.0.4.30-CUDA-11.1.1, 8.2.2.26-CUDA-11.4.1, 8.5.0.96-CUDA-11.7.0, 8.8.0.121-CUDA-12.0.0, 8.9.7.29-CUDA-12.3.0, 9.1.1.17-CUDA-12.4.0	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		0.19.4-Python-3.6.6, 2.8.0-Python-3.7.4, 2021.2.0	Desc Dask natively scales Python. Dask provides advanced parallelism for analytics, enabling performance at scale for the tools you love.
flatbuffers		1.12.0	Desc FlatBuffers: Memory Efficient Serialization Library
flit		3.9.0	Desc A simple packaging tool for simple packages.
foss		2016a, 2016b, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.

Modules	Documentation	Versions	Description
fosscuda		2018b, 2019a, 2019b, 2020b	Desc GCC based compiler toolchain with CUDA support, and including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
futile		1.8.3	Desc The FUTILE project (Fortran Utilities for the Treatment of Innermost Level of Executables) is a set of modules and wrapper that encapsulate the most common low-level operations of a Fortran code.
gappa		0.8.0	Desc gappa is a collection of commands for working with phylogenetic data. Its main focus are evolutionary placements of short environmental sequences on a reference phylogenetic tree. Such data is typically produced by tools like EPA-ng, RAxML-EPA or pplacer and usually stored in jplace files.
gcccuda		2018b, 2019a, 2019b, 2020b	Desc GNU Compiler Collection (GCC) based compiler toolchain, along with CUDA toolkit.
geopandas		0.7.0-Python-3.7.4, 0.8.2	Desc GeoPandas is a project to add support for geographic data to pandas objects. It currently implements GeoSeries and GeoDataFrame types which are subclasses of pandas.Series and pandas.DataFrame respectively. GeoPandas objects can act on shapely geometry objects and perform geometric operations.
gfbf		2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including FlexiBLAS (BLAS and LAPACK support) and (serial) FFTW.
git		2.8.0, 2.16.1, 2.23.0-nodocs, 2.28.0-nodocs, 2.32.0-nodocs, 2.33.1-nodocs, 2.38.1-nodocs, 2.42.0	Desc Git is a free and open source distributed version control system designed to handle everything from small to very large projects with speed and efficiency.
gmpy2		2.1.5	Desc GMP/MPIR, MPFR, and MPC interface to Python 2.6+ and 3.x
gnuplot		4.6.0, 5.0.3, 5.2.5, 5.2.8, 5.4.1, 5.4.2, 5.4.6	Desc Portable interactive, function plotting utility
gompi		2016a, 2016b, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021a, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support.
gompic		2018b, 2019a, 2019b, 2020b	Desc GNU Compiler Collection (GCC) based compiler toolchain along with CUDA toolkit, including OpenMPI for MPI support with CUDA features enabled.
graph-tool		2.22-Python-3.5.2	Desc Graph-tool is an efficient Python module for manipulation and statistical analysis of graphs (a.k.a. networks). Contrary to most other python modules with similar functionality, the core data structures and algorithms are implemented in C+ +, making extensive use of template metaprogramming, based heavily on the Boost Graph Library. This confers it a level of performance that is comparable (both in memory usage and computation time) to that of a pure C/C+ + library.
h5py		2.6.0-Python-2.7.11, 2.8.0-Python-2.7.15, 2.8.0-Python-3.6.6, 2.10.0-Python-3.7.4, 3.1.0, 3.6.0	Desc HDF5 for Python (h5py) is a general-purpose Python interface to the Hierarchical Data Format library, version 5. HDF5 is a versatile, mature scientific software library designed for the fast, flexible storage of enormous amounts of data.
hatchling		1.18.0	Desc Extensible, standards compliant build backend used by Hatch, a modern, extensible Python project manager.
horton		2.0.0-Python-2.7.11	Desc Horton is a development platform for electronic structure methods.
hypothesis		4.5.0-Python-3.6.6, 4.44.2-Python-3.7.4, 5.41.2, 5.41.5, 6.14.6, 6.68.2, 6.90.0	Desc Hypothesis is an advanced testing library for Python. It lets you write tests which are parametrized by a source of examples, and then generates simple and comprehensible examples that make your tests fail. This lets you find more bugs in your code with less work.
iTensor		3.1.11	Desc An efficient and flexible C+ + library for performing tensor network calculations
icc		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc C and C+ + compiler from Intel
iccifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32, 2019.5.281, 2020.1.217	Desc Intel C, C+ + and Fortran compilers
ifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc Fortran compiler from Intel
iimpi		7.2.3-GCC-4.9.2, 8.1.5-GCC-4.9.3-2.25, 2016b, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel C/C+ + and Fortran compilers, alongside Intel MPI.
imkl		11.2.1.133, 11.3.1.150, 11.3.3.210, 2018.3.222, 2019.3.199, 2019.5.281, 2020.1.217, 2021.2.0, 2022.2.1, 2023.2.0	Desc Intel oneAPI Math Kernel Library

Modules	Documentation	Versions	Description
imkl-FFTW		2022.2.1, 2023.2.0	Desc FFTW interfaces using Intel oneAPI Math Kernel Library
impi		5.0.2.044, 5.1.2.150, 5.1.3.181, 2018.3.222, 2018.5.288, 2019.3.199, 2019.7.217, 2021.2.0, 2021.7.1, 2021.10.0	Desc The Intel(R) MPI Library for Linux* OS is a multi-fabric message passing library based on ANL MPICH2 and OSU MVAPICH2. The Intel MPI Library for Linux OS implements the Message Passing Interface, version 3.0 (MPI-3) specification.
intel		2015a, 2016a, 2016b, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel Cluster Toolkit Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MPI & Intel MKL.
intel-compilers		2021.2.0, 2022.2.1, 2023.2.1	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)
iomkl		2016b	Desc Intel Cluster Toolchain Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MKL & OpenMPI.
iompi		2016b	Desc Toolchain with Intel C, C+ + and Fortran compilers, alongside OpenMPI.
ipp		9.0.4.258, 2019.3.199	Desc Intel Integrated Performance Primitives (Intel IPP) is an extensive library of multicore-ready, highly optimized software functions for multimedia, data processing, and communications applications. Intel IPP offers thousands of optimized functions covering frequently used fundamental algorithms.
itac		9.1.2.024, 2019.3.032, 2021.10.0	Desc The Intel Trace Collector is a low-overhead tracing library that performs event-based tracing in applications. The Intel Trace Analyzer provides a convenient way to monitor application activities gathered by the Intel Trace Collector through graphical displays.
json-c		0.16	Desc JSON-C implements a reference counting object model that allows you to easily construct JSON objects in C, output them as JSON formatted strings and parse JSON formatted strings back into the C representation of JSON objects.
lammps		11Aug17-Python-2.7.11-mpi, 11Aug17-Python-2.7.11, 14May16-Python-2.7.11-mpi, 14May16-Python-2.7.11	Desc LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers.
libAfterImage		1.20	Desc libAfterImage is a generic image manipulation library
libarchive		3.4.2	Desc Multi-format archive and compression library
libfabric		1.13.2	Desc Libfabric is a core component of OFI. It is the library that defines and exports the user-space API of OFI, and is typically the only software that applications deal with directly. It works in conjunction with provider libraries, which are often integrated directly into libfabric.
libgpuarray		0.7.6-Python-3.7.4	Desc Library to manipulate tensors on the GPU.
libopus		1.3.1	Desc Opus is a totally open, royalty-free, highly versatile audio codec. Opus is unmatched for interactive speech and music transmission over the Internet, but is also intended for storage and streaming applications. It is standardized by the Internet Engineering Task Force (IETF) as RFC 6716 which incorporated technology from Skype's SILK codec and Xiph.Org's CELT codec.
libsigc+ +		libsigc+ 2.4.1	Desc The libsigc+ + package implements a typesafe callback system for standard C+ +.
libsodium		1.0.8, 1.0.16	Desc Sodium is a modern, easy-to-use software library for encryption, decryption, signatures, password hashing and more.
lmod		lmod	Desc Lmod: An Environment Module System
magma		2.5.0, 2.5.1, 2.5.4, 2.7.1-CUDA-12.0.0, 2.7.2-CUDA-12.4.0	Desc The MAGMA project aims to develop a dense linear algebra library similar to LAPACK but for heterogeneous/hybrid architectures, starting with current Multicore+GPU systems.
make		4.3, 4.4.1	Desc GNU version of make utility
matplotlib		1.4.3-Python-2.7.11, 1.5.1-Python-2.7.11, 1.5.1-Python-3.4.3, 1.5.1-Python-3.5.1, 1.5.1-Python-3.5.2, 2.0.2-Python-3.5.1, 2.0.2-Python-3.6.1, 3.0.0-Python-3.6.6, 3.0.3-Python-3.7.2, 3.1.1-Python-3.7.4, 3.2.1-Python-3.8.2, 3.3.3, 3.4.3	Desc matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell, web application servers, and six graphical user interface toolkits.
meson-python		0.15.0	Desc Python build backend (PEP 517) for Meson projects
molmod		1.4.5-Python-3.7.4	Desc MolMod is a Python library with many compoments that are useful to write molecular modeling programs.
mpi4py		2.0.0-Python-2.7.11, 3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.0.3-Python-3.8.2, 3.1.4	Desc MPI for Python (mpi4py) provides bindings of the Message Passing Interface (MPI) standard for the Python programming language, allowing any Python program to exploit multiple processors.
mpifileutils	mpiFileUtils	0.10.1, 0.11, 0.11.1	Desc MPI-Based File Utilities For Distributed Systems
mpmath		0.19-Python-2.7.11	Desc mpmath can be used as an arbitrary-precision substitute for Python's float/complex types and math/cmath modules, but also does much more advanced mathematics. Almost any calculation can be performed just as well at 10-digit or 1000-digit precision, with either real or complex numbers, and in many cases mpmath implements efficient algorithms that scale well for extremely high precision work.
ncview		2.1.8	Desc Ncview is a visual browser for netCDF format files. Typically you would use ncview to get a quick and easy, push-button look at your netCDF files. You can view simple movies of the data, view along various dimensions, take a look at the actual data values, change color maps, invert the data, etc.

Modules	Documentation	Versions	Description
netCDF		4.4.0, 4.4.1, 4.6.1, 4.7.1, 4.7.4, 4.8.0, 4.8.1, 4.9.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
netCDF-Fortran		4.4.3, 4.4.4, 4.5.3, 4.6.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
nettle		3.2	Desc Nettle is a cryptographic library that is designed to fit easily in more or less any context: In crypto toolkits for object-oriented languages (C+ +, Python, Pike, ...), in applications like LSH or GNUPG, or even in kernel space.
networkx		1.10-Python-2.7.11, 2.2-Python-3.5.1, 2.4-Python-3.7.4, 2.5, 2.6.3, 3.0, 3.2.1	Desc NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.
nlohmann_json		3.11.2	Desc JSON for Modern C+ +
nsync		1.24.0	Desc nsync is a C library that exports various synchronization primitives, such as mutexes
numba		0.53.1	Desc Numba is an Open Source NumPy-aware optimizing compiler for Python sponsored by Continuum Analytics, Inc. It uses the remarkable LLVM compiler infrastructure to compile Python syntax to machine code.
numpy		1.8.2-Python-2.7.11, 1.9.2-Python-2.7.11, 1.10.1-Python-2.7.11, 1.10.1-Python-3.4.3, 1.10.1-Python-3.5.1, 1.13.0-Python-3.5.1, 1.18.5-Python-3.7.4, 1.18.5-Python-3.8.2	Desc NumPy is the fundamental package for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C+ + and Fortran code, useful linear algebra, Fourier transform, and random number capabilities. Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases.
parallel		20190922, 20210322	Desc parallel: Build and execute shell commands in parallel
pcp		2.0.0_39-Python-2.7.16	Desc A parallel copy program for lustre
phenix		1.10.1-2155	Desc PHENIX is a software suite for the automated determination of molecular structures using X-ray crystallography and other methods.
pigz		2.6	Desc pigz, which stands for parallel implementation of gzip, is a fully functional replacement for gzip that exploits multiple processors and multiple cores to the hilt when compressing data. pigz was written by Mark Adler, and uses the zlib and pthread libraries.
pkgconf		1.8.0, 1.9.3, 2.0.3	Desc pkgconf is a program which helps to configure compiler and linker flags for development libraries. It is similar to pkg-config from freedesktop.org.
poetry		1.6.1	Desc Python packaging and dependency management made easy. Poetry helps you declare, manage and install dependencies of Python projects, ensuring you have the right stack everywhere.
protobuf		3.2.0, 3.4.0	Desc Google Protocol Buffers
protobuf-python		3.2.0-Python-3.5.1, 3.4.0-Python-3.5.1, 3.10.0-Python-3.7.4	Desc Python Protocol Buffers runtime library.
psutil		5.6.3-Python-3.6.6, 5.9.4	Desc A cross-platform process and system utilities module for Python
pytest		7.1.3	Desc pytest: simple powerful testing with Python
qutip		2.2.0-Python-2.7.11, 3.1.0-Python-2.7.11, 4.0.2-Python-3.4.3	Desc QuTiP : Quantum Toolbox in Python
rioxarray		0.1.1-Python-3.7.4	Desc geospatial xarray extension powered by rasterio
scikit-build		0.17.2, 0.17.6	Desc Scikit-Build, or skbuild, is an improved build system generator for CPython C/C+ +/Fortran/Cython extensions.
scikit-image		0.12.3-Python-3.5.1, 0.14.1-Python-3.6.6, 0.14.5-Python-3.6.6, 0.16.2-Python-3.7.4, 0.18.1	Desc scikit-image is a collection of algorithms for image processing.
scikit-learn		0.18.1-Python-3.5.1, 0.20.0-Python-3.6.6, 0.20.3-Python-3.6.6, 0.21.3-Python-3.7.4, 0.23.2	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-umfpack		0.2.1-Python-2.7.11	Desc scikit-umfpack provides a wrapper of UMFPACK sparse direct solver to SciPy.
scipy		0.16.1-Python-2.7.11, 0.17.1-Python-2.7.11, 0.17.1-Python-3.4.3, 0.19.1-Python-3.5.1, 1.4.1-Python-3.7.4	Desc SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension for Python.
settarg		settarg	Desc
setuptools-rust		1.8.0	Desc setuptools-rust is a plugin for setuptools to build Rust Python extensions implemented with PyO3 or rust-cpython.
sparsehash		2.0.2	Desc An extremely memory-efficient hash_map implementation. 2 bits/entry overhead! The SparseHash library contains several hash-map implementations, including implementations that optimize for space or speed.

Modules	Documentation	Versions	Description
sympy		1.0-Python-2.7.11, 1.12	Desc SymPy is a Python library for symbolic mathematics. It aims to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries.
tbb		4.4.6.258, 2019_U9, 2019.2.187, 2020.3, 2021.10.0	Desc Intel Threading Building Blocks 4.0 (Intel TBB) is a widely used, award-winning C+ + template library for creating reliable, portable, and scalable parallel applications. Use Intel TBB for a simple and rapid way of developing robust task-based parallel applications that scale to available processor cores, are compatible with multiple environments, and are easier to maintain. Intel TBB is the most proficient way to implement future-proof parallel applications that tap into the power and performance of multicore and manycore hardware platforms.
texlive		20200406, 20210324, 20240312	Desc TeX is a typesetting language. Instead of visually formatting your text, you enter your manuscript text intertwined with TeX commands in a plain text file. You then run TeX to produce formatted output, such as a PDF file. Thus, in contrast to standard word processors, your document is a separate file that does not pretend to be a representation of the final typeset output, and so can be easily edited and manipulated.
torchvision		0.14.1-PyTorch-1.13.1-CUDA-12.0.0	Desc Datasets, Transforms and Models specific to Computer Vision
typing-extensions		3.7.4.3	Desc Typing Extensions – Backported and Experimental Type Hints for Python
utf8proc		2.2.0	Desc utf8proc is a small, clean C library that provides Unicode normalization, case-folding, and other operations for data in the UTF-8 encoding.
virtualenv		20.24.6	Desc A tool for creating isolated virtual python environments.
wheel		0.29.0-Python-3.5.1, 0.31.1-Python-2.7.15, 0.31.1-Python-3.6.6	Desc A built-package format for Python.
xtb		6.4.1, 6.5.1, 6.6.1	Desc xtb - An extended tight-binding semi-empirical program package.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

Haswell(AVX2)

Installed software as of Wed, 23 Oct 2024 07:35:11 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	6.14-2, 2016, 2017-hotfix-1819, 2017, 2018, 2019-hotfix-1939, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341	Desc Finite Element Analysis software for modeling, visualization and best-in-class implicit and explicit dynamics FEA.
AMPL-MP		3.1.0	Desc An open-source library for mathematical programming.
ANSYS	ANSYS / CFX	15.0, 16.0, 16.2, 17.2, 18.0, 18.2, 19.0, 19.2, 19.3, 2019.2, 2019.3, 2020.1, 2020.2, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ANSYSEM		17.2, 18.0, 18.1, 18.2, 19.0, 19.1, 20.2, 2022.2, 2023.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ARIA		2.3.1-Python-2.7.11	Desc ARIA (Ambiguous Restraints for Iterative Assignment) is a software for automated NOE assignment and NMR structure calculation
ASE		3.12.0-Python-2.7.11, 3.16.0-Python-2.7.11, 3.16.2-Python-3.6.6, 3.21.1	Desc ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language. From version 3.20.1 we also include the ase-ext package, it contains optional reimplementations in C of functions in ASE. ASE uses it automatically when installed.
ATK		2.20.0	Desc ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications. - Homepage: https://developer.gnome.org/ATK/stable/
ATSAS		2.7.2-5.el6.x86_64	Desc ATSAS is a program suite for small-angle scattering data analysis from biological macromolecules. - Homepage: http://www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html
Advisor		2016_update3, 2019_update3, 2023.2.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain - Homepage: https://software.intel.com/intel-advisor-xe
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		14-AmberTools-15-patchlevel-0-0, 18-AmberTools-18-patchlevel-9-5-CUDA	Desc Amber (originally Assisted Model Building with Energy Refinement) is software for performing molecular dynamics and structure prediction.
Armadillo		11.4.3	Desc Armadillo is an open-source C+ + linear algebra library (matrix maths) aiming towards a good balance between speed and ease of use. Integer, floating point and complex numbers are supported, as well as a subset of trigonometric and statistics functions.
BLAST+		2.2.31-Python-2.7.11	Desc Basic Local Alignment Search Tool, or BLAST, is an algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences. - Homepage: http://blast.ncbi.nlm.nih.gov/
BLIS		0.8.1, 0.9.0	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
BWA		0.7.17	Desc Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome.

Modules	Documentation	Versions	Description
Bazel		0.5.2, 0.7.0, 0.18.0, 2.0.0, 3.4.1, 3.7.2, 4.2.2, 6.3.1	Desc Bazel is a build tool that builds code quickly and reliably. It is used to build the majority of Google's software.
Biopython		1.71-Python-2.7.11, 1.78	Desc Biopython is a set of freely available tools for biological computation written in Python by an international team of developers. It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics.
Bonnie+ +		Bonnie+ 1.97	Desc Bonnie+ +-1.97: Enhanced performance Test of Filesystem I/O - Homepage: http://www.coker.com.au/bonnie+ +/
Boost		1.47.0, 1.58.0-Python-2.7.11, 1.59.0-Python-2.7.11, 1.60.0-Python-2.7.11, 1.60.0, 1.61.0-Python-2.7.11, 1.61.0, 1.63.0-Python-3.5.2, 1.66.0, 1.67.0, 1.68.0-Python-2.7.15, 1.71.0, 1.74.0, 1.77.0, 1.81.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Boost.Python		1.67.0-Python-2.7.15	Desc Boost.Python is a C+ + library which enables seamless interoperability between C+ + and the Python programming language.
Brunsli		0.1	Desc Brunsli is a lossless JPEG repacking library.
CFITSIO		3.38, 3.45, 4.2.0	Desc CFITSIO is a library of C and Fortran subroutines for reading and writing data files in FITS (Flexible Image Transport System) data format.
CGAL		4.7-Python-2.7.11, 4.8-Python-2.7.11, 4.8.1-Python-3.5.2, 4.8.1, 4.11.1-Python-2.7.15, 4.14.1-Python-3.7.4, 4.14.3, 5.2	Desc The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C+ + library.
CGNS		2.5.5, 3.3.1	Desc The CGNS system is designed to facilitate the exchange of data between sites and applications, and to help stabilize the archiving of aerodynamic data.
CLooG		0.18.1	Desc CLooG is a free software and library to generate code for scanning Z-polyhedra. That is, it finds a code (e.g. in C, FORTRAN...) that reaches each integral point of one or more parameterized polyhedra. CLooG has been originally written to solve the code generation problem for optimizing compilers based on the polytope model. Nevertheless it is used now in various area e.g. to build control automata for high-level synthesis or to find the best polynomial approximation of a function. CLooG may help in any situation where scanning polyhedra matters. While the user has full control on generated code quality, CLooG is designed to avoid control overhead and to produce a very effective code. - Homepage: http://www.bastoul.net/cloog/index.php
CMake		2.8.4, 3.4.1, 3.4.3, 3.5.2, 3.6.1, 3.7.1, 3.9.6, 3.11.4, 3.12.1, 3.15.3, 3.16.4, 3.18.4, 3.20.1, 3.21.1, 3.22.1, 3.24.3, 3.27.6	Desc CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software. - Homepage: http://www.cmake.org
CNS		1.3-haddock-2.2, 1.3-haddock-2.4, 1.21-aria2.3	Desc Crystallography & NMR System (CNS) has been designed to provide a flexible multi-level hierachical approach for the most commonly used algorithms in macromolecular structure determination
COMSOL	COMSOL	5.1, 5.2, 5.4, 5.5, 5.6, 6.0, 6.1, 6.2	Desc COMSOL Multiphysics is a finite element analysis, solver and simulation software/FEA software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. - Homepage: https://www.comsol.com/
CPMD	CPMD	4.1, 4.3-omp, 4.3	Desc CPMD The CPMD code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. - Homepage: http://www.cpmd.org/
CREST		2.11.2, 2.12	Desc CREST is an utility/driver program for the xtb program. Originally it was designed as conformer sampling program, hence the abbreviation Conformer–Rotamer Ensemble Sampling Tool, but now offers also some utility functions for calculations with the GFNn–xTB methods. Generally the program functions as an IO based OMP scheduler (i.e., calculations are performed by the xtb program) and tool for the creation and analysation of structure ensembles.
CRYSTAL14		1.0.4	Desc Crystal is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations - Homepage: http://www.crystalsolutions.eu/
CUDA		7.5.18, 8.0.44, 9.2.88, 11.1.1, 11.4.1, 11.7.0, 12.0.0, 12.3.0, 12.3.2, 12.4.0	Desc CUDA (formerly Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. CUDA gives developers access to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs.
CheMPS2		1.8.11	Desc CheMPS2 is a scientific library which contains a spin-adapted implementation of the density matrix renormalization group (DMRG) for ab initio quantum chemistry.
Clang		9.0.1, 16.0.4	Desc C, C+ +, Objective-C compiler, based on LLVM. Does not include C+ + standard library – use libstdc+ + from GCC.
CoordgenLibs		3.0.0	Desc Schrodinger-developed 2D Coordinate Generation
Cython		0.24-Python-2.7.11, 0.24-Python-3.4.3, 0.29.22	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
DMTCP		2.6.0	Desc DMTCP is a tool to transparently checkpoint the state of multiple simultaneous applications, including multi-threaded and distributed applications. It operates directly on the user binary executable, without any Linux kernel modules or other kernel modifications.
DendroPy		4.5.2	Desc A Python library for phylogenetics and phylogenetic computing: reading, writing, simulation, processing and manipulation of phylogenetic trees (phylogenies) and characters.
Doxygen		1.8.11	Desc Doxygen is a documentation system for C+ +, C, Java, Objective-C, Python, IDL (Corba and Microsoft flavors), Fortran, VHDL, PHP, C#, and to some extent D.
ELPA		2021.05.001	Desc Eigenvalue SoLvers for Petaflop-Applications .
EPA-ng		0.3.8	Desc EPA-ng - Fast, parallel, highly accurate Maximum Likelihood Phylogenetic Placement of genetic sequences on a user-supplied reference tree and alignment
EasyBuild-custom		1.0	Desc EasyBuild is a software build and installation framework - Homepage: http://hpcugent.github.com/easybuild/
Eigen		3.2.9, 3.3.4, 3.3.7, 3.3.8, 3.3.9, 3.4.0	Desc Eigen is a C+ + template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
FDS		6.4.0, 6.5.2, 6.6.0, 6.7.3, 6.7.4	Desc Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires. - Homepage: http://firemodels.github.io/fds-smv/
FEKO	FEKO	2017.2_hw, 2017.2.5_hw, 2018_hw, 2019_hw, 2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering
FFTW		3.3.4-PFFT-20150905, 3.3.4, 3.3.6, 3.3.8, 3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FFTW.MPI		3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FLANN		1.8.4-Python-2.7.15	Desc FLANN is a library for performing fast approximate nearest neighbor searches in high dimensional spaces.
Fiona		1.8.13-Python-3.7.4, 1.8.20	Desc Fiona is designed to be simple and dependable. It focuses on reading and writing data in standard Python IO style and relies upon familiar Python types and protocols such as files, dictionaries, mappings, and iterators instead of classes specific to OGR. Fiona can read and write real-world data using multi-layered GIS formats and zipped virtual file systems and integrates readily with other Python GIS packages such as pyproj, Rtree, and Shapely.
FlexiBLAS		3.0.4, 3.2.1, 3.3.1	Desc FlexiBLAS is a wrapper library that enables the exchange of the BLAS and LAPACK implementation used by a program without recompiling or relinking it.

Modules	Documentation	Versions	Description
Flux		2019	Desc Altair Flux captures the complexity of electromagnetic and thermal phenomena to predict the behavior of future products with precision.
FriBidi		1.0.5, 1.0.10, 1.0.12	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		24.5.4, 24.5.6_nhus, 24.7.4_nhus, 24.7.4, 26.1.0_nhus, 26.1.0, 30.3.0, 45.7.0, 46.5.0	Desc The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. - Homepage: https://www.gams.com/
GCC		4.8.3, 4.9.2, 4.9.3-binutils-2.25, 4.9.3-2.25, 5.3.0-2.26, 5.4.0-2.26, 6.3.0-2.27, 6.4.0-2.28, 7.3.0-2.30, 8.3.0, 9.3.0, 10.2.0, 10.3.0, 11.2.0, 12.2.0, 13.2.0	Desc The GNU Compiler Collection includes front ends for C, C+ +, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc+ +, libgcj,...).
GDB		9.1-Python-3.7.4	Desc The GNU Project Debugger
GEOS		3.6.1-Python-2.7.12	Desc GEOS (Geometry Engine - Open Source) is a C+ + port of the Java Topology Suite (JTS)
GMP		6.1.0, 6.1.1, 6.1.2, 6.2.0, 6.2.1	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers. - Homepage: http://gmplib.org/
GNUGo		3.8	Desc GNU Go is a free program that plays the game of Go
GObject-Introspection		1.47.1	Desc GObject introspection is a middleware layer between C libraries (using GObject) and language bindings. The C library can be scanned at compile time and generate a metadata file, in addition to the actual native C library. Then at runtime, language bindings can read this metadata and automatically provide bindings to call into the C library. - Homepage: https://wiki.gnome.org/GObjectIntrospection/
GPAW		1.1.0-Python-2.7.11, 1.4.0-Python-2.7.11, 1.4.0-Python-3.6.6	Desc GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.
GROMACS		5.1.2-hybrid, 2016.5-hybrid, 2018.4, 2019	Desc GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.
GSL		1.16, 2.1, 2.5, 2.6, 2.7	Desc The GNU Scientific Library (GSL) is a numerical library for C and C+ + programmers. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting.
GST-plugins-base		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/
GStreamer		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/
GTK+		2.24.30	Desc The GTK+ 2 package contains libraries used for creating graphical user interfaces for applications. - Homepage: https://developer.gnome.org/gtk+/stable/
GTK3		3.24.35	Desc GTK+ is the primary library used to construct user interfaces in GNOME. It provides all the user interface controls, or widgets, used in a common graphical application. Its object-oriented API allows you to construct user interfaces without dealing with the low-level details of drawing and device interaction.
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g09.D01, g09.E01, g16.A03, g16.B01	Desc Gaussian provides state-of-the-art capabilities for electronic structure modeling.
GitPython		2.1.11-Python-3.6.6	Desc GitPython is a python library used to interact with Git repositories
Go		1.16.6	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
GraphicsMagick		1.3.23	Desc GraphicsMagick is the swiss army knife of image processing.
Graphviz		2.50.0	Desc Graphviz is open source graph visualization software. Graph visualization is a way of representing structural information as diagrams of abstract graphs and networks. It has important applications in networking, bioinformatics, software engineering, database and web design, machine learning, and in visual interfaces for other technical domains.
Guile		1.8.8	Desc Guile is a programming language, designed to help programmers create flexible applications that can be extended by users or other programmers with plug-ins, modules, or scripts.
Gurobi		6.5.0, 7.0.2, 7.5.2, 8.1.0, 9.0.1, 9.1.2, 9.5.0, 11.0.0	Desc The Gurobi Optimizer is a state-of-the-art solver for mathematical programming. The solvers in the Gurobi Optimizer were designed from the ground up to exploit modern architectures and multi-core processors, using the most advanced implementations of the latest algorithms.
HADDOCK		2.2-Python-2.7.11, 2.4-Python-2.7.16	Desc HADDOCK (High Ambiguity Driven biomolecular DOCKing) is an information-driven flexible docking approach for the modelling of biomolecular complexes
HDF		4.2.15	Desc HDF (also known as HDF4) is a library and multi-object file format for storing and managing data between machines.
HDF5		1.8.16-serial, 1.8.16, 1.8.17, 1.10.2, 1.10.5, 1.10.6, 1.10.7, 1.12.1, 1.14.0	Desc HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.
HDFView		2.14-Java-1.8.0_152-centos7	Desc HDFView is a visual tool for browsing and editing HDF4 and HDF5 files.
HH-suite		3.3.0	Desc The HH-suite is an open-source software package for sensitive protein sequence searching based on the pairwise alignment of hidden Markov models (HMMs).
HMMER		3.2.1, 3.3.2	Desc HMMER is used for searching sequence databases for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs). Compared to BLAST, FASTA, and other sequence alignment and database search tools based on older scoring methodology, HMMER aims to be significantly more accurate and more able to detect remote homologs because of the strength of its underlying mathematical models. In the past, this strength came at significant computational expense, but in the new HMMER3 project, HMMER is now essentially as fast as BLAST.
HPL		2.2	Desc HPL is a software package that solves a (random) dense linear system in double precision (64 bits) arithmetic on distributed-memory computers. It can thus be regarded as a portable as well as freely available implementation of the High Performance Computing Linpack Benchmark.
Hadoop-cluster		1.0	Desc Framework for deploying Hadoop clusters on traditional HPC - Homepage: http://luis.uni-hannover.de
Highway		1.0.3	Desc Highway is a C+ + library for SIMD (Single Instruction, Multiple Data), i.e. applying the same operation to 'lanes'.
ICU		61.1, 64.2, 67.1, 69.1, 72.1	Desc ICU is a mature, widely used set of C/C+ + and Java libraries providing Unicode and Globalization support for software applications.
IPython		3.2.3-Python-2.7.11, 6.2.1-Python-3.6.4, 7.2.0-Python-3.6.6, 7.9.0-Python-3.7.4, 7.18.1-Python-3.7.4, 7.25.0	Desc IPython provides a rich architecture for interactive computing with: Powerful interactive shells (terminal and Qt-based). A browser-based notebook with support for code, text, mathematical expressions, inline plots and other rich media. Support for interactive data visualization and use of GUI toolkits. Flexible, embeddable interpreters to load into your own projects. Easy to use, high performance tools for parallel computing.
ImageMagick		7.0.8-11, 7.0.9-5, 7.0.10-35, 7.1.0-4, 7.1.0-53	Desc ImageMagick is a software suite to create, edit, compose, or convert bitmap images
Imath		3.1.6	Desc Imath is a C+ + and python library of 2D and 3D vector, matrix, and math operations for computer graphics
Inspector		2016_update3, 2019_update3, 2023.2.0	Desc Intel Inspector XE is an easy to use memory error checker and thread checker for serial and parallel applications - Homepage: http://software.intel.com/en-us/intel-inspector-xe

Modules	Documentation	Versions	Description
Ipopt		3.14.4	Desc IPOPT (Interior Point Optimizer, pronounced Eye-Pea-Opt) is an open source software package for large-scale nonlinear optimization.
Java		1.8.0_45, 1.8.0_72, 1.8.0_92, 1.8.0_144, 1.8.0_152, 11.0.2, 11.0.16, 11.0.18	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.
Julia		1.6.1-linux-x86_64, 1.7.0-linux-x86_64, 1.7.2-linux-x86_64, 1.10.2-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter in the cluster	2.2.8-Python-3.7.4, 3.1.14	Desc JupyterLab is the next-generation user interface for Project Jupyter offering all the familiar building blocks of the classic Jupyter Notebook (notebook, terminal, text editor, file browser, rich outputs, etc.) in a flexible and powerful user interface. JupyterLab will eventually replace the classic Jupyter Notebook.
Kalign		3.3.1	Desc Kalign is a fast multiple sequence alignment program for biological sequences.
LAME		3.100	Desc LAME is a high quality MPEG Audio Layer III (MP3) encoder licensed under the LGPL.
LAMMPS		3Mar2020-Python-3.7.4-kokkos, 23Jun2022-kokkos	Desc LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.
LAPACK		3.5.0	Desc LAPACK is written in Fortran90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems. - Homepage: http://www.netlib.org/lapack/
LERC		4.0.0	Desc LERC is an open-source image or raster format which supports rapid encoding and decoding for any pixel type (not just RGB or Byte). Users set the maximum compression error per pixel while encoding, so the precision of the original input image is preserved (within user defined error bounds).
Lua		5.4.2, 5.4.3, 5.4.4	Desc Lua is a powerful, fast, lightweight, embeddable scripting language. Lua combines simple procedural syntax with powerful data description constructs based on associative arrays and extensible semantics. Lua is dynamically typed, runs by interpreting bytecode for a register-based virtual machine, and has automatic memory management with incremental garbage collection, making it ideal for configuration, scripting, and rapid prototyping.
Lumerical		2020-2.4, 2021-2.3, 2022-1, 2023-1, 2024-1.02	Desc Ansys Lumerical photonic multiphysics and circuit simulation suites. Design components and analyze electrical, thermal and optical effects at the physical level. Simulate and optimize the performance of photonic integrated circuits
MATLAB	MATLAB	2015a, 2016b, 2017a, 2017b, 2018a, 2018b, 2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b	Desc MATLAB is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran. - Homepage: http://www.mathworks.com/products/matlab
METIS		5.1.0, 5.1.0-32bitIDX	Desc METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms implemented in METIS are based on the multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning schemes.
MPC		1.0.3	Desc Gnu Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It extends the principles of the IEEE-754 standard for fixed precision real floating point numbers to complex numbers, providing well-defined semantics for every operation. At the same time, speed of operation at high precision is a major design goal. - Homepage: http://www.multiprecision.org/
MPFR		3.1.4, 4.0.1, 4.0.2, 4.1.0, 4.2.0	Desc The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.
MUMPS		5.2.1-metis, 5.3.5-metis, 5.4.1-metis, 5.6.1-metis	Desc A parallel sparse direct solver
Mako		1.0.4-Python-2.7.12, 1.0.7-Python-2.7.15, 1.1.0, 1.1.3, 1.1.4, 1.2.4	Desc A super-fast templating language that borrows the best ideas from the existing templating languages
Maple		17, 18, 2015.0, 2017, 2020.1, 2021.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface. - Homepage: http://www.maplesoft.com/products/maple/
Mathematica		10.4.1, 11.3.0, 12.1.1, 12.3.0, 13.0.0, 13.2.1	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields. - Homepage: http://www.wolfram.com/mathematica
Meson		0.51.2-Python-3.7.4, 0.53.2-Python-3.8.2, 0.55.3, 0.58.0, 0.58.2, 0.64.0	Desc Meson is a cross-platform build system designed to be both as fast and as user friendly as possible.
Mesquite		2.3.0	Desc Mesh-Quality Improvement Library - Homepage: https://software.sandia.gov/mesquite/
Miniconda2		4.5.1, 4.5.12, 4.7.10	Desc Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.
Miniconda3	Conda	4.10.3, 22.11.1-1, 23.5.2-0	Desc Miniconda is a free minimal installer for conda. It is a small, bootstrap version of Anaconda that includes only conda, Python, the packages they depend on, and a small number of other useful packages.
Modeller		9.19-Python-2.7.11	Desc MODELLER is used for homology or comparative modeling of protein three-dimensional structures (1,2). The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.
Molden		5.0, 5.6, 5.7, 5.9, 5.9.4	Desc Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK, GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac - Homepage: http://www.cmbi.ru.nl/molden/
Mothur		1.40.3-Python-2.7.11, 1.40.5-Python-2.7.11, 1.41.3-Python-2.7.15, 1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.
NAMD		2.12-mpi, 2.13-mpi	Desc NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
NCCL		2.3.7, 2.8.3-CUDA-11.1.1, 2.10.3-CUDA-11.4.1, 2.16.2-CUDA-11.7.0, 2.16.2-CUDA-12.0.0	Desc The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.
NFFT	NFFT	3.1.3, 3.3.0, 3.3.1, 3.5.0	Desc The NFFT (nonequispaced fast Fourier transform or nonuniform fast Fourier transform) is a C subroutine library for computing the nonequispaced discrete Fourier transform (NDFT) and its generalisations in one or more dimensions, of arbitrary input size, and of complex data.
NVHPC		23.1-CUDA-12.0.0	Desc C, C++ and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
NWChem		6.6.revision27746-2015-10-20-Python-2.7.11	Desc NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters. NWChem software can handle: biomolecules, nanostructures, and solid-state; from quantum to classical, and all combinations; Gaussian basis functions or plane-waves; scaling from one to thousands of processors; properties and relativity. - Homepage: http://www.nwchem-sw.org
Ninja		1.9.0, 1.10.0, 1.10.1, 1.10.2, 1.11.1	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1, 5.0.4	Desc ORCA is a flexible, efficient and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated ab initio methods. It can also treat environmental and relativistic effects.

Modules	Documentation	Versions	Description
Octave		3.8.2, 4.0.0, 4.4.1, 5.1.0, 9.1.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations.
Octopus		5.0.0-mpi, 5.0.0, 7.3-mpi, 7.3, 9.1-mpi, 11.4, 13.0	Desc Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory (DFT), in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation.
OpenBLAS		0.2.9-LAPACK-3.5.0, 0.2.13-LAPACK-3.5.0, 0.2.14-LAPACK-3.5.0, 0.2.15-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.1, 0.2.19-LAPACK-3.7.0, 0.2.20, 0.3.1, 0.3.7, 0.3.9, 0.3.12, 0.3.18, 0.3.21, 0.3.24	Desc OpenBLAS is an optimized BLAS library based on GotoBLAS2 1.13 BSD version.
OpenBabel		3.1.1-Python-3.7.4	Desc Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.
OpenCV		2.4.12, 3.1.0, 4.0.1-Python-2.7.15, 4.2.0-Python-3.7.4, 4.5.1-contrib	Desc OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products. Includes extra modules for OpenCV from the contrib repository.
OpenEXR		2.5.5, 3.1.5	Desc OpenEXR is a high dynamic-range (HDR) image file format developed by Industrial Light & Magic for use in computer imaging applications
OpenFAST		2.3.0, 2.4.0, 3.1.0	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.
OpenFOAM		v1612+, v1906, v1912, v2012, v2106, v2112, v2212, 2.3.0, 2.3.1, 3.0.0, 4.0, 4.1, 6, 7, 8, 9, 10	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.
OpenFOAM-Extend		3.2, 4.0	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. - Homepage: http://www.extend-project.de/
OpenMPI		1.8.1, 1.8.8, 1.10.2, 1.10.3, 2.0.2, 2.1.1, 3.1.1, 3.1.4, 4.0.3, 4.0.5, 4.1.1, 4.1.4, 4.1.6	Desc The Open MPI Project is an open source MPI-3 implementation.
OpenPGM		5.2.122	Desc OpenPGM is an open source implementation of the Pragmatic General Multicast (PGM) specification in RFC 3208 available at www.ietf.org. PGM is a reliable and scalable multicast protocol that enables receivers to detect loss, request retransmission of lost data, or notify an application of unrecoverable loss. PGM is a receiver-reliable protocol, which means the receiver is responsible for ensuring all data is received, absolving the sender of reception responsibility.
OpenSSL		1.0.1s, 1.0.2g, 1.0.2h, 1.1, 1.1.1d	Desc The OpenSSL Project is a collaborative effort to develop a robust, commercial-grade, full-featured, and Open Source toolchain implementing the Secure Sockets Layer (SSL v2/v3) and Transport Layer Security (TLS v1) protocols as well as a full-strength general purpose cryptography library. - Homepage: http://www.openssl.org/
PCL		1.9.1-Python-2.7.15, 1.12.1-Python-3.8.6	Desc The Point Cloud Library (PCL) is a standalone, large scale, open project for 2D/3D image and point cloud processing.
PFFT		1.0.8-alpha	Desc PFFT is a software library for computing massively parallel, fast Fourier transformations on distributed memory architectures. PFFT can be understood as a generalization of FFTW-MPI to multidimensional data decomposition.
PGI		16.5-GCC-5.4.0-2.26	Desc C, C+ + and Fortran compilers from The Portland Group - PGI
PICRUSt2		2.5.0-Python-3.9.6	Desc PICRUSt2 (Phylogenetic Investigation of Communities by Reconstruction of Unobserved States) is a software for predicting functional abundances based only on marker gene sequences. Check out the pre-print here.
PIL		1.1.7-Python-2.7.11	Desc The Python Imaging Library (PIL) adds image processing capabilities to your Python interpreter. This library supports many file formats, and provides powerful image processing and graphics capabilities. - Homepage: http://www.pythonware.com/products/pil
PLUMED		2.5.3-Python-3.7.4, 2.7.3	Desc PLUMED is an open source library for free energy calculations in molecular systems which works together with some of the most popular molecular dynamics engines. Free energy calculations can be performed as a function of many order parameters with a particular focus on biological problems, using state of the art methods such as metadynamics, umbrella sampling and Jarzynski-equation based steered MD. The software, written in C+ +, can be easily interfaced with both fortran and C/C+ + codes.
POV-Ray		3.7.0.8	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. POV-Ray is a high-quality, Free Software tool for creating stunning three-dimensional graphics. The source code is available for those wanting to do their own ports.
POVRay		3.6.1	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. - Homepage: www.povray.org
PSI4		1.7	Desc PSI4 is an open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties. We can routinely perform computations with more than 2500 basis functions running serially or in parallel.
PSolver		1.8.3	Desc Interpolating scaling function Poisson Solver Library
Pandoc		3.1.8	Desc If you need to convert files from one markup format into another, pandoc is your swiss-army knife
ParMETIS		3.2.0, 4.0.3	Desc ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. ParMETIS extends the functionality provided by METIS and includes routines that are especially suited for parallel AMR computations and large scale numerical simulations. The algorithms implemented in ParMETIS are based on the parallel multilevel k-way graph-partitioning, adaptive repartitioning, and parallel multi-constrained partitioning schemes.
ParMGridGen		1.0	Desc ParMGridGen is an MPI-based parallel library that is based on the serial package MGridGen, that implements (serial) algorithms for obtaining a sequence of successive coarse grids that are well-suited for geometric multigrid methods. - Homepage: http://www-users.cs.umn.edu/~moulitsa/software.html
ParaView		4.4.0-mpi, 4.4.0, 5.1.2-mpi, 5.2.0-mpi, 5.4.1-mpi, 5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi, 5.11.1	Desc ParaView is a scientific parallel visualizer.
Perl		5.22.1-bare, 5.22.1, 5.28.0, 5.30.0, 5.30.2, 5.32.0-minimal, 5.32.0, 5.32.1-minimal, 5.32.1, 5.34.0, 5.36.0-minimal, 5.36.0, 5.38.0	Desc Larry Wall's Practical Extraction and Report Language This is a minimal build without any modules. Should only be used for build dependencies.
Pies		1.3	Desc GNU Pies stands for the Program Invocation and Execution Supervisor.
Pillow		3.4.2-Python-3.5.1, 4.2.0-Python-3.5.1, 5.3.0-Python-3.6.6, 6.2.1, 8.0.1, 8.3.2, 9.4.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
Pillow-SIMD		9.5.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.

Modules	Documentation	Versions	Description
PnetCDF		1.12.3	Desc Parallel netCDF: A Parallel I/O Library for NetCDF File Access
ProFit		3.1, 3.3	Desc ProFit is the protein least squares fitting program
Pth		2.0.7	Desc GNU Pth - The GNU Portable Threads
PyQt5		5.11.3-Python-3.6.6, 5.13.1-Python-3.7.4, 5.15.1	Desc PyQt5 is a set of Python bindings for v5 of the Qt application framework from The Qt Company. This bundle includes PyQtWebEngine, a set of Python bindings for The Qt Company's Qt WebEngine framework.
PyTorch		1.2.0-Python-3.6.6, 1.9.0, 1.13.1-CUDA-12.0.0, 1.13.1	Desc Tensors and Dynamic neural networks in Python with strong GPU acceleration. PyTorch is a deep learning framework that puts Python first.
PyTorch-bundle		2022.1	Desc PyTorch Geometric (PyG) is a geometric deep learning extension library for PyTorch.
PyZMQ		15.2.0-Python-2.7.11-zmq4	Desc Python bindings for ZeroMQ - Homepage: http://www.zeromq.org/bindings:python
Python		2.7.11, 2.7.12, 2.7.15-bare, 2.7.15, 2.7.16, 2.7.18-bare, 2.7.18, 3.4.3, 3.5.1, 3.5.2, 3.6.1, 3.6.4, 3.6.6, 3.7.0, 3.7.4, 3.8.2, 3.8.6, 3.9.5-bare, 3.9.5, 3.9.6-bare, 3.9.6, 3.10.8-bare, 3.10.8, 3.11.5	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Qt		4.8.7	Desc Qt is a comprehensive cross-platform C+ + application framework. - Homepage: http://qt.io/
Qt5		5.6.0, 5.7.0, 5.10.1, 5.13.1, 5.14.2, 5.15.2, 5.15.7	Desc Qt is a comprehensive cross-platform C+ + application framework.
QuTiP		4.3.1-Python-3.6.6	Desc QuTiP is open-source software for simulating the dynamics of open quantum systems.
R	Conda, Jupyter in the cluster	3.3.1, 3.4.1-X11-20160819, 3.5.1, 3.6.1, 4.0.3, 4.1.0, 4.1.2, 4.2.2	Desc R is a free software environment for statistical computing and graphics.
ROOT		v5.34.36-Python-2.7.11, 6.14.06-Python-2.7.15	Desc The ROOT system provides a set of OO frameworks with all the functionality needed to handle and analyze large amounts of data in a very efficient way. - Homepage: http://root.cern.ch/drupal/
Rust		1.52.1, 1.54.0, 1.65.0	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAS		9.4	Desc SAS is a software suite for advanced analytics, multivariate analyses, business intelligence, data management, and predictive analytics.
SCIPOptSuite		8.0.1, 8.0.4-Gurobi-9.5.0, 8.0.4, 9.0.1	Desc SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access of detailed information down to the guts of the solver.
SCOTCH		6.0.4, 6.0.6, 6.0.9, 6.1.0, 6.1.2-no-thread, 6.1.2, 7.0.2, 7.0.3	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.
SCons		2.4.1-Python-2.7.11	Desc SCons is a software construction tool. - Homepage: http://www.scons.org/
SEPP		4.5.1	Desc SATe-enabled Phylogenetic Placement - addresses the problem of phylogenetic placement of short reads into reference alignments and trees.
SQLite		3.13.0	Desc SQLite: SQL Database Engine in a C Library - Homepage: http://www.sqlite.org/
SUMO		1.9.2-Python-3.7.4, 1.16.0-Python-3.9.6	Desc "Simulation of Urban MObility" (SUMO) is an open source, highly portable, microscopic and continuous traffic simulation package designed to handle large networks. It allows for intermodal simulation including pedestrians and comes with a large set of tools for scenario creation.
ScaFaCoS		1.0.1	Desc ScaFaCoS is a library of scalable fast coulomb solvers.
ScaLAPACK		2.0.2-OpenBLAS-0.2.9-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.14-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.15-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.1, 2.0.2-OpenBLAS-0.2.19-LAPACK-3.7.0, 2.0.2-OpenBLAS-0.2.20, 2.0.2-OpenBLAS-0.3.1, 2.0.2, 2.1.0-fb, 2.1.0, 2.2.0-fb	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.
Schrodinger		2015-3_Linux-x86_64	Desc Schrödinger aims to provide integrated software solutions and services that truly meet its customers' needs. We want to empower researchers around the world to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials. - Homepage: http://www.schrodinger.com/
SciPy-bundle		2019.10-Python-3.7.4, 2020.03-Python-3.8.2, 2020.11, 2021.10, 2023.02	Desc Bundle of Python packages for scientific software
Shapely		1.7.0-Python-3.7.4, 1.8a1	Desc Shapely is a BSD-licensed Python package for manipulation and analysis of planar geometric objects. It is based on the widely deployed GEOS (the engine of PostGIS) and JTS (from which GEOS is ported) libraries.
Siesta		4.1.5	Desc SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
Singularity		2.3.1, 2.4.2, 2.6.1, 3.5.3	Desc Singularity is a portable application stack packaging and runtime utility. - Homepage: http://gmkurtzer.github.io/singularity
Sphinx		1.8.1-Python-3.6.6	Desc Sphinx is a tool that makes it easy to create intelligent and beautiful documentation. It was originally created for the new Python documentation, and it has excellent facilities for the documentation of Python projects, but C/C+ + is already supported as well, and it is planned to add special support for other languages as well.
Spyder		3.3.6-Python-3.6.6, 4.1.5-Python-3.7.4, 5.1.5	Desc Spyder is an interactive Python development environment providing MATLAB-like features in a simple and light-weighted software.
Subversion		1.12.0	Desc Subversion is an open source version control system.
SuiteSparse		4.2.1-ParMETIS-4.0.3, 4.4.5-METIS-5.1.0, 4.5.3-METIS-5.1.0, 5.1.2-METIS-5.1.0, 5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0, 5.13.0-METIS-5.1.0	Desc SuiteSparse is a collection of libraries manipulate sparse matrices.
Tcl		8.6.3, 8.6.4, 8.6.5, 8.6.6, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13	Desc Tcl (Tool Command Language) is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. - Homepage: http://www.tcl.tk/
Tecplot360ex		2021.1	Desc Quickly plot and animate your CFD results exactly the way you want. Analyze complex solutions, arrange multiple layouts, and communicate your results with professional images and animations.
TensorFlow		1.2.0-Python-3.5.1, 1.4.0-Python-3.5.1, 1.12.0-Python-2.7.15, 1.12.0-Python-3.6.6, 2.2.0-Python-3.7.4, 2.3.1-Python-3.7.4, 2.4.1, 2.8.4-CUDA-11.4.1	Desc An open-source software library for Machine Intelligence
TensorRT		4.0.1.6-Python-2.7.15	Desc NVIDIA TensorRT is a platform for high-performance deep learning inference
Tk		8.6.4-no-X11, 8.6.5, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12	Desc Tk is an open source, cross-platform widget toolchain that provides a library of basic elements for building a graphical user interface (GUI) in many different programming languages. - Homepage: http://www.tcl.tk/
TurboVNC		2.1.2, 2.2.1	Desc TurboVNC is a derivative of VNC (Virtual Network Computing) that is tuned to provide peak performance for 3D and video workloads.

Modules	Documentation	Versions	Description
VMD		1.9.3-Python-2.7.11, 1.9.3-Python-2.7.15, 1.9.4a51	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.
VSEARCH		2.8.0, 2.9.1, 2.22.1	Desc VSEARCH supports de novo and reference based chimera detection, clustering, full-length and prefix dereplication, rereplication, reverse complementation, masking, all-vs-all pairwise global alignment, exact and global alignment searching, shuffling, subsampling and sorting. It also supports FASTQ file analysis, filtering, conversion and merging of paired-end reads.
VTK		5.4.2, 6.3.0-Python-2.7.11, 7.0.0-Python-2.7.11, 8.1.1-Python-2.7.15, 9.0.1, 9.1.0	Desc The Visualization Toolkit (VTK) is an open-source, freely available software system for 3D computer graphics, image processing and visualization. VTK consists of a C+ + class library and several interpreted interface layers including Tcl/Tk, Java, and Python. VTK supports a wide variety of visualization algorithms including: scalar, vector, tensor, texture, and volumetric methods; and advanced modeling techniques such as: implicit modeling, polygon reduction, mesh smoothing, cutting, contouring, and Delaunay triangulation.
VTune		2016_update3, 2019_update3, 2022.3.0, 2023.2.0	Desc Intel VTune Amplifier XE is the premier performance profiler for C, C+ +, C#, Fortran, Assembly and Java. - Homepage: http://software.intel.com/en-us/intel-vtune-amplifier-xe
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools
VirtualGL		2.5.2, 2.6.2, 2.6.4	Desc VirtualGL is an open source toolkit that gives any Linux or Unix remote display software the ability to run OpenGL applications with full hardware acceleration.
Voro+ +		Voro+ 0.4.6	Desc Voro+ + is a software library for carrying out three-dimensional computations of the Voronoi tessellation. A distinguishing feature of the Voro+ + library is that it carries out cell-based calculations, computing the Voronoi cell for each particle individually. It is particularly well-suited for applications that rely on cell-based statistics, where features of Voronoi cells (eg. volume, centroid, number of faces) can be used to analyze a system of particles.
WPS		4.4-dmpar	Desc WRF Preprocessing System (WPS) for WRF. The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
WRF		4.4.1-dmpar	Desc The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
X11		20200222	Desc The X Window System (X11) is a windowing system for bitmap displays
XCFun		2.1.1-Python-3.7.4	Desc Arbitrary order exchange-correlation functional library
Xvfb		1.20.8	Desc Xvfb is an X server that can run on machines with no display hardware and no physical input devices. It emulates a dumb framebuffer using virtual memory.
YACS		0.1.8	Desc YACS was created as a lightweight library to define and manage system configurations, such as those commonly found in software designed for scientific experimentation. These “configurations” typically cover concepts like hyperparameters used in training a machine learning model or configurable model hyperparameters, such as the depth of a convolutional neural network.
Z3		4.12.2	Desc Z3 is a theorem prover from Microsoft Research.
ZeroMQ		4.1.4, 4.2.2, 4.2.5, 4.3.2, 4.3.3	Desc ZeroMQ looks like an embeddable networking library but acts like a concurrency framework. It gives you sockets that carry atomic messages across various transports like in-process, inter-process, TCP, and multicast. You can connect sockets N-to-N with patterns like fanout, pub-sub, task distribution, and request-reply. It's fast enough to be the fabric for clustered products. Its asynchronous I/O model gives you scalable multicore applications, built as asynchronous message-processing tasks. It has a score of language APIs and runs on most operating systems.
arpack-ng		3.3.0, 3.5.0, 3.7.0, 3.8.0, 3.9.1	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
at-spi2-atk		2.34.1, 2.38.0	Desc AT-SPI 2 toolkit bridge
at-spi2-core		2.34.0, 2.38.0, 2.46.0	Desc Assistive Technology Service Provider Interface.
cURL		7.47.0, 7.49.1, 7.55.1, 7.60.0, 7.66.0, 7.69.1, 7.72.0, 7.76.0, 7.78.0, 7.86.0, 8.3.0	Desc libcurl is a free and easy-to-use client-side URL transfer library, supporting DICT, FILE, FTP, FTPS, Gopher, HTTP, HTTPS, IMAP, IMAPS, LDAP, LDAPS, POP3, POP3S, RTMP, RTSP, SCP, SFTP, SMTP, SMTPS, Telnet and TFTP. libcurl supports SSL certificates, HTTP POST, HTTP PUT, FTP uploading, HTTP form based upload, proxies, cookies, user+password authentication (Basic, Digest, NTLM, Negotiate, Kerberos), file transfer resume, http proxy tunneling and more.
ccpnmr		2.4.2-Python-2.7.11	Desc CcpNmr Analysis is a graphics-based interactive NMR spectrum visualisation, resonance assignment and data analysis program
cuDNN		7.1.4.18, 8.0.4.30-CUDA-11.1.1, 8.2.2.26-CUDA-11.4.1, 8.5.0.96-CUDA-11.7.0, 8.8.0.121-CUDA-12.0.0, 8.9.7.29-CUDA-12.3.0	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		0.19.4-Python-3.6.6, 2021.2.0	Desc Dask natively scales Python. Dask provides advanced parallelism for analytics, enabling performance at scale for the tools you love.
flatbuffers		1.12.0	Desc FlatBuffers: Memory Efficient Serialization Library
foss		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK. - Homepage: (none)
fosscuda		2018b, 2020b	Desc GCC based compiler toolchain with CUDA support, and including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
futile		1.8.3	Desc The FUTILE project (Fortran Utilities for the Treatment of Innermost Level of Executables) is a set of modules and wrapper that encapsulate the most common low-level operations of a Fortran code.
gappa		0.8.0	Desc gappa is a collection of commands for working with phylogenetic data. Its main focus are evolutionary placements of short environmental sequences on a reference phylogenetic tree. Such data is typically produced by tools like EPA-ng, RAxML-EPA or pplacer and usually stored in jplace files.
gcccuda		2018b, 2020b	Desc GNU Compiler Collection (GCC) based compiler toolchain, along with CUDA toolkit.
geopandas		0.7.0-Python-3.7.4, 0.8.2	Desc GeoPandas is a project to add support for geographic data to pandas objects. It currently implements GeoSeries and GeoDataFrame types which are subclasses of pandas.Series and pandas.DataFrame respectively. GeoPandas objects can act on shapely geometry objects and perform geometric operations.
gfbf		2022b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including FlexiBLAS (BLAS and LAPACK support) and (serial) FFTW.
git		2.8.0, 2.16.1, 2.23.0-nodocs, 2.28.0-nodocs, 2.32.0-nodocs, 2.33.1-nodocs, 2.38.1-nodocs	Desc Git is a free and open source distributed version control system designed to handle everything from small to very large projects with speed and efficiency.
gmsh		2.9.1	Desc Gmsh is a 3D finite element grid generator with a build-in CAD engine and post-processor. - Homepage: http://geuz.org/gmsh
gnuplot		4.6.0, 5.0.3, 5.2.5, 5.2.8, 5.4.1, 5.4.2, 5.4.6	Desc Portable interactive, function plotting utility
gompi		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021a, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support. - Homepage: (none)
gompic		2018b, 2020b	Desc GNU Compiler Collection (GCC) based compiler toolchain along with CUDA toolkit, including OpenMPI for MPI support with CUDA features enabled.

Modules	Documentation	Versions	Description
graph-tool		2.22-Python-3.5.2	Desc Graph-tool is an efficient Python module for manipulation and statistical analysis of graphs (a.k.a. networks). Contrary to most other python modules with similar functionality, the core data structures and algorithms are implemented in C+ +, making extensive use of template metaprogramming, based heavily on the Boost Graph Library. This confers it a level of performance that is comparable (both in memory usage and computation time) to that of a pure C/C+ + library. - Homepage: https://graph-tool.skewed.de/
h5py		2.6.0-Python-2.7.11, 2.8.0-Python-2.7.15, 2.8.0-Python-3.6.6, 2.10.0-Python-3.7.4, 3.1.0, 3.6.0	Desc HDF5 for Python (h5py) is a general-purpose Python interface to the Hierarchical Data Format library, version 5. HDF5 is a versatile, mature scientific software library designed for the fast, flexible storage of enormous amounts of data.
help2man		1.47.4	Desc help2man produces simple manual pages from the '–help' and '–version' output of other commands.
horton		2.0.0-Python-2.7.11	Desc Horton is a development platform for electronic structure methods. - Homepage: http://theochem.github.io/horton
hypothesis		4.5.0-Python-3.6.6, 5.41.2, 5.41.5, 6.14.6, 6.68.2	Desc Hypothesis is an advanced testing library for Python. It lets you write tests which are parametrized by a source of examples, and then generates simple and comprehensible examples that make your tests fail. This lets you find more bugs in your code with less work.
iTensor		3.1.11	Desc An efficient and flexible C+ + library for performing tensor network calculations
icc		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc C and C+ + compiler from Intel
iccifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32, 2019.5.281, 2020.1.217	Desc Intel C, C+ + and Fortran compilers
ifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc Fortran compiler from Intel
iimpi		7.2.3-GCC-4.9.2, 8.1.5-GCC-4.9.3-2.25, 2016b, 2016.01-GCC-4.9.3-2.25, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel C/C+ + and Fortran compilers, alongside Intel MPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
imkl		11.2.1.133, 11.3.1.150, 11.3.3.210, 2018.3.222, 2019.3.199, 2019.5.281, 2020.1.217, 2021.2.0, 2022.2.1, 2023.2.0	Desc Intel oneAPI Math Kernel Library
imkl-FFTW		2022.2.1, 2023.2.0	Desc FFTW interfaces using Intel oneAPI Math Kernel Library
impi		5.0.2.044, 5.1.2.150, 5.1.3.181, 2018.3.222, 2018.5.288, 2019.3.199, 2019.7.217, 2021.2.0, 2021.7.1, 2021.10.0	Desc The Intel(R) MPI Library for Linux* OS is a multi-fabric message passing library based on ANL MPICH2 and OSU MVAPICH2. The Intel MPI Library for Linux OS implements the Message Passing Interface, version 3.0 (MPI-3) specification.
intel		2015a, 2016a, 2016b, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel Cluster Toolkit Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MPI & Intel MKL.
intel-compilers		2021.2.0, 2022.2.1, 2023.2.1	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)
iomkl		2016b	Desc Intel Cluster Toolchain Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MKL & OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
iompi		2016b	Desc Toolchain with Intel C, C+ + and Fortran compilers, alongside OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
ipp		9.0.4.258, 2019.3.199	Desc Intel Integrated Performance Primitives (Intel IPP) is an extensive library of multicore-ready, highly optimized software functions for multimedia, data processing, and communications applications. Intel IPP offers thousands of optimized functions covering frequently used fundamental algorithms.
itac		9.1.2.024, 2019.3.032, 2021.10.0	Desc The Intel Trace Collector is a low-overhead tracing library that performs event-based tracing in applications. The Intel Trace Analyzer provides a convenient way to monitor application activities gathered by the Intel Trace Collector through graphical displays.
json-c		0.16	Desc JSON-C implements a reference counting object model that allows you to easily construct JSON objects in C, output them as JSON formatted strings and parse JSON formatted strings back into the C representation of JSON objects.
lammps		11Aug17-Python-2.7.11-mpi, 11Aug17-Python-2.7.11, 14May16-Python-2.7.11-mpi, 14May16-Python-2.7.11	Desc LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers.
libAfterImage		1.20	Desc libAfterImage is a generic image manipulation library - Homepage: http://www.afterstep.org/
libarchive		3.4.2	Desc Multi-format archive and compression library
libffi		3.2.1	Desc The libffi library provides a portable, high level programming interface to various calling conventions. This allows a programmer to call any function specified by a call interface description at run-time.
libopus		1.3.1	Desc Opus is a totally open, royalty-free, highly versatile audio codec. Opus is unmatched for interactive speech and music transmission over the Internet, but is also intended for storage and streaming applications. It is standardized by the Internet Engineering Task Force (IETF) as RFC 6716 which incorporated technology from Skype's SILK codec and Xiph.Org's CELT codec.
libreadline		6.3	Desc The GNU Readline library provides a set of functions for use by applications that allow users to edit command lines as they are typed in. Both Emacs and vi editing modes are available. The Readline library includes additional functions to maintain a list of previously-entered command lines, to recall and perhaps reedit those lines, and perform csh-like history expansion on previous commands. - Homepage: http://cnswww.cns.cwru.edu/php/chet/readline/rltop.html
libsigc+ +		libsigc+ 2.4.1	Desc The libsigc+ + package implements a typesafe callback system for standard C+ +. - Homepage: http://www.gtk.org/
libsodium		1.0.8, 1.0.13, 1.0.16	Desc Sodium is a modern, easy-to-use software library for encryption, decryption, signatures, password hashing and more.
lmod		lmod	Desc Lmod: An Environment Module System
ls-dyna		8.1.105897_mpp_d, 9.0.1.109912_mpp_d, 9.1.113698_mpp_d, 9.2.119543_mpp_d, 10_0_118302_mpp_d	Desc LS-DYNA is a general-purpose finite element program capable of simulating complex real world problems. It is used by the automobile, aerospace, construction, military, manufacturing, and bioengineering industries. - Homepage: http://www.lstc.com/products/ls-dyna
magma		2.5.0, 2.5.4, 2.7.1-CUDA-11.7.0, 2.7.1-CUDA-12.0.0	Desc The MAGMA project aims to develop a dense linear algebra library similar to LAPACK but for heterogeneous/hybrid architectures, starting with current Multicore+GPU systems.
make		4.3, 4.4.1	Desc GNU version of make utility
matplotlib		1.4.3-Python-2.7.11, 1.5.1-Python-2.7.11, 1.5.1-Python-3.4.3, 1.5.1-Python-3.5.1, 1.5.1-Python-3.5.2, 2.0.2-Python-3.5.1, 2.0.2-Python-3.6.1, 3.0.0-Python-3.6.6, 3.1.1-Python-3.7.4, 3.2.1-Python-3.8.2, 3.3.3, 3.4.3	Desc matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell, web application servers, and six graphical user interface toolkits.
molmod		1.4.5-Python-3.7.4	Desc MolMod is a Python library with many compoments that are useful to write molecular modeling programs.

Modules	Documentation	Versions	Description
mpi4py		2.0.0-Python-2.7.11, 3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.0.3-Python-3.8.2	Desc MPI for Python (mpi4py) provides bindings of the Message Passing Interface (MPI) standard for the Python programming language, allowing any Python program to exploit multiple processors. - Homepage: https://bitbucket.org/mpi4py/mpi4py
mpifileutils	mpiFileUtils	0.10.1, 0.11, 0.11.1	Desc MPI-Based File Utilities For Distributed Systems
mpmath		0.19-Python-2.7.11, 0.19-Python-3.4.3	Desc mpmath can be used as an arbitrary-precision substitute for Python's float/complex types and math/cmath modules, but also does much more advanced mathematics. Almost any calculation can be performed just as well at 10-digit or 1000-digit precision, with either real or complex numbers, and in many cases mpmath implements efficient algorithms that scale well for extremely high precision work. - Homepage: http://mpmath.org/
msindo		3.6	Desc Semiempirical SCF MO program for systems with first-, second-, third-, and fourth-row elements - Homepage: http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=MSINDO&lang=english
ncurses		6.0	Desc The Ncurses (new curses) library is a free software emulation of curses in System V Release 4.0, and more. It uses Terminfo format, supports pads and color and multiple highlights and forms characters and function-key mapping, and has all the other SYSV-curses enhancements over BSD Curses. - Homepage: http://www.gnu.org/software/ncurses/
ncview		2.1.8	Desc Ncview is a visual browser for netCDF format files. Typically you would use ncview to get a quick and easy, push-button look at your netCDF files. You can view simple movies of the data, view along various dimensions, take a look at the actual data values, change color maps, invert the data, etc.
netCDF		4.4.0, 4.4.1, 4.6.1, 4.7.1, 4.7.4, 4.8.0, 4.8.1, 4.9.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
netCDF-Fortran		4.4.3, 4.4.4, 4.5.2, 4.5.3, 4.6.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
nettle		3.2	Desc Nettle is a cryptographic library that is designed to fit easily in more or less any context: In crypto toolkits for object-oriented languages (C+ +, Python, Pike, ...), in applications like LSH or GNUPG, or even in kernel space. - Homepage: http://www.lysator.liu.se/~nisse/nettle/
networkx		1.10-Python-2.7.11, 2.2-Python-3.5.1, 2.4-Python-3.7.4, 2.5, 2.6.3	Desc NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.
nlohmann_json		3.11.2	Desc JSON for Modern C+ +
nsync		1.24.0	Desc nsync is a C library that exports various synchronization primitives, such as mutexes
numba		0.29.0-Python-2.7.11, 0.53.1	Desc Numba is an Open Source NumPy-aware optimizing compiler for Python sponsored by Continuum Analytics, Inc. It uses the remarkable LLVM compiler infrastructure to compile Python syntax to machine code.
numpy		1.8.2-Python-2.7.11, 1.9.2-Python-2.7.11, 1.10.1-Python-2.7.11, 1.10.1-Python-3.4.3, 1.10.1-Python-3.5.1, 1.13.0-Python-3.5.1, 1.18.5-Python-3.7.4, 1.18.5-Python-3.8.2	Desc NumPy is the fundamental package for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C+ + and Fortran code, useful linear algebra, Fourier transform, and random number capabilities. Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases. - Homepage: http://www.numpy.org
pandas		0.18.0-Python-2.7.11, 0.18.0-Python-3.5.1	Desc pandas is an open source, BSD-licensed library providing high-performance, easy-to-use data structures and data analysis tools for the Python programming language. - Homepage: https://pypi.python.org/pypi/pandas/
parallel		20190922, 20210322	Desc parallel: Build and execute shell commands in parallel
pcp		2.0.0_39-Python-2.7.16	Desc A parallel copy program for lustre
phenix		1.10.1-2155	Desc PHENIX is a software suite for the automated determination of molecular structures using X-ray crystallography and other methods. - Homepage: http://www.phenix-online.org
pigz		2.6	Desc pigz, which stands for parallel implementation of gzip, is a fully functional replacement for gzip that exploits multiple processors and multiple cores to the hilt when compressing data. pigz was written by Mark Adler, and uses the zlib and pthread libraries.
pkgconf		1.8.0, 1.9.3, 2.0.3	Desc pkgconf is a program which helps to configure compiler and linker flags for development libraries. It is similar to pkg-config from freedesktop.org.
protobuf		3.2.0	Desc Google Protocol Buffers - Homepage: https://github.com/google/protobuf/
protobuf-python		3.2.0-Python-3.4.3, 3.2.0-Python-3.5.1, 3.10.0-Python-3.7.4	Desc Python Protocol Buffers runtime library. - Homepage: https://github.com/google/protobuf/
psutil		5.6.3-Python-3.6.6, 5.9.4	Desc A cross-platform process and system utilities module for Python
pytest		7.1.3	Desc pytest: simple powerful testing with Python
qutip		2.2.0-Python-2.7.11, 3.1.0-Python-2.7.11, 4.0.2-Python-3.4.3	Desc QuTiP : Quantum Toolbox in Python - Homepage: http://qutip.org/
scikit-image		0.12.3-Python-3.5.1, 0.14.1-Python-3.6.6, 0.18.1	Desc scikit-image is a collection of algorithms for image processing.
scikit-learn		0.18.1-Python-3.5.1, 0.20.0-Python-3.6.6, 0.20.3-Python-3.6.6, 0.21.3-Python-3.7.4, 0.23.2	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-umfpack		0.2.1-Python-2.7.11	Desc scikit-umfpack provides a wrapper of UMFPACK sparse direct solver to SciPy. - Homepage: http://rc.github.io/scikit-umfpack/
scipy		0.16.1-Python-2.7.11, 0.17.1-Python-2.7.11, 0.17.1-Python-3.4.3, 0.19.1-Python-3.5.1	Desc SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension for Python. - Homepage: http://www.scipy.org
settarg		settarg	Desc
sparsehash		2.0.2	Desc An extremely memory-efficient hash_map implementation. 2 bits/entry overhead! The SparseHash library contains several hash-map implementations, including implementations that optimize for space or speed. - Homepage: https://code.google.com/p/sparsehash/
sympy		1.0-Python-2.7.11, 1.0-Python-3.4.3	Desc SymPy is a Python library for symbolic mathematics. It aims to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries. - Homepage: http://sympy.org/
tbb		4.4.6.258, 2019_U9, 2019.2.187, 2020.3, 2021.10.0	Desc Intel(R) Threading Building Blocks (Intel(R) TBB) lets you easily write parallel C+ + programs that take full advantage of multicore performance, that are portable, composable and have future-proof scalability.
texlive		20200406, 20210324, 20240312	Desc TeX is a typesetting language. Instead of visually formatting your text, you enter your manuscript text intertwined with TeX commands in a plain text file. You then run TeX to produce formatted output, such as a PDF file. Thus, in contrast to standard word processors, your document is a separate file that does not pretend to be a representation of the final typeset output, and so can be easily edited and manipulated.
torchvision		0.14.1-PyTorch-1.13.1-CUDA-12.0.0	Desc Datasets, Transforms and Models specific to Computer Vision
typing-extensions		3.7.4.3	Desc Typing Extensions – Backported and Experimental Type Hints for Python
utf8proc		2.2.0	Desc utf8proc is a small, clean C library that provides Unicode normalization, case-folding, and other operations for data in the UTF-8 encoding.

Modules	Documentation	Versions	Description
wheel		0.29.0-Python-3.4.3, 0.29.0-Python-3.5.1, 0.31.1-Python-2.7.15, 0.31.1-Python-3.6.6	Desc A built-package format for Python.
xtb		6.4.1, 6.5.1, 6.6.1	Desc xtb - An extended tight-binding semi-empirical program package.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

Sandy&Ivy-Bridge(AVX)

Installed software as of Wed, 23 Oct 2024 07:35:20 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	6.14-2, 2016, 2017-hotfix-1819, 2017, 2018, 2019-hotfix-1939, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341	Desc Finite Element Analysis software for modeling, visualization and best-in-class implicit and explicit dynamics FEA.
AMPL-MP		3.1.0	Desc An open-source library for mathematical programming.
ANSYS	ANSYS / CFX	15.0, 16.0, 16.2, 17.2, 18.0, 18.2, 19.0, 19.2, 19.3, 2019.2, 2019.3, 2020.1, 2020.2, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ANSYSEM		17.2, 18.0, 18.1, 18.2, 19.0, 19.1, 20.2, 2022.2, 2023.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ARIA		2.3.1-Python-2.7.11	Desc ARIA (Ambiguous Restraints for Iterative Assignment) is a software for automated NOE assignment and NMR structure calculation
ASE		3.12.0-Python-2.7.11, 3.16.0-Python-2.7.11, 3.16.2-Python-3.6.6	Desc ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language.
ATK		2.20.0	Desc ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications. - Homepage: https://developer.gnome.org/ATK/stable/
ATSAS		2.7.2-5.el6.x86_64	Desc ATSAS is a program suite for small-angle scattering data analysis from biological macromolecules. - Homepage: http://www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html
Advisor		2016_update3, 2019_update3, 2023.2.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain - Homepage: https://software.intel.com/intel-advisor-xe
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		14-AmberTools-15-patchlevel-0-0, 18-AmberTools-18-patchlevel-9-5-CUDA	Desc Amber (originally Assisted Model Building with Energy Refinement) is software for performing molecular dynamics and structure prediction.
Armadillo		11.4.3	Desc Armadillo is an open-source C+ + linear algebra library (matrix maths) aiming towards a good balance between speed and ease of use. Integer, floating point and complex numbers are supported, as well as a subset of trigonometric and statistics functions.
BLAST+		2.2.31-Python-2.7.11	Desc Basic Local Alignment Search Tool, or BLAST, is an algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences. - Homepage: http://blast.ncbi.nlm.nih.gov/
BLIS		0.8.1, 0.9.0	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
BWA		0.7.17	Desc Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome.
Bazel		0.5.2, 0.7.0, 0.18.0, 2.0.0, 3.4.1, 3.7.2, 6.3.1	Desc Bazel is a build tool that builds code quickly and reliably. It is used to build the majority of Google's software.
Biopython		1.71-Python-2.7.11, 1.78	Desc Biopython is a set of freely available tools for biological computation written in Python by an international team of developers. It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics.
Bonnie+ +		Bonnie+ 1.97	Desc Bonnie+ +-1.97: Enhanced performance Test of Filesystem I/O - Homepage: http://www.coker.com.au/bonnie+ +/
Boost		1.47.0, 1.58.0-Python-2.7.11, 1.59.0-Python-2.7.11, 1.60.0-Python-2.7.11, 1.60.0, 1.61.0-Python-2.7.11, 1.61.0, 1.63.0-Python-3.5.2, 1.66.0, 1.67.0, 1.68.0-Python-2.7.15, 1.71.0, 1.74.0, 1.77.0, 1.81.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Boost.Python		1.67.0-Python-2.7.15	Desc Boost.Python is a C+ + library which enables seamless interoperability between C+ + and the Python programming language.
Brunsli		0.1	Desc Brunsli is a lossless JPEG repacking library.
CFITSIO		3.38, 3.45, 4.2.0	Desc CFITSIO is a library of C and Fortran subroutines for reading and writing data files in FITS (Flexible Image Transport System) data format.
CGAL		4.8-Python-2.7.11, 4.8.1-Python-3.5.2, 4.8.1, 4.11.1-Python-2.7.15, 4.14.1-Python-3.7.4, 4.14.3, 5.2	Desc The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C+ + library.
CGNS		2.5.5, 3.3.1	Desc The CGNS system is designed to facilitate the exchange of data between sites and applications, and to help stabilize the archiving of aerodynamic data.
CLooG		0.18.1	Desc CLooG is a free software and library to generate code for scanning Z-polyhedra. That is, it finds a code (e.g. in C, FORTRAN...) that reaches each integral point of one or more parameterized polyhedra. CLooG has been originally written to solve the code generation problem for optimizing compilers based on the polytope model. Nevertheless it is used now in various area e.g. to build control automata for high-level synthesis or to find the best polynomial approximation of a function. CLooG may help in any situation where scanning polyhedra matters. While the user has full control on generated code quality, CLooG is designed to avoid control overhead and to produce a very effective code. - Homepage: http://www.bastoul.net/cloog/index.php
CMake		2.8.4, 3.4.1, 3.4.3, 3.5.2, 3.6.1, 3.7.1, 3.9.6, 3.11.4, 3.12.1, 3.15.3, 3.16.4, 3.18.4, 3.20.1, 3.21.1, 3.22.1, 3.24.3, 3.27.6	Desc CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software. - Homepage: http://www.cmake.org
CNS		1.3-haddock-2.2, 1.3-haddock-2.4, 1.21-aria2.3	Desc Crystallography & NMR System (CNS) has been designed to provide a flexible multi-level hierachical approach for the most commonly used algorithms in macromolecular structure determination

Modules	Documentation	Versions	Description
COMSOL	COMSOL	5.1, 5.2, 5.4, 5.5, 5.6, 6.0, 6.1, 6.2	Desc COMSOL Multiphysics is a finite element analysis, solver and simulation software/FEA software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. - Homepage: https://www.comsol.com/
CPMD	CPMD	4.1, 4.3-omp, 4.3	Desc CPMD The CPMD code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. - Homepage: http://www.cpmd.org/
CREST		2.12	Desc CREST is an utility/driver program for the xtb program. Originally it was designed as conformer sampling program, hence the abbreviation Conformer–Rotamer Ensemble Sampling Tool, but now offers also some utility functions for calculations with the GFNn–xTB methods. Generally the program functions as an IO based OMP scheduler (i.e., calculations are performed by the xtb program) and tool for the creation and analysation of structure ensembles.
CRYSTAL14		1.0.4	Desc Crystal is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations - Homepage: http://www.crystalsolutions.eu/
CUDA		7.5.18, 8.0.44, 9.2.88	Desc CUDA (formerly Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. CUDA gives developers access to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs. - Homepage: https://developer.nvidia.com/cuda-toolkit
Catch2		2.13.9	Desc A modern, C+ +-native, header-only, test framework for unit-tests, TDD and BDD - using C+ +11, C+ +14, C+ +17 and later
CheMPS2		1.8.11	Desc CheMPS2 is a scientific library which contains a spin-adapted implementation of the density matrix renormalization group (DMRG) for ab initio quantum chemistry.
Clang		9.0.1, 16.0.4	Desc C, C+ +, Objective-C compiler, based on LLVM. Does not include C+ + standard library – use libstdc+ + from GCC.
CoordgenLibs		3.0.0	Desc Schrodinger-developed 2D Coordinate Generation
Cython		0.24-Python-2.7.11, 0.24-Python-3.4.3, 0.29.22	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
DMTCP		2.6.0	Desc DMTCP is a tool to transparently checkpoint the state of multiple simultaneous applications, including multi-threaded and distributed applications. It operates directly on the user binary executable, without any Linux kernel modules or other kernel modifications.
DendroPy		4.5.2	Desc A Python library for phylogenetics and phylogenetic computing: reading, writing, simulation, processing and manipulation of phylogenetic trees (phylogenies) and characters.
Doxygen		1.8.11	Desc Doxygen is a documentation system for C+ +, C, Java, Objective-C, Python, IDL (Corba and Microsoft flavors), Fortran, VHDL, PHP, C#, and to some extent D.
ELPA		2021.05.001	Desc Eigenvalue SoLvers for Petaflop-Applications .
EPA-ng		0.3.8	Desc EPA-ng - Fast, parallel, highly accurate Maximum Likelihood Phylogenetic Placement of genetic sequences on a user-supplied reference tree and alignment
EasyBuild-custom		1.0	Desc EasyBuild is a software build and installation framework - Homepage: http://hpcugent.github.com/easybuild/
Eigen		3.2.9, 3.3.4, 3.3.7, 3.3.8, 3.3.9, 3.4.0	Desc Eigen is a C+ + template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
FDS		6.4.0, 6.5.2, 6.6.0, 6.7.3, 6.7.4	Desc Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires. - Homepage: http://firemodels.github.io/fds-smv/
FEKO	FEKO	2017.2_hw, 2017.2.5_hw, 2018_hw, 2019_hw, 2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering
FFTW		3.3.4-PFFT-20150905, 3.3.4, 3.3.6, 3.3.8, 3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FFTW.MPI		3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FLANN		1.8.4-Python-2.7.15	Desc FLANN is a library for performing fast approximate nearest neighbor searches in high dimensional spaces.
Fiona		1.8.13-Python-3.7.4, 1.8.20	Desc Fiona is designed to be simple and dependable. It focuses on reading and writing data in standard Python IO style and relies upon familiar Python types and protocols such as files, dictionaries, mappings, and iterators instead of classes specific to OGR. Fiona can read and write real-world data using multi-layered GIS formats and zipped virtual file systems and integrates readily with other Python GIS packages such as pyproj, Rtree, and Shapely.
FlexiBLAS		3.0.4, 3.2.1, 3.3.1	Desc FlexiBLAS is a wrapper library that enables the exchange of the BLAS and LAPACK implementation used by a program without recompiling or relinking it.
Flux		2019	Desc Altair Flux captures the complexity of electromagnetic and thermal phenomena to predict the behavior of future products with precision.
FriBidi		1.0.5, 1.0.10, 1.0.12	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		24.5.4, 24.5.6_nhus, 24.7.4_nhus, 24.7.4, 26.1.0_nhus, 26.1.0, 30.3.0, 45.7.0, 46.5.0	Desc The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. - Homepage: https://www.gams.com/
GCC		4.8.3, 4.9.2, 4.9.3-binutils-2.25, 4.9.3-2.25, 5.3.0-2.26, 5.4.0-2.26, 6.3.0-2.27, 6.4.0-2.28, 7.3.0-2.30, 8.3.0, 9.3.0, 10.2.0, 10.3.0, 11.2.0, 12.2.0, 13.2.0	Desc The GNU Compiler Collection includes front ends for C, C+ +, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc+ +, libgcj,...).
GDB		9.1-Python-3.7.4	Desc The GNU Project Debugger
GEOS		3.6.1-Python-2.7.12	Desc GEOS (Geometry Engine - Open Source) is a C+ + port of the Java Topology Suite (JTS)
GMP		6.1.0, 6.1.1, 6.1.2, 6.2.0, 6.2.1	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers. - Homepage: http://gmplib.org/
GNUGo		3.8	Desc GNU Go is a free program that plays the game of Go
GPAW		1.1.0-Python-2.7.11, 1.4.0-Python-2.7.11, 1.4.0-Python-3.6.6	Desc GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.
GROMACS		5.1.2-hybrid, 2016.5-hybrid, 2018.4, 2019	Desc GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.
GSL		1.16, 2.1, 2.5, 2.6, 2.7	Desc The GNU Scientific Library (GSL) is a numerical library for C and C+ + programmers. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting.
GST-plugins-base		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/
GStreamer		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/

Modules	Documentation	Versions	Description
GTK+		2.24.30	Desc The GTK+ 2 package contains libraries used for creating graphical user interfaces for applications. - Homepage: https://developer.gnome.org/gtk+/stable/
GTK3		3.24.35	Desc GTK+ is the primary library used to construct user interfaces in GNOME. It provides all the user interface controls, or widgets, used in a common graphical application. Its object-oriented API allows you to construct user interfaces without dealing with the low-level details of drawing and device interaction.
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g09.D01, g09.E01, g16.A03, g16.B01	Desc Gaussian provides state-of-the-art capabilities for electronic structure modeling.
GitPython		2.1.11-Python-3.6.6	Desc GitPython is a python library used to interact with Git repositories
Go		1.16.6	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
GraphicsMagick		1.3.23	Desc GraphicsMagick is the swiss army knife of image processing.
Graphviz		2.50.0	Desc Graphviz is open source graph visualization software. Graph visualization is a way of representing structural information as diagrams of abstract graphs and networks. It has important applications in networking, bioinformatics, software engineering, database and web design, machine learning, and in visual interfaces for other technical domains.
Guile		1.8.8	Desc Guile is a programming language, designed to help programmers create flexible applications that can be extended by users or other programmers with plug-ins, modules, or scripts.
Gurobi		6.5.0, 7.0.2, 7.5.2, 8.1.0, 9.0.1, 9.1.2, 9.5.0, 11.0.0	Desc The Gurobi Optimizer is a state-of-the-art solver for mathematical programming. The solvers in the Gurobi Optimizer were designed from the ground up to exploit modern architectures and multi-core processors, using the most advanced implementations of the latest algorithms.
HADDOCK		2.2-Python-2.7.11, 2.4-Python-2.7.16	Desc HADDOCK (High Ambiguity Driven biomolecular DOCKing) is an information-driven flexible docking approach for the modelling of biomolecular complexes
HDF		4.2.15	Desc HDF (also known as HDF4) is a library and multi-object file format for storing and managing data between machines.
HDF5		1.8.16-serial, 1.8.16, 1.8.17, 1.10.2, 1.10.5, 1.10.6, 1.10.7, 1.12.1, 1.14.0	Desc HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.
HDFView		2.14-Java-1.8.0_152-centos7	Desc HDFView is a visual tool for browsing and editing HDF4 and HDF5 files.
HH-suite		3.3.0	Desc The HH-suite is an open-source software package for sensitive protein sequence searching based on the pairwise alignment of hidden Markov models (HMMs).
HMMER		3.2.1, 3.3.2	Desc HMMER is used for searching sequence databases for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs). Compared to BLAST, FASTA, and other sequence alignment and database search tools based on older scoring methodology, HMMER aims to be significantly more accurate and more able to detect remote homologs because of the strength of its underlying mathematical models. In the past, this strength came at significant computational expense, but in the new HMMER3 project, HMMER is now essentially as fast as BLAST.
HPL		2.2	Desc HPL is a software package that solves a (random) dense linear system in double precision (64 bits) arithmetic on distributed-memory computers. It can thus be regarded as a portable as well as freely available implementation of the High Performance Computing Linpack Benchmark.
Hadoop-cluster		1.0	Desc Framework for deploying Hadoop clusters on traditional HPC - Homepage: http://luis.uni-hannover.de
Highway		1.0.3	Desc Highway is a C+ + library for SIMD (Single Instruction, Multiple Data), i.e. applying the same operation to 'lanes'.
ICU		61.1, 64.2, 67.1, 69.1, 72.1	Desc ICU is a mature, widely used set of C/C+ + and Java libraries providing Unicode and Globalization support for software applications.
IPython		3.2.3-Python-2.7.11, 6.2.1-Python-3.6.4, 7.2.0-Python-3.6.6, 7.9.0-Python-3.7.4, 7.18.1-Python-3.7.4, 7.25.0	Desc IPython provides a rich architecture for interactive computing with: Powerful interactive shells (terminal and Qt-based). A browser-based notebook with support for code, text, mathematical expressions, inline plots and other rich media. Support for interactive data visualization and use of GUI toolkits. Flexible, embeddable interpreters to load into your own projects. Easy to use, high performance tools for parallel computing.
ImageMagick		7.0.8-11, 7.0.9-5, 7.0.10-35, 7.1.0-4, 7.1.0-53	Desc ImageMagick is a software suite to create, edit, compose, or convert bitmap images
Imath		3.1.6	Desc Imath is a C+ + and python library of 2D and 3D vector, matrix, and math operations for computer graphics
Inspector		2016_update3, 2019_update3, 2023.2.0	Desc Intel Inspector XE is an easy to use memory error checker and thread checker for serial and parallel applications - Homepage: http://software.intel.com/en-us/intel-inspector-xe
Ipopt		3.14.4	Desc IPOPT (Interior Point Optimizer, pronounced Eye-Pea-Opt) is an open source software package for large-scale nonlinear optimization.
Java		1.8.0_45, 1.8.0_72, 1.8.0_92, 1.8.0_144, 1.8.0_152, 11.0.2, 11.0.16, 11.0.18	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.
Julia		1.6.1-linux-x86_64, 1.7.0-linux-x86_64, 1.7.2-linux-x86_64, 1.10.2-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter in the cluster	2.2.8-Python-3.7.4, 3.1.14	Desc JupyterLab is the next-generation user interface for Project Jupyter offering all the familiar building blocks of the classic Jupyter Notebook (notebook, terminal, text editor, file browser, rich outputs, etc.) in a flexible and powerful user interface. JupyterLab will eventually replace the classic Jupyter Notebook.
Kalign		3.3.1	Desc Kalign is a fast multiple sequence alignment program for biological sequences.
LAME		3.100	Desc LAME is a high quality MPEG Audio Layer III (MP3) encoder licensed under the LGPL.
LAMMPS		3Mar2020-Python-3.7.4-kokkos, 23Jun2022-kokkos	Desc LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.
LAPACK		3.5.0	Desc LAPACK is written in Fortran90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems. - Homepage: http://www.netlib.org/lapack/
LERC		4.0.0	Desc LERC is an open-source image or raster format which supports rapid encoding and decoding for any pixel type (not just RGB or Byte). Users set the maximum compression error per pixel while encoding, so the precision of the original input image is preserved (within user defined error bounds).
Lua		5.4.2, 5.4.3, 5.4.4	Desc Lua is a powerful, fast, lightweight, embeddable scripting language. Lua combines simple procedural syntax with powerful data description constructs based on associative arrays and extensible semantics. Lua is dynamically typed, runs by interpreting bytecode for a register-based virtual machine, and has automatic memory management with incremental garbage collection, making it ideal for configuration, scripting, and rapid prototyping.
Lumerical		2020-2.4, 2021-2.3, 2022-1, 2023-1, 2024-1.02	Desc Ansys Lumerical photonic multiphysics and circuit simulation suites. Design components and analyze electrical, thermal and optical effects at the physical level. Simulate and optimize the performance of photonic integrated circuits

Modules	Documentation	Versions	Description
MATLAB	MATLAB	2015a, 2016b, 2017a, 2017b, 2018a, 2018b, 2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b	Desc MATLAB is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran. - Homepage: http://www.mathworks.com/products/matlab
METIS		5.1.0, 5.1.0-32bitIDX	Desc METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms implemented in METIS are based on the multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning schemes.
MPC		1.0.3	Desc Gnu Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It extends the principles of the IEEE-754 standard for fixed precision real floating point numbers to complex numbers, providing well-defined semantics for every operation. At the same time, speed of operation at high precision is a major design goal. - Homepage: http://www.multiprecision.org/
MPFR		3.1.4, 4.0.1, 4.0.2, 4.1.0, 4.2.0	Desc The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.
MUMPS		5.2.1-metis, 5.3.5-metis, 5.4.1-metis, 5.6.1-metis	Desc A parallel sparse direct solver
Mako		1.0.4-Python-2.7.12, 1.0.7-Python-2.7.15, 1.1.0, 1.1.3, 1.1.4, 1.2.4	Desc A super-fast templating language that borrows the best ideas from the existing templating languages
Maple		17, 18, 2015.0, 2017, 2020.1, 2021.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface. - Homepage: http://www.maplesoft.com/products/maple/
Mathematica		10.4.1, 11.3.0, 12.1.1, 12.3.0, 13.0.0, 13.2.1	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields. - Homepage: http://www.wolfram.com/mathematica
Meson		0.51.2-Python-3.7.4, 0.53.2-Python-3.8.2, 0.55.3, 0.58.0, 0.58.2, 0.64.0	Desc Meson is a cross-platform build system designed to be both as fast and as user friendly as possible.
Mesquite		2.3.0	Desc Mesh-Quality Improvement Library - Homepage: https://software.sandia.gov/mesquite/
Miniconda2		4.5.1, 4.5.12, 4.7.10	Desc Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.
Miniconda3	Conda	4.10.3, 22.11.1-1, 23.5.2-0	Desc Miniconda is a free minimal installer for conda. It is a small, bootstrap version of Anaconda that includes only conda, Python, the packages they depend on, and a small number of other useful packages.
Modeller		9.19-Python-2.7.11	Desc MODELLER is used for homology or comparative modeling of protein three-dimensional structures (1,2). The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.
Molden		5.0, 5.6, 5.7, 5.9, 5.9.4	Desc Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK, GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac - Homepage: http://www.cmbi.ru.nl/molden/
Mothur		1.40.3-Python-2.7.11, 1.40.5-Python-2.7.11, 1.41.3-Python-2.7.15, 1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.
NAMD		2.12-mpi, 2.13-mpi	Desc NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
NCCL		2.3.7	Desc The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.
NFFT	NFFT	3.1.3, 3.3.0, 3.3.1, 3.5.0	Desc The NFFT (nonequispaced fast Fourier transform or nonuniform fast Fourier transform) is a C subroutine library for computing the nonequispaced discrete Fourier transform (NDFT) and its generalisations in one or more dimensions, of arbitrary input size, and of complex data.
NVHPC		23.1-CUDA-12.0.0	Desc C, C+ + and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
NWChem		6.6.revision27746-2015-10-20-Python-2.7.11	Desc NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters. NWChem software can handle: biomolecules, nanostructures, and solid-state; from quantum to classical, and all combinations; Gaussian basis functions or plane-waves; scaling from one to thousands of processors; properties and relativity. - Homepage: http://www.nwchem-sw.org
Ninja		1.8.2, 1.9.0, 1.10.0, 1.10.1, 1.10.2, 1.11.1	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1, 5.0.4	Desc ORCA is a flexible, efficient and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated ab initio methods. It can also treat environmental and relativistic effects.
Octave		3.8.2, 4.0.0, 4.4.1, 5.1.0, 9.1.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations.
Octopus		5.0.0-mpi, 5.0.0, 7.3-mpi, 7.3, 9.1-mpi, 11.4, 13.0	Desc Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory (DFT), in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation.
OpenBLAS		0.2.9-LAPACK-3.5.0, 0.2.13-LAPACK-3.5.0, 0.2.14-LAPACK-3.5.0, 0.2.15-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.1, 0.2.19-LAPACK-3.7.0, 0.2.20, 0.3.1, 0.3.7, 0.3.9, 0.3.12, 0.3.18, 0.3.21, 0.3.24	Desc OpenBLAS is an optimized BLAS library based on GotoBLAS2 1.13 BSD version.
OpenBabel		3.1.1-Python-3.7.4	Desc Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.
OpenCV		2.4.12, 3.1.0, 4.0.1-Python-2.7.15, 4.2.0-Python-3.7.4, 4.5.1-contrib	Desc OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products. Includes extra modules for OpenCV from the contrib repository.
OpenEXR		2.5.5, 3.1.5	Desc OpenEXR is a high dynamic-range (HDR) image file format developed by Industrial Light & Magic for use in computer imaging applications
OpenFAST		2.3.0, 2.4.0, 3.1.0	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.
OpenFOAM		v1612+, v1906, v1912, v2012, v2106, v2112, v2212, 2.3.0, 2.3.1, 3.0.0, 4.0, 4.1, 6, 7, 8, 9, 10	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.
OpenFOAM-Extend		3.2, 4.0	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. - Homepage: http://www.extend-project.de/
OpenMPI		1.8.1, 1.8.8, 1.10.2, 1.10.3, 2.0.2, 2.1.1, 3.1.1, 3.1.4, 4.0.3, 4.0.5, 4.1.1, 4.1.4, 4.1.6	Desc The Open MPI Project is an open source MPI-3 implementation.

Modules	Documentation	Versions	Description
OpenPGM		5.2.122	Desc OpenPGM is an open source implementation of the Pragmatic General Multicast (PGM) specification in RFC 3208 available at www.ietf.org. PGM is a reliable and scalable multicast protocol that enables receivers to detect loss, request retransmission of lost data, or notify an application of unrecoverable loss. PGM is a receiver-reliable protocol, which means the receiver is responsible for ensuring all data is received, absolving the sender of reception responsibility.
OpenSSL		1.0.1s, 1.0.2g, 1.0.2h, 1.1, 1.1.1d	Desc The OpenSSL Project is a collaborative effort to develop a robust, commercial-grade, full-featured, and Open Source toolchain implementing the Secure Sockets Layer (SSL v2/v3) and Transport Layer Security (TLS v1) protocols as well as a full-strength general purpose cryptography library. - Homepage: http://www.openssl.org/
PCL		1.9.1-Python-2.7.15, 1.12.1-Python-3.8.6	Desc The Point Cloud Library (PCL) is a standalone, large scale, open project for 2D/3D image and point cloud processing.
PFFT		1.0.8-alpha	Desc PFFT is a software library for computing massively parallel, fast Fourier transformations on distributed memory architectures. PFFT can be understood as a generalization of FFTW-MPI to multidimensional data decomposition.
PGI		16.5-GCC-5.4.0-2.26	Desc C, C+ + and Fortran compilers from The Portland Group - PGI
PICRUSt2		2.5.0-Python-3.9.6	Desc PICRUSt2 (Phylogenetic Investigation of Communities by Reconstruction of Unobserved States) is a software for predicting functional abundances based only on marker gene sequences. Check out the pre-print here.
PIL		1.1.7-Python-2.7.11	Desc The Python Imaging Library (PIL) adds image processing capabilities to your Python interpreter. This library supports many file formats, and provides powerful image processing and graphics capabilities. - Homepage: http://www.pythonware.com/products/pil
PLUMED		2.5.3-Python-3.7.4, 2.7.3	Desc PLUMED is an open source library for free energy calculations in molecular systems which works together with some of the most popular molecular dynamics engines. Free energy calculations can be performed as a function of many order parameters with a particular focus on biological problems, using state of the art methods such as metadynamics, umbrella sampling and Jarzynski-equation based steered MD. The software, written in C+ +, can be easily interfaced with both fortran and C/C+ + codes.
POV-Ray		3.7.0.8	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. POV-Ray is a high-quality, Free Software tool for creating stunning three-dimensional graphics. The source code is available for those wanting to do their own ports.
POVRay		3.6.1	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. - Homepage: www.povray.org
PSI4		1.7	Desc PSI4 is an open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties. We can routinely perform computations with more than 2500 basis functions running serially or in parallel.
PSolver		1.8.3	Desc Interpolating scaling function Poisson Solver Library
Pandoc		3.1.8	Desc If you need to convert files from one markup format into another, pandoc is your swiss-army knife
ParMETIS		3.2.0, 4.0.3	Desc ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. ParMETIS extends the functionality provided by METIS and includes routines that are especially suited for parallel AMR computations and large scale numerical simulations. The algorithms implemented in ParMETIS are based on the parallel multilevel k-way graph-partitioning, adaptive repartitioning, and parallel multi-constrained partitioning schemes.
ParMGridGen		1.0	Desc ParMGridGen is an MPI-based parallel library that is based on the serial package MGridGen, that implements (serial) algorithms for obtaining a sequence of successive coarse grids that are well-suited for geometric multigrid methods. - Homepage: http://www-users.cs.umn.edu/~moulitsa/software.html
ParaView		4.4.0-mpi, 4.4.0, 5.1.2-mpi, 5.2.0-mpi, 5.4.1-mpi, 5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi, 5.11.1	Desc ParaView is a scientific parallel visualizer.
Perl		5.22.1-bare, 5.22.1, 5.28.0, 5.30.0, 5.30.2, 5.32.0-minimal, 5.32.0, 5.32.1-minimal, 5.32.1, 5.34.0, 5.36.0-minimal, 5.36.0, 5.38.0	Desc Larry Wall's Practical Extraction and Report Language This is a minimal build without any modules. Should only be used for build dependencies.
Pies		1.3	Desc GNU Pies stands for the Program Invocation and Execution Supervisor.
Pillow		3.4.2-Python-3.5.1, 4.2.0-Python-3.5.1, 5.3.0-Python-3.6.6, 6.2.1, 8.0.1, 8.3.2	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
ProFit		3.1, 3.3	Desc ProFit is the protein least squares fitting program
Pth		2.0.7	Desc GNU Pth - The GNU Portable Threads
PyQt5		5.11.3-Python-3.6.6, 5.13.1-Python-3.7.4, 5.15.1	Desc PyQt5 is a set of Python bindings for v5 of the Qt application framework from The Qt Company. This bundle includes PyQtWebEngine, a set of Python bindings for The Qt Company's Qt WebEngine framework.
PyTorch		1.2.0-Python-3.6.6, 1.9.0	Desc Tensors and Dynamic neural networks in Python with strong GPU acceleration. PyTorch is a deep learning framework that puts Python first.
PyZMQ		15.2.0-Python-2.7.11-zmq4	Desc Python bindings for ZeroMQ - Homepage: http://www.zeromq.org/bindings:python
Python		2.7.11, 2.7.12, 2.7.15-bare, 2.7.15, 2.7.16, 2.7.18-bare, 2.7.18, 3.4.3, 3.5.1, 3.5.2, 3.6.1, 3.6.4, 3.6.6, 3.7.0, 3.7.4, 3.8.2, 3.8.6, 3.9.5-bare, 3.9.5, 3.9.6-bare, 3.9.6, 3.10.8-bare, 3.10.8, 3.11.5	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Qt		4.8.7	Desc Qt is a comprehensive cross-platform C+ + application framework. - Homepage: http://qt.io/
Qt5		5.6.0, 5.7.0, 5.10.1, 5.13.1, 5.14.2, 5.15.2, 5.15.7	Desc Qt is a comprehensive cross-platform C+ + application framework.
QuTiP		4.3.1-Python-3.6.6	Desc QuTiP is open-source software for simulating the dynamics of open quantum systems.
R	Conda, Jupyter in the cluster	3.3.1, 3.4.1-X11-20160819, 3.5.1, 3.6.1, 4.0.3, 4.1.0, 4.1.2, 4.2.2	Desc R is a free software environment for statistical computing and graphics.
ROOT		v5.34.36-Python-2.7.11, 6.14.06-Python-2.7.15	Desc The ROOT system provides a set of OO frameworks with all the functionality needed to handle and analyze large amounts of data in a very efficient way. - Homepage: http://root.cern.ch/drupal/
Rust		1.52.1, 1.54.0, 1.65.0	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAS		9.4	Desc SAS is a software suite for advanced analytics, multivariate analyses, business intelligence, data management, and predictive analytics.
SCIPOptSuite		8.0.1, 8.0.4-Gurobi-9.5.0, 8.0.4, 9.0.1	Desc SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access of detailed information down to the guts of the solver.
SCOTCH		6.0.4, 6.0.6, 6.0.9, 6.1.0, 6.1.2-no-thread, 6.1.2, 7.0.2, 7.0.3	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.

Modules	Documentation	Versions	Description
SCons		2.4.1-Python-2.7.11	Desc SCons is a software construction tool. - Homepage: http://www.scons.org/
SEPP		4.5.1	Desc SATe-enabled Phylogenetic Placement - addresses the problem of phylogenetic placement of short reads into reference alignments and trees.
SQLite		3.13.0	Desc SQLite: SQL Database Engine in a C Library - Homepage: http://www.sqlite.org/
SUMO		1.9.2-Python-3.7.4, 1.16.0-Python-3.9.6	Desc “Simulation of Urban MObility” (SUMO) is an open source, highly portable, microscopic and continuous traffic simulation package designed to handle large networks. It allows for intermodal simulation including pedestrians and comes with a large set of tools for scenario creation.
ScaFaCoS		1.0.1	Desc ScaFaCoS is a library of scalable fast coulomb solvers.
ScaLAPACK		2.0.2-OpenBLAS-0.2.9-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.14-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.15-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.1, 2.0.2-OpenBLAS-0.2.19-LAPACK-3.7.0, 2.0.2-OpenBLAS-0.2.20, 2.0.2-OpenBLAS-0.3.1, 2.0.2, 2.1.0-fb, 2.1.0, 2.2.0-fb	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.
Schrodinger		2015-3_Linux-x86_64	Desc Schrödinger aims to provide integrated software solutions and services that truly meet its customers’ needs. We want to empower researchers around the world to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials. - Homepage: http://www.schrodinger.com/
SciPy-bundle		2019.10-Python-3.7.4, 2020.03-Python-3.8.2, 2020.11, 2021.10, 2023.02	Desc Bundle of Python packages for scientific software
Shapely		1.7.0-Python-3.7.4, 1.8a1	Desc Shapely is a BSD-licensed Python package for manipulation and analysis of planar geometric objects. It is based on the widely deployed GEOS (the engine of PostGIS) and JTS (from which GEOS is ported) libraries.
Siesta		4.1.5	Desc SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
Singularity		2.3.1, 2.4.2, 2.6.1, 3.5.3	Desc Singularity is a portable application stack packaging and runtime utility. - Homepage: http://gmkurtzer.github.io/singularity
Sphinx		1.8.1-Python-3.6.6	Desc Sphinx is a tool that makes it easy to create intelligent and beautiful documentation. It was originally created for the new Python documentation, and it has excellent facilities for the documentation of Python projects, but C/C+ + is already supported as well, and it is planned to add special support for other languages as well.
Spyder		3.3.6-Python-3.6.6, 4.1.5-Python-3.7.4, 5.1.5	Desc Spyder is an interactive Python development environment providing MATLAB-like features in a simple and light-weighted software.
Subversion		1.12.0	Desc Subversion is an open source version control system.
SuiteSparse		4.2.1-ParMETIS-4.0.3, 4.4.5-METIS-5.1.0, 4.5.3-METIS-5.1.0, 5.1.2-METIS-5.1.0, 5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0, 5.13.0-METIS-5.1.0	Desc SuiteSparse is a collection of libraries manipulate sparse matrices.
Tcl		8.6.3, 8.6.4, 8.6.5, 8.6.6, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13	Desc Tcl (Tool Command Language) is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. - Homepage: http://www.tcl.tk/
Tecplot360ex		2021.1	Desc Quickly plot and animate your CFD results exactly the way you want. Analyze complex solutions, arrange multiple layouts, and communicate your results with professional images and animations.
TensorFlow		1.2.0-Python-3.5.1, 1.4.0-Python-3.5.1, 1.12.0-Python-3.6.6, 2.2.0-Python-3.7.4, 2.3.1-Python-3.7.4, 2.4.1	Desc An open-source software library for Machine Intelligence
TensorRT		4.0.1.6-Python-2.7.15	Desc NVIDIA TensorRT is a platform for high-performance deep learning inference
Tk		8.6.4-no-X11, 8.6.5, 8.6.8, 8.6.9, 8.6.10, 8.6.11, 8.6.12	Desc Tk is an open source, cross-platform widget toolchain that provides a library of basic elements for building a graphical user interface (GUI) in many different programming languages. - Homepage: http://www.tcl.tk/
TurboVNC		2.1.2, 2.2.1	Desc TurboVNC is a derivative of VNC (Virtual Network Computing) that is tuned to provide peak performance for 3D and video workloads.
VMD		1.9.3-Python-2.7.11, 1.9.3-Python-2.7.15, 1.9.4a51	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.
VSEARCH		2.8.0, 2.9.1, 2.22.1	Desc VSEARCH supports de novo and reference based chimera detection, clustering, full-length and prefix dereplication, rereplication, reverse complementation, masking, all-vs-all pairwise global alignment, exact and global alignment searching, shuffling, subsampling and sorting. It also supports FASTQ file analysis, filtering, conversion and merging of paired-end reads.
VTK		5.4.2, 6.3.0-Python-2.7.11, 7.0.0-Python-2.7.11, 8.1.1-Python-2.7.15, 9.0.1, 9.1.0	Desc The Visualization Toolkit (VTK) is an open-source, freely available software system for 3D computer graphics, image processing and visualization. VTK consists of a C+ + class library and several interpreted interface layers including Tcl/Tk, Java, and Python. VTK supports a wide variety of visualization algorithms including: scalar, vector, tensor, texture, and volumetric methods; and advanced modeling techniques such as: implicit modeling, polygon reduction, mesh smoothing, cutting, contouring, and Delaunay triangulation.
VTune		2016_update3, 2019_update3, 2022.3.0, 2023.2.0	Desc Intel VTune Amplifier XE is the premier performance profiler for C, C+ +, C#, Fortran, Assembly and Java. - Homepage: http://software.intel.com/en-us/intel-vtune-amplifier-xe
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools
VirtualGL		2.5.2, 2.6.2, 2.6.4	Desc VirtualGL is an open source toolkit that gives any Linux or Unix remote display software the ability to run OpenGL applications with full hardware acceleration.
Voro+ +		Voro+ 0.4.6	Desc Voro+ + is a software library for carrying out three-dimensional computations of the Voronoi tessellation. A distinguishing feature of the Voro+ + library is that it carries out cell-based calculations, computing the Voronoi cell for each particle individually. It is particularly well-suited for applications that rely on cell-based statistics, where features of Voronoi cells (eg. volume, centroid, number of faces) can be used to analyze a system of particles.
WPS		4.4-dmpar	Desc WRF Preprocessing System (WPS) for WRF. The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
WRF		4.4.1-dmpar	Desc The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
X11		20200222	Desc The X Window System (X11) is a windowing system for bitmap displays
XCFun		2.1.1-Python-3.7.4	Desc Arbitrary order exchange-correlation functional library
Xvfb		1.20.8	Desc Xvfb is an X server that can run on machines with no display hardware and no physical input devices. It emulates a dumb framebuffer using virtual memory.
Z3		4.12.2	Desc Z3 is a theorem prover from Microsoft Research.

Modules	Documentation	Versions	Description
ZeroMQ		4.1.4, 4.2.2, 4.2.5, 4.3.2, 4.3.3	Desc ZeroMQ looks like an embeddable networking library but acts like a concurrency framework. It gives you sockets that carry atomic messages across various transports like in-process, inter-process, TCP, and multicast. You can connect sockets N-to-N with patterns like fanout, pub-sub, task distribution, and request-reply. It's fast enough to be the fabric for clustered products. Its asynchronous I/O model gives you scalable multicore applications, built as asynchronous message-processing tasks. It has a score of language APIs and runs on most operating systems.
arpack-ng		3.3.0, 3.5.0, 3.7.0, 3.8.0, 3.9.1	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
at-spi2-atk		2.34.1, 2.38.0	Desc AT-SPI 2 toolkit bridge
at-spi2-core		2.34.0, 2.38.0, 2.46.0	Desc Assistive Technology Service Provider Interface.
cURL		7.47.0, 7.49.1, 7.55.1, 7.60.0, 7.66.0, 7.69.1, 7.72.0, 7.76.0, 7.78.0, 7.86.0, 8.3.0	Desc libcurl is a free and easy-to-use client-side URL transfer library, supporting DICT, FILE, FTP, FTPS, Gopher, HTTP, HTTPS, IMAP, IMAPS, LDAP, LDAPS, POP3, POP3S, RTMP, RTSP, SCP, SFTP, SMTP, SMTPS, Telnet and TFTP. libcurl supports SSL certificates, HTTP POST, HTTP PUT, FTP uploading, HTTP form based upload, proxies, cookies, user+password authentication (Basic, Digest, NTLM, Negotiate, Kerberos), file transfer resume, http proxy tunneling and more.
ccpnmr		2.4.2-Python-2.7.11	Desc CcpNmr Analysis is a graphics-based interactive NMR spectrum visualisation, resonance assignment and data analysis program
cuDNN		7.1.4.18	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		0.19.4-Python-3.6.6	Desc Dask provides multi-core execution on larger-than-memory datasets using blocked algorithms and task scheduling.
flatbuffers		1.12.0	Desc FlatBuffers: Memory Efficient Serialization Library
foss		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK. - Homepage: (none)
fosscuda		2018b	Desc GCC based compiler toolchain with CUDA support, and including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
futile		1.8.3	Desc The FUTILE project (Fortran Utilities for the Treatment of Innermost Level of Executables) is a set of modules and wrapper that encapsulate the most common low-level operations of a Fortran code.
gappa		0.8.0	Desc gappa is a collection of commands for working with phylogenetic data. Its main focus are evolutionary placements of short environmental sequences on a reference phylogenetic tree. Such data is typically produced by tools like EPA-ng, RAxML-EPA or pplacer and usually stored in jplace files.
gcccuda		2018b	Desc GNU Compiler Collection (GCC) based compiler toolchain, along with CUDA toolkit.
geopandas		0.7.0-Python-3.7.4, 0.8.2	Desc GeoPandas is a project to add support for geographic data to pandas objects. It currently implements GeoSeries and GeoDataFrame types which are subclasses of pandas.Series and pandas.DataFrame respectively. GeoPandas objects can act on shapely geometry objects and perform geometric operations.
gfbf		2022b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including FlexiBLAS (BLAS and LAPACK support) and (serial) FFTW.
git		2.8.0, 2.16.1, 2.23.0-nodocs, 2.28.0-nodocs, 2.32.0-nodocs, 2.33.1-nodocs, 2.38.1-nodocs	Desc Git is a free and open source distributed version control system designed to handle everything from small to very large projects with speed and efficiency.
gmsh		2.9.1	Desc Gmsh is a 3D finite element grid generator with a build-in CAD engine and post-processor. - Homepage: http://geuz.org/gmsh
gnuplot		4.6.0, 5.0.3, 5.2.5, 5.2.8, 5.4.1, 5.4.2, 5.4.6	Desc Portable interactive, function plotting utility
gompi		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021a, 2021b, 2022b, 2023b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support. - Homepage: (none)
gompic		2018b	Desc GNU Compiler Collection (GCC) based compiler toolchain along with CUDA toolkit, including OpenMPI for MPI support with CUDA features enabled.
graph-tool		2.22-Python-3.5.2	Desc Graph-tool is an efficient Python module for manipulation and statistical analysis of graphs (a.k.a. networks). Contrary to most other python modules with similar functionality, the core data structures and algorithms are implemented in C+ +, making extensive use of template metaprogramming, based heavily on the Boost Graph Library. This confers it a level of performance that is comparable (both in memory usage and computation time) to that of a pure C/C+ + library. - Homepage: https://graph-tool.skewed.de/
h5py		2.6.0-Python-2.7.11, 2.8.0-Python-2.7.15, 2.8.0-Python-3.6.6, 2.10.0-Python-3.7.4, 3.6.0	Desc HDF5 for Python (h5py) is a general-purpose Python interface to the Hierarchical Data Format library, version 5. HDF5 is a versatile, mature scientific software library designed for the fast, flexible storage of enormous amounts of data.
help2man		1.47.4	Desc help2man produces simple manual pages from the '–help' and '–version' output of other commands.
horton		2.0.0-Python-2.7.11	Desc Horton is a development platform for electronic structure methods. - Homepage: http://theochem.github.io/horton
hypothesis		4.5.0-Python-3.6.6, 5.41.2, 5.41.5, 6.14.6, 6.68.2	Desc Hypothesis is an advanced testing library for Python. It lets you write tests which are parametrized by a source of examples, and then generates simple and comprehensible examples that make your tests fail. This lets you find more bugs in your code with less work.
iTensor		3.1.11	Desc An efficient and flexible C+ + library for performing tensor network calculations
icc		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc C and C+ + compiler from Intel
iccifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32, 2019.5.281, 2020.1.217	Desc Intel C, C+ + and Fortran compilers
ifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc Fortran compiler from Intel
iimpi		7.2.3-GCC-4.9.2, 8.1.5-GCC-4.9.3-2.25, 2016b, 2016.01-GCC-4.9.3-2.25, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel C/C+ + and Fortran compilers, alongside Intel MPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
imkl		11.2.1.133, 11.3.1.150, 11.3.3.210, 2018.3.222, 2019.3.199, 2019.5.281, 2020.1.217, 2021.2.0, 2022.2.1, 2023.2.0	Desc Intel oneAPI Math Kernel Library
imkl-FFTW		2022.2.1, 2023.2.0	Desc FFTW interfaces using Intel oneAPI Math Kernel Library
impi		5.0.2.044, 5.1.2.150, 5.1.3.181, 2018.3.222, 2018.5.288, 2019.3.199, 2019.7.217, 2021.2.0, 2021.7.1, 2021.10.0	Desc The Intel(R) MPI Library for Linux* OS is a multi-fabric message passing library based on ANL MPICH2 and OSU MVAPICH2. The Intel MPI Library for Linux OS implements the Message Passing Interface, version 3.0 (MPI-3) specification.

Modules	Documentation	Versions	Description
intel		2015a, 2016a, 2016b, 2018b, 2019b, 2019.03, 2020a, 2021a, 2022b, 2023b	Desc Intel Cluster Toolkit Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MPI & Intel MKL.
intel-compilers		2021.2.0, 2022.2.1, 2023.2.1	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)
iomkl		2016b	Desc Intel Cluster Toolchain Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MKL & OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
iompi		2016b	Desc Toolchain with Intel C, C+ + and Fortran compilers, alongside OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
ipp		9.0.4.258, 2019.3.199	Desc Intel Integrated Performance Primitives (Intel IPP) is an extensive library of multicore-ready, highly optimized software functions for multimedia, data processing, and communications applications. Intel IPP offers thousands of optimized functions covering frequently used fundamental algorithms.
itac		9.1.2.024, 2019.3.032, 2021.10.0	Desc The Intel Trace Collector is a low-overhead tracing library that performs event-based tracing in applications. The Intel Trace Analyzer provides a convenient way to monitor application activities gathered by the Intel Trace Collector through graphical displays.
json-c		0.16	Desc JSON-C implements a reference counting object model that allows you to easily construct JSON objects in C, output them as JSON formatted strings and parse JSON formatted strings back into the C representation of JSON objects.
lammps		11Aug17-Python-2.7.11-mpi, 11Aug17-Python-2.7.11, 14May16-Python-2.7.11-mpi, 14May16-Python-2.7.11	Desc LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers.
libAfterImage		1.20	Desc libAfterImage is a generic image manipulation library - Homepage: http://www.afterstep.org/
libarchive		3.4.2	Desc Multi-format archive and compression library
libopus		1.3.1	Desc Opus is a totally open, royalty-free, highly versatile audio codec. Opus is unmatched for interactive speech and music transmission over the Internet, but is also intended for storage and streaming applications. It is standardized by the Internet Engineering Task Force (IETF) as RFC 6716 which incorporated technology from Skype's SILK codec and Xiph.Org's CELT codec.
libsigc+ +		libsigc+ 2.4.1	Desc The libsigc+ + package implements a typesafe callback system for standard C+ +. - Homepage: http://www.gtk.org/
libsodium		1.0.8, 1.0.13, 1.0.16	Desc Sodium is a modern, easy-to-use software library for encryption, decryption, signatures, password hashing and more.
lmod		lmod	Desc Lmod: An Environment Module System
ls-dyna		8.1.105897_mpp_d, 9.0.1.109912_mpp_d, 9.1.113698_mpp_d, 9.2.119543_mpp_d, 10_0_118302_mpp_d	Desc LS-DYNA is a general-purpose finite element program capable of simulating complex real world problems. It is used by the automobile, aerospace, construction, military, manufacturing, and bioengineering industries. - Homepage: http://www.lstc.com/products/ls-dyna
magma		2.5.0	Desc The MAGMA project aims to develop a dense linear algebra library similar to LAPACK but for heterogeneous/hybrid architectures, starting with current Multicore+GPU systems.
make		4.3, 4.4.1	Desc GNU version of make utility
matplotlib		1.4.3-Python-2.7.11, 1.5.1-Python-2.7.11, 1.5.1-Python-3.4.3, 1.5.1-Python-3.5.1, 1.5.1-Python-3.5.2, 2.0.2-Python-3.5.1, 2.0.2-Python-3.6.1, 3.0.0-Python-3.6.6, 3.1.1-Python-3.7.4, 3.2.1-Python-3.8.2, 3.3.3, 3.4.3	Desc matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell, web application servers, and six graphical user interface toolkits.
molmod		1.4.5-Python-3.7.4	Desc MolMod is a Python library with many compoments that are useful to write molecular modeling programs.
mpi4py		2.0.0-Python-2.7.11, 3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.0.3-Python-3.8.2	Desc MPI for Python (mpi4py) provides bindings of the Message Passing Interface (MPI) standard for the Python programming language, allowing any Python program to exploit multiple processors. - Homepage: https://bitbucket.org/mpi4py/mpi4py
mpifileutils	mpiFileUtils	0.10.1, 0.11, 0.11.1	Desc MPI-Based File Utilities For Distributed Systems
mpmath		0.19-Python-2.7.11, 0.19-Python-3.4.3	Desc mpmath can be used as an arbitrary-precision substitute for Python's float/complex types and math/cmath modules, but also does much more advanced mathematics. Almost any calculation can be performed just as well at 10-digit or 1000-digit precision, with either real or complex numbers, and in many cases mpmath implements efficient algorithms that scale well for extremely high precision work. - Homepage: http://mpmath.org/
msindo		3.6	Desc Semiempirical SCF MO program for systems with first-, second-, third-, and fourth-row elements - Homepage: http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=MSINDO&lang=english
ncview		2.1.8	Desc Ncview is a visual browser for netCDF format files. Typically you would use ncview to get a quick and easy, push-button look at your netCDF files. You can view simple movies of the data, view along various dimensions, take a look at the actual data values, change color maps, invert the data, etc.
netCDF		4.4.0, 4.4.1, 4.6.1, 4.7.1, 4.7.4, 4.8.0, 4.8.1, 4.9.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
netCDF-Fortran		4.4.3, 4.4.4, 4.5.2, 4.5.3, 4.6.0	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
nettle		3.2	Desc Nettle is a cryptographic library that is designed to fit easily in more or less any context: In crypto toolkits for object-oriented languages (C+ +, Python, Pike, ...), in applications like LSH or GNUPG, or even in kernel space. - Homepage: http://www.lysator.liu.se/~nisse/nettle/
networkx		1.10-Python-2.7.11, 2.2-Python-3.5.1, 2.4-Python-3.7.4, 2.5, 2.6.3	Desc NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.
nlohmann_json		3.11.2	Desc JSON for Modern C+ +
nsync		1.24.0	Desc nsync is a C library that exports various synchronization primitives, such as mutexes
numba		0.29.0-Python-2.7.11	Desc Numba is an Open Source NumPy-aware optimizing compiler for Python sponsored by Continuum Analytics, Inc. It uses the remarkable LLVM compiler infrastructure to compile Python syntax to machine code. - Homepage: http://numba.pydata.org/
numpy		1.8.2-Python-2.7.11, 1.9.2-Python-2.7.11, 1.10.1-Python-2.7.11, 1.10.1-Python-3.4.3, 1.10.1-Python-3.5.1, 1.13.0-Python-3.5.1, 1.18.5-Python-3.7.4, 1.18.5-Python-3.8.2	Desc NumPy is the fundamental package for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C+ + and Fortran code, useful linear algebra, Fourier transform, and random number capabilities. Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases. - Homepage: http://www.numpy.org
pandas		0.18.0-Python-2.7.11, 0.18.0-Python-3.5.1	Desc pandas is an open source, BSD-licensed library providing high-performance, easy-to-use data structures and data analysis tools for the Python programming language. - Homepage: https://pypi.python.org/pypi/pandas/
parallel		20190922, 20210322	Desc parallel: Build and execute shell commands in parallel
pcp		2.0.0_39-Python-2.7.16	Desc A parallel copy program for lustre
phenix		1.10.1-2155	Desc PHENIX is a software suite for the automated determination of molecular structures using X-ray crystallography and other methods. - Homepage: http://www.phenix-online.org

Modules	Documentation	Versions	Description
pigz		2.6	Desc pigz, which stands for parallel implementation of gzip, is a fully functional replacement for gzip that exploits multiple processors and multiple cores to the hilt when compressing data. pigz was written by Mark Adler, and uses the zlib and pthread libraries.
pkgconf		1.8.0, 1.9.3, 2.0.3	Desc pkgconf is a program which helps to configure compiler and linker flags for development libraries. It is similar to pkg-config from freedesktop.org.
protobuf		3.2.0	Desc Google Protocol Buffers - Homepage: https://github.com/google/protobuf/
protobuf-python		3.2.0-Python-3.4.3, 3.2.0-Python-3.5.1, 3.10.0-Python-3.7.4	Desc Python Protocol Buffers runtime library. - Homepage: https://github.com/google/protobuf/
psutil		5.6.3-Python-3.6.6, 5.9.4	Desc A cross-platform process and system utilities module for Python
pytest		7.1.3	Desc pytest: simple powerful testing with Python
qutip		2.2.0-Python-2.7.11, 3.1.0-Python-2.7.11, 4.0.2-Python-3.4.3	Desc QuTiP : Quantum Toolbox in Python - Homepage: http://qutip.org/
scikit-image		0.12.3-Python-3.5.1, 0.14.1-Python-3.6.6	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-learn		0.18.1-Python-3.5.1, 0.20.0-Python-3.6.6, 0.20.3-Python-3.6.6, 0.21.3-Python-3.7.4, 0.23.2	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-umfpack		0.2.1-Python-2.7.11	Desc scikit-umfpack provides a wrapper of UMFPACK sparse direct solver to SciPy. - Homepage: http://rc.github.io/scikit-umfpack/
scipy		0.16.1-Python-2.7.11, 0.17.1-Python-2.7.11, 0.17.1-Python-3.4.3, 0.19.1-Python-3.5.1	Desc SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension for Python. - Homepage: http://www.scipy.org
settarg		settarg	Desc
sparsehash		2.0.2	Desc An extremely memory-efficient hash_map implementation. 2 bits/entry overhead! The SparseHash library contains several hash-map implementations, including implementations that optimize for space or speed. - Homepage: https://code.google.com/p/sparsehash/
sympy		1.0-Python-2.7.11, 1.0-Python-3.4.3	Desc SymPy is a Python library for symbolic mathematics. It aims to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries. - Homepage: http://sympy.org/
tbb		4.4.6.258, 2019_U9, 2019.2.187, 2020.3, 2021.10.0	Desc Intel Threading Building Blocks 4.0 (Intel TBB) is a widely used, award-winning C+ + template library for creating reliable, portable, and scalable parallel applications. Use Intel TBB for a simple and rapid way of developing robust task-based parallel applications that scale to available processor cores, are compatible with multiple environments, and are easier to maintain. Intel TBB is the most proficient way to implement future-proof parallel applications that tap into the power and performance of multicore and manycore hardware platforms.
texlive		20200406, 20210324, 20240312	Desc TeX is a typesetting language. Instead of visually formatting your text, you enter your manuscript text intertwined with TeX commands in a plain text file. You then run TeX to produce formatted output, such as a PDF file. Thus, in contrast to standard word processors, your document is a separate file that does not pretend to be a representation of the final typeset output, and so can be easily edited and manipulated.
typing-extensions		3.7.4.3	Desc Typing Extensions – Backported and Experimental Type Hints for Python
utf8proc		2.2.0	Desc utf8proc is a small, clean C library that provides Unicode normalization, case-folding, and other operations for data in the UTF-8 encoding.
wheel		0.29.0-Python-3.4.3, 0.29.0-Python-3.5.1, 0.31.1-Python-2.7.15, 0.31.1-Python-3.6.6	Desc A built-package format for Python.
xtb		6.4.1, 6.5.1, 6.6.1	Desc xtb - An extended tight-binding semi-empirical program package.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

Nehalem(SSE)

Installed software as of Wed, 23 Oct 2024 07:35:24 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	6.14-2, 2016, 2017-hotfix-1819, 2017, 2018, 2019-hotfix-1939, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341	Desc Finite Element Analysis software for modeling, visualization and best-in-class implicit and explicit dynamics FEA.
AMPL-MP		3.1.0	Desc An open-source library for mathematical programming.
ANSYS	ANSYS / CFX	15.0, 16.0, 16.2, 17.2, 18.0, 18.2, 19.0, 19.2, 19.3, 2019.2, 2019.3, 2020.1, 2020.2, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ANSYSEM		17.2, 18.0, 18.1, 18.2, 19.0, 19.1, 20.2, 2022.2, 2023.1	Desc ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater. - Homepage: http://www.ansys.com
ARIA		2.3.1-Python-2.7.11	Desc ARIA (Ambiguous Restraints for Iterative Assignment) is a software for automated NOE assignment and NMR structure calculation
ASE		3.12.0-Python-2.7.11, 3.16.0-Python-2.7.11, 3.16.2-Python-3.6.6	Desc ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language.
ATK		2.20.0, 2.22.0	Desc ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications. - Homepage: https://developer.gnome.org/ATK/stable/
ATSAS		2.7.2-5.el6.x86_64	Desc ATSAS is a program suite for small-angle scattering data analysis from biological macromolecules. - Homepage: http://www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html
Advisor		2016_update3, 2019_update3, 2023.2.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain - Homepage: https://software.intel.com/intel-advisor-xe
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		14-AmberTools-15-patchlevel-0-0, 18-AmberTools-18-patchlevel-9-5-CUDA	Desc Amber (originally Assisted Model Building with Energy Refinement) is software for performing molecular dynamics and structure prediction.

Modules	Documentation	Versions	Description
BLAST+		2.2.31-Python-2.7.11	Desc Basic Local Alignment Search Tool, or BLAST, is an algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences. - Homepage: http://blast.ncbi.nlm.nih.gov/
BLIS		0.8.1	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
BWA		0.7.17	Desc Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome.
Bazel		0.5.2, 0.7.0, 0.18.0, 2.0.0, 3.4.1, 3.7.2	Desc Bazel is a build tool that builds code quickly and reliably. It is used to build the majority of Google's software.
Biopython		1.71-Python-2.7.11, 1.78	Desc Biopython is a set of freely available tools for biological computation written in Python by an international team of developers. It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics.
Bonnie+ +		Bonnie+ 1.97	Desc Bonnie+ +-1.97: Enhanced performance Test of Filesystem I/O - Homepage: http://www.coker.com.au/bonnie+ +/
Boost		1.47.0, 1.58.0-Python-2.7.11, 1.59.0-Python-2.7.11, 1.60.0-Python-2.7.11, 1.60.0, 1.61.0-Python-2.7.11, 1.61.0, 1.63.0-Python-3.5.2, 1.66.0, 1.67.0, 1.68.0-Python-2.7.15, 1.71.0, 1.74.0, 1.77.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Boost.Python		1.67.0-Python-2.7.15	Desc Boost.Python is a C+ + library which enables seamless interoperability between C+ + and the Python programming language.
CFITSIO		3.38, 3.45	Desc CFITSIO is a library of C and Fortran subroutines for reading and writing data files in FITS (Flexible Image Transport System) data format.
CGAL		4.7-Python-2.7.11, 4.8-Python-2.7.11, 4.8.1-Python-3.5.2, 4.8.1, 4.11.1-Python-2.7.15, 4.14.1-Python-3.7.4, 4.14.3, 5.2	Desc The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C+ + library.
CGNS		2.5.5, 3.3.1	Desc The CGNS system is designed to facilitate the exchange of data between sites and applications, and to help stabilize the archiving of aerodynamic data.
CLooG		0.18.1	Desc CLooG is a free software and library to generate code for scanning Z-polyhedra. That is, it finds a code (e.g. in C, FORTRAN...) that reaches each integral point of one or more parameterized polyhedra. CLooG has been originally written to solve the code generation problem for optimizing compilers based on the polytope model. Nevertheless it is used now in various area e.g. to build control automata for high-level synthesis or to find the best polynomial approximation of a function. CLooG may help in any situation where scanning polyhedra matters. While the user has full control on generated code quality, CLooG is designed to avoid control overhead and to produce a very effective code. - Homepage: http://www.bastoul.net/cloog/index.php
CMake		2.8.4, 3.4.1, 3.4.3, 3.5.2, 3.6.1, 3.7.1, 3.9.6, 3.11.4, 3.12.1, 3.15.3, 3.16.4, 3.18.4, 3.20.1, 3.21.1, 3.22.1	Desc CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software. - Homepage: http://www.cmake.org
CNS		1.3-haddock-2.2, 1.3-haddock-2.4, 1.21-aria2.3	Desc Crystallography & NMR System (CNS) has been designed to provide a flexible multi-level hierachical approach for the most commonly used algorithms in macromolecular structure determination
COMSOL	COMSOL	5.1, 5.2, 5.4, 5.5, 5.6, 6.0, 6.1, 6.2	Desc COMSOL Multiphysics is a finite element analysis, solver and simulation software/FEA software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. - Homepage: https://www.comsol.com/
CPMD	CPMD	4.1, 4.3	Desc CPMD The CPMD code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. - Homepage: http://www.cpmd.org/
CRYSTAL14		1.0.4	Desc Crystal is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations - Homepage: http://www.crystalsolutions.eu/
CUDA		7.5.18, 8.0.44, 9.2.88	Desc CUDA (formerly Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. CUDA gives developers access to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs. - Homepage: https://developer.nvidia.com/cuda-toolkit
Cython		0.24-Python-2.7.11, 0.24-Python-3.4.3, 0.29.22	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
DMTCP		2.6.0	Desc DMTCP is a tool to transparently checkpoint the state of multiple simultaneous applications, including multi-threaded and distributed applications. It operates directly on the user binary executable, without any Linux kernel modules or other kernel modifications.
DendroPy		4.5.2	Desc A Python library for phylogenetics and phylogenetic computing: reading, writing, simulation, processing and manipulation of phylogenetic trees (phylogenies) and characters.
Doxygen		1.8.11	Desc Doxygen is a documentation system for C+ +, C, Java, Objective-C, Python, IDL (Corba and Microsoft flavors), Fortran, VHDL, PHP, C#, and to some extent D.
ELPA		2021.05.001	Desc Eigenvalue SoLvers for Petaflop-Applications .
EasyBuild-custom		1.0	Desc EasyBuild is a software build and installation framework - Homepage: http://hpcugent.github.com/easybuild/
Eigen		3.2.9, 3.3.4, 3.3.7, 3.3.8, 3.3.9, 3.4.0	Desc Eigen is a C+ + template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
FDS		6.4.0, 6.5.2, 6.6.0, 6.7.3, 6.7.4	Desc Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires. - Homepage: http://firemodels.github.io/fds-smv/
FEKO	FEKO	2017.2_hw, 2017.2.5_hw, 2018_hw, 2019_hw, 2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering
FFTW		3.3.4-PFFT-20150905, 3.3.4, 3.3.6, 3.3.8, 3.3.10	Desc FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data.
FLANN		1.8.4-Python-2.7.15	Desc FLANN is a library for performing fast approximate nearest neighbor searches in high dimensional spaces.
Fiona		1.8.13-Python-3.7.4, 1.8.20	Desc Fiona is designed to be simple and dependable. It focuses on reading and writing data in standard Python IO style and relies upon familiar Python types and protocols such as files, dictionaries, mappings, and iterators instead of classes specific to OGR. Fiona can read and write real-world data using multi-layered GIS formats and zipped virtual file systems and integrates readily with other Python GIS packages such as pyproj, Rtree, and Shapely.
FlexiBLAS		3.0.4	Desc FlexiBLAS is a wrapper library that enables the exchange of the BLAS and LAPACK implementation used by a program without recompiling or relinking it.
Flux		2019	Desc Altair Flux captures the complexity of electromagnetic and thermal phenomena to predict the behavior of future products with precision.
FriBidi		1.0.5, 1.0.10	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		24.5.4, 24.5.6_nhus, 24.7.4_nhus, 24.7.4, 26.1.0_nhus, 26.1.0, 30.3.0, 45.7.0, 46.5.0	Desc The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. - Homepage: https://www.gams.com/

Modules	Documentation	Versions	Description
GCC		4.8.3, 4.9.2, 4.9.3-binutils-2.25, 4.9.3-2.25, 5.3.0-2.26, 5.4.0-2.26, 6.3.0-2.27, 6.4.0-2.28, 7.3.0-2.30, 8.3.0, 9.3.0, 10.2.0, 10.3.0, 11.2.0	Desc The GNU Compiler Collection includes front ends for C, C+ +, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc+ +, libgcj,...).
GDB		9.1-Python-3.7.4	Desc The GNU Project Debugger
GEOS		3.6.1-Python-2.7.12	Desc GEOS (Geometry Engine - Open Source) is a C+ + port of the Java Topology Suite (JTS)
GMP		6.1.0, 6.1.1, 6.1.2, 6.2.0, 6.2.1	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers. - Homepage: http://gmplib.org/
GNUGo		3.8	Desc GNU Go is a free program that plays the game of Go
GPAW		1.1.0-Python-2.7.11, 1.4.0-Python-2.7.11, 1.4.0-Python-3.6.6	Desc GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.
GROMACS		5.1.2-hybrid, 2016.5-hybrid, 2018.4, 2019	Desc GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.
GSL		1.16, 2.1, 2.5, 2.6, 2.7	Desc The GNU Scientific Library (GSL) is a numerical library for C and C+ + programmers. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting.
GST-plugins-base		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/
GStreamer		1.6.4	Desc GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing. - Homepage: http://gstreamer.freedesktop.org/
GTK+		2.24.30, 2.24.31	Desc The GTK+ 2 package contains libraries used for creating graphical user interfaces for applications. - Homepage: https://developer.gnome.org/gtk+/stable/
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g09.D01, g09.E01, g16.A03, g16.B01	Desc Gaussian provides state-of-the-art capabilities for electronic structure modeling.
GitPython		2.1.11-Python-3.6.6	Desc GitPython is a python library used to interact with Git repositories
Go		1.16.6	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
GraphicsMagick		1.3.23	Desc GraphicsMagick is the swiss army knife of image processing.
Guile		1.8.8	Desc Guile is a programming language, designed to help programmers create flexible applications that can be extended by users or other programmers with plug-ins, modules, or scripts.
Gurobi		6.5.0, 7.0.2, 7.5.2, 8.1.0, 9.0.1, 9.1.2, 9.5.0, 11.0.0	Desc The Gurobi Optimizer is a state-of-the-art solver for mathematical programming. The solvers in the Gurobi Optimizer were designed from the ground up to exploit modern architectures and multi-core processors, using the most advanced implementations of the latest algorithms.
HADDOCK		2.2-Python-2.7.11, 2.4-Python-2.7.16	Desc HADDOCK (High Ambiguity Driven biomolecular DOCKing) is an information-driven flexible docking approach for the modelling of biomolecular complexes
HDF		4.2.15	Desc HDF (also known as HDF4) is a library and multi-object file format for storing and managing data between machines.
HDF5		1.8.16-serial, 1.8.16, 1.8.17, 1.10.2, 1.10.5, 1.10.7, 1.12.1	Desc HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.
HDFView		2.14-Java-1.8.0_152-centos7	Desc HDFView is a visual tool for browsing and editing HDF4 and HDF5 files.
HH-suite		3.3.0	Desc The HH-suite is an open-source software package for sensitive protein sequence searching based on the pairwise alignment of hidden Markov models (HMMs).
HMMER		3.3.2	Desc HMMER is used for searching sequence databases for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs). Compared to BLAST, FASTA, and other sequence alignment and database search tools based on older scoring methodology, HMMER aims to be significantly more accurate and more able to detect remote homologs because of the strength of its underlying mathematical models. In the past, this strength came at significant computational expense, but in the new HMMER3 project, HMMER is now essentially as fast as BLAST.
HPL		2.2	Desc HPL is a software package that solves a (random) dense linear system in double precision (64 bits) arithmetic on distributed-memory computers. It can thus be regarded as a portable as well as freely available implementation of the High Performance Computing Linpack Benchmark.
Hadoop-cluster		1.0	Desc Framework for deploying Hadoop clusters on traditional HPC - Homepage: http://luis.uni-hannover.de
ICU		61.1, 64.2, 67.1, 69.1	Desc ICU is a mature, widely used set of C/C+ + and Java libraries providing Unicode and Globalization support for software applications.
IPython		3.2.3-Python-2.7.11, 6.2.1-Python-3.6.4, 7.2.0-Python-3.6.6, 7.9.0-Python-3.7.4, 7.18.1-Python-3.7.4, 7.25.0	Desc IPython provides a rich architecture for interactive computing with: Powerful interactive shells (terminal and Qt-based). A browser-based notebook with support for code, text, mathematical expressions, inline plots and other rich media. Support for interactive data visualization and use of GUI toolkits. Flexible, embeddable interpreters to load into your own projects. Easy to use, high performance tools for parallel computing.
ImageMagick		7.0.8-11, 7.0.9-5, 7.1.0-4	Desc ImageMagick is a software suite to create, edit, compose, or convert bitmap images
Inspector		2016_update3, 2019_update3, 2023.2.0	Desc Intel Inspector XE is an easy to use memory error checker and thread checker for serial and parallel applications - Homepage: http://software.intel.com/en-us/intel-inspector-xe
Ipopt		3.14.4	Desc IPOPT (Interior Point Optimizer, pronounced Eye-Pea-Opt) is an open source software package for large-scale nonlinear optimization.
Java		1.8.0_45, 1.8.0_72, 1.8.0_92, 1.8.0_144, 1.8.0_152, 11.0.2, 11.0.16	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.
Julia		1.6.1-linux-x86_64, 1.7.0-linux-x86_64, 1.7.2-linux-x86_64, 1.10.2-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter in the cluster	2.2.8-Python-3.7.4, 3.1.14	Desc JupyterLab is the next-generation user interface for Project Jupyter offering all the familiar building blocks of the classic Jupyter Notebook (notebook, terminal, text editor, file browser, rich outputs, etc.) in a flexible and powerful user interface. JupyterLab will eventually replace the classic Jupyter Notebook.
Kalign		3.3.1	Desc Kalign is a fast multiple sequence alignment program for biological sequences.
LAME		3.100	Desc LAME is a high quality MPEG Audio Layer III (MP3) encoder licensed under the LGPL.
LAMMPS		3Mar2020-Python-3.7.4-kokkos	Desc LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.

Modules	Documentation	Versions	Description
LAPACK		3.5.0	Desc LAPACK is written in Fortran90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems. - Homepage: http://www.netlib.org/lapack/
Lua		5.4.2, 5.4.3	Desc Lua is a powerful, fast, lightweight, embeddable scripting language. Lua combines simple procedural syntax with powerful data description constructs based on associative arrays and extensible semantics. Lua is dynamically typed, runs by interpreting bytecode for a register-based virtual machine, and has automatic memory management with incremental garbage collection, making it ideal for configuration, scripting, and rapid prototyping.
Lumerical		2020-2.4, 2021-2.3, 2022-1, 2023-1, 2024-1.02	Desc Ansys Lumerical photonic multiphysics and circuit simulation suites. Design components and analyze electrical, thermal and optical effects at the physical level. Simulate and optimize the performance of photonic integrated circuits
MATLAB	MATLAB	2015a, 2016b, 2017a, 2017b, 2018a, 2018b, 2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b	Desc MATLAB is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran. - Homepage: http://www.mathworks.com/products/matlab
METIS		5.1.0, 5.1.0-32bitIDX	Desc METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms implemented in METIS are based on the multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning schemes.
MPC		1.0.3	Desc Gnu Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It extends the principles of the IEEE-754 standard for fixed precision real floating point numbers to complex numbers, providing well-defined semantics for every operation. At the same time, speed of operation at high precision is a major design goal. - Homepage: http://www.multiprecision.org/
MPFR		3.1.4, 4.0.1, 4.0.2, 4.1.0	Desc The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.
MUMPS		5.2.1-metis, 5.3.5-metis	Desc A parallel sparse direct solver
Mako		1.0.4-Python-2.7.12, 1.0.7-Python-2.7.15, 1.1.0, 1.1.3, 1.1.4	Desc A super-fast templating language that borrows the best ideas from the existing templating languages
Maple		17, 18, 2015.0, 2017, 2020.1, 2021.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface. - Homepage: http://www.maplesoft.com/products/maple/
Mathematica		10.4.1, 11.3.0, 12.1.1, 12.3.0, 13.0.0, 13.2.1	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields. - Homepage: http://www.wolfram.com/mathematica
Meson		0.51.2-Python-3.7.4, 0.53.2-Python-3.8.2, 0.55.3, 0.58.2	Desc Meson is a cross-platform build system designed to be both as fast and as user friendly as possible.
Mesquite		2.3.0	Desc Mesh-Quality Improvement Library - Homepage: https://software.sandia.gov/mesquite/
Miniconda2		4.5.1, 4.5.12, 4.7.10	Desc Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.
Miniconda3	Conda	4.10.3, 22.11.1-1, 23.5.2-0	Desc Miniconda is a free minimal installer for conda. It is a small, bootstrap version of Anaconda that includes only conda, Python, the packages they depend on, and a small number of other useful packages.
Modeller		9.19-Python-2.7.11	Desc MODELLER is used for homology or comparative modeling of protein three-dimensional structures (1,2). The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.
Molden		5.0, 5.6, 5.7, 5.9, 5.9.4	Desc Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK, GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac - Homepage: http://www.cmbi.ru.nl/molden/
Mothur		1.40.3-Python-2.7.11, 1.40.5-Python-2.7.11, 1.41.3-Python-2.7.15, 1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.
NAMD		2.12-mpi, 2.13-mpi	Desc NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
NCCL		2.3.7	Desc The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.
NFFT	NFFT	3.1.3, 3.3.0, 3.3.1, 3.5.0	Desc The NFFT (nonequispaced fast Fourier transform or nonuniform fast Fourier transform) is a C subroutine library for computing the nonequispaced discrete Fourier transform (NDFT) and its generalisations in one or more dimensions, of arbitrary input size, and of complex data.
NVHPC		23.1-CUDA-12.0.0	Desc C, C+ + and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
NWChem		6.6.revision27746-2015-10-20-Python-2.7.11	Desc NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters. NWChem software can handle: biomolecules, nanostructures, and solid-state; from quantum to classical, and all combinations; Gaussian basis functions or plane-waves; scaling from one to thousands of processors; properties and relativity. - Homepage: http://www.nwchem-sw.org
Ninja		1.9.0, 1.10.0, 1.10.1, 1.10.2	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1	Desc ORCA is a flexible, efficient and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated ab initio methods. It can also treat environmental and relativistic effects.
Octave		3.8.2, 4.0.0, 4.4.1, 5.1.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations. - Homepage: http://www.gnu.org/software/octave/
Octopus		5.0.0-mpi, 5.0.0, 7.3-mpi, 7.3, 9.1-mpi, 11.4	Desc Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory (DFT), in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation.
OpenBLAS		0.2.9-LAPACK-3.5.0, 0.2.13-LAPACK-3.5.0, 0.2.14-LAPACK-3.5.0, 0.2.15-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.0, 0.2.18-LAPACK-3.6.1, 0.2.19-LAPACK-3.7.0, 0.2.20, 0.3.1, 0.3.7, 0.3.9, 0.3.12, 0.3.18	Desc OpenBLAS is an optimized BLAS library based on GotoBLAS2 1.13 BSD version.
OpenBabel		3.1.1-Python-3.7.4	Desc Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.
OpenCV		2.4.12, 3.1.0, 4.0.1-Python-2.7.15, 4.2.0-Python-3.7.4, 4.5.1-contrib	Desc OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products. Includes extra modules for OpenCV from the contrib repository.
OpenEXR		2.5.5	Desc OpenEXR is a high dynamic-range (HDR) image file format developed by Industrial Light & Magic for use in computer imaging applications
OpenFAST		2.3.0, 2.4.0, 3.1.0	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.

Modules	Documentation	Versions	Description
OpenFOAM		v1612+, v1906, v1912, v2012, v2106, v2112, 2.3.0, 2.3.1, 3.0.0, 4.0, 4.1, 6, 7, 8, 9	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.
OpenFOAM-Extend		3.2, 4.0	Desc OpenFOAM is a free, open source CFD software package. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. - Homepage: http://www.extend-project.de/
OpenMPI		1.8.1, 1.8.8, 1.10.2, 1.10.3, 2.0.2, 2.1.1, 3.1.1, 3.1.4, 4.0.3, 4.0.5, 4.1.1	Desc The Open MPI Project is an open source MPI-3 implementation.
OpenPGM		5.2.122	Desc OpenPGM is an open source implementation of the Pragmatic General Multicast (PGM) specification in RFC 3208 available at www.ietf.org. PGM is a reliable and scalable multicast protocol that enables receivers to detect loss, request retransmission of lost data, or notify an application of unrecoverable loss. PGM is a receiver-reliable protocol, which means the receiver is responsible for ensuring all data is received, absolving the sender of reception responsibility.
OpenSSL		1.0.1s, 1.0.2g, 1.0.2h, 1.1, 1.1.1d	Desc The OpenSSL Project is a collaborative effort to develop a robust, commercial-grade, full-featured, and Open Source toolchain implementing the Secure Sockets Layer (SSL v2/v3) and Transport Layer Security (TLS v1) protocols as well as a full-strength general purpose cryptography library. - Homepage: http://www.openssl.org/
PCL		1.9.1-Python-2.7.15, 1.12.1-Python-3.8.6	Desc The Point Cloud Library (PCL) is a standalone, large scale, open project for 2D/3D image and point cloud processing.
PFFT		1.0.8-alpha	Desc PFFT is a software library for computing massively parallel, fast Fourier transformations on distributed memory architectures. PFFT can be understood as a generalization of FFTW-MPI to multidimensional data decomposition.
PGI		16.5-GCC-5.4.0-2.26	Desc C, C+ + and Fortran compilers from The Portland Group - PGI
PICRUSt2		2.5.0-Python-3.9.6	Desc PICRUSt2 (Phylogenetic Investigation of Communities by Reconstruction of Unobserved States) is a software for predicting functional abundances based only on marker gene sequences. Check out the pre-print here.
PIL		1.1.7-Python-2.7.11	Desc The Python Imaging Library (PIL) adds image processing capabilities to your Python interpreter. This library supports many file formats, and provides powerful image processing and graphics capabilities. - Homepage: http://www.pythonware.com/products/pil
PLUMED		2.5.3-Python-3.7.4, 2.7.3	Desc PLUMED is an open source library for free energy calculations in molecular systems which works together with some of the most popular molecular dynamics engines. Free energy calculations can be performed as a function of many order parameters with a particular focus on biological problems, using state of the art methods such as metadynamics, umbrella sampling and Jarzynski-equation based steered MD. The software, written in C+ +, can be easily interfaced with both fortran and C/C+ + codes.
POVRay		3.6.1	Desc The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. - Homepage: www.povray.org
PSolver		1.8.3	Desc Interpolating scaling function Poisson Solver Library
Pandoc		3.1.8	Desc If you need to convert files from one markup format into another, pandoc is your swiss-army knife
ParMETIS		3.2.0, 4.0.3	Desc ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. ParMETIS extends the functionality provided by METIS and includes routines that are especially suited for parallel AMR computations and large scale numerical simulations. The algorithms implemented in ParMETIS are based on the parallel multilevel k-way graph-partitioning, adaptive repartitioning, and parallel multi-constrained partitioning schemes.
ParMGridGen		1.0	Desc ParMGridGen is an MPI-based parallel library that is based on the serial package MGridGen, that implements (serial) algorithms for obtaining a sequence of successive coarse grids that are well-suited for geometric multigrid methods. - Homepage: http://www-users.cs.umn.edu/~moulitsa/software.html
ParaView		4.4.0-mpi, 4.4.0, 5.1.2-mpi, 5.2.0-mpi, 5.4.1-mpi, 5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi	Desc ParaView is a scientific parallel visualizer.
Perl		5.22.1-bare, 5.22.1, 5.28.0, 5.30.0, 5.30.2, 5.32.0-minimal, 5.32.0, 5.32.1-minimal, 5.32.1, 5.34.0	Desc Larry Wall's Practical Extraction and Report Language This is a minimal build without any modules. Should only be used for build dependencies.
Pies		1.3	Desc GNU Pies stands for the Program Invocation and Execution Supervisor.
Pillow		3.4.2-Python-3.5.1, 4.2.0-Python-3.5.1, 5.3.0-Python-3.6.6, 6.2.1, 8.0.1, 8.3.2	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
ProFit		3.1, 3.3	Desc ProFit is the protein least squares fitting program
Pth		2.0.7	Desc GNU Pth - The GNU Portable Threads
PyQt5		5.11.3-Python-3.6.6, 5.13.1-Python-3.7.4, 5.15.1	Desc PyQt5 is a set of Python bindings for v5 of the Qt application framework from The Qt Company. This bundle includes PyQtWebEngine, a set of Python bindings for The Qt Company's Qt WebEngine framework.
PyTorch		1.2.0-Python-3.6.6	Desc Tensors and Dynamic neural networks in Python with strong GPU acceleration. PyTorch is a deep learning framework that puts Python first.
PyZMQ		15.2.0-Python-2.7.11-zmq4	Desc Python bindings for ZeroMQ - Homepage: http://www.zeromq.org/bindings:python
Python		2.7.11, 2.7.12, 2.7.15-bare, 2.7.15, 2.7.16, 2.7.18-bare, 2.7.18, 3.4.3, 3.5.1, 3.5.2, 3.6.1, 3.6.4, 3.6.6, 3.7.0, 3.7.4, 3.8.2, 3.8.6, 3.9.6-bare, 3.9.6	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Qt		4.8.7	Desc Qt is a comprehensive cross-platform C+ + application framework. - Homepage: http://qt.io/
Qt5		5.6.0, 5.7.0, 5.10.1, 5.13.1, 5.14.2, 5.15.2	Desc Qt is a comprehensive cross-platform C+ + application framework.
QuTiP		4.3.1-Python-3.6.6	Desc QuTiP is open-source software for simulating the dynamics of open quantum systems.
R	Conda, Jupyter in the cluster	3.3.1, 3.4.1-X11-20160819, 3.5.1, 3.6.1, 4.0.3, 4.1.0	Desc R is a free software environment for statistical computing and graphics. - Homepage: http://www.r-project.org/
ROOT		v5.34.36-Python-2.7.11, 6.14.06-Python-2.7.15	Desc The ROOT system provides a set of OO frameworks with all the functionality needed to handle and analyze large amounts of data in a very efficient way. - Homepage: http://root.cern.ch/drupal/
Rust		1.54.0	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAS		9.4	Desc SAS is a software suite for advanced analytics, multivariate analyses, business intelligence, data management, and predictive analytics.
SCIPOptSuite		8.0.1	Desc SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access of detailed information down to the guts of the solver.
SCOTCH		6.0.4, 6.0.6, 6.0.9, 6.1.0, 6.1.2	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.

Modules	Documentation	Versions	Description
SCons		2.4.1-Python-2.7.11	Desc SCons is a software construction tool. - Homepage: http://www.scons.org/
SQLite		3.13.0	Desc SQLite: SQL Database Engine in a C Library - Homepage: http://www.sqlite.org/
SUMO		1.9.2-Python-3.7.4	Desc “Simulation of Urban MObility” (SUMO) is an open source, highly portable, microscopic and continuous traffic simulation package designed to handle large networks. It allows for intermodal simulation including pedestrians and comes with a large set of tools for scenario creation.
ScaFaCoS		1.0.1	Desc ScaFaCoS is a library of scalable fast coulomb solvers.
ScaLAPACK		2.0.2-OpenBLAS-0.2.9-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.14-LAPACK-3.5.0, 2.0.2-OpenBLAS-0.2.15-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.0, 2.0.2-OpenBLAS-0.2.18-LAPACK-3.6.1, 2.0.2-OpenBLAS-0.2.19-LAPACK-3.7.0, 2.0.2-OpenBLAS-0.2.20, 2.0.2-OpenBLAS-0.3.1, 2.0.2, 2.1.0-fb, 2.1.0	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.
Schrodinger		2015-3_Linux-x86_64	Desc Schrödinger aims to provide integrated software solutions and services that truly meet its customers’ needs. We want to empower researchers around the world to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials. - Homepage: http://www.schrodinger.com/
SciPy-bundle		2019.10-Python-3.7.4, 2020.03-Python-3.8.2, 2020.11, 2021.10	Desc Bundle of Python packages for scientific software
Shapely		1.7.0-Python-3.7.4, 1.8a1	Desc Shapely is a BSD-licensed Python package for manipulation and analysis of planar geometric objects. It is based on the widely deployed GEOS (the engine of PostGIS) and JTS (from which GEOS is ported) libraries.
Siesta		4.1.5	Desc SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
Singularity		2.3.1, 2.4.2, 2.6.1, 3.5.3	Desc Singularity is a portable application stack packaging and runtime utility. - Homepage: http://gmkurtzer.github.io/singularity
Sphinx		1.8.1-Python-3.6.6	Desc Sphinx is a tool that makes it easy to create intelligent and beautiful documentation. It was originally created for the new Python documentation, and it has excellent facilities for the documentation of Python projects, but C/C+ + is already supported as well, and it is planned to add special support for other languages as well.
Spyder		3.3.6-Python-3.6.6, 4.1.5-Python-3.7.4, 5.1.5	Desc Spyder is an interactive Python development environment providing MATLAB-like features in a simple and light-weighted software.
Subversion		1.12.0	Desc Subversion is an open source version control system.
SuiteSparse		4.2.1-ParMETIS-4.0.3, 4.4.5-METIS-5.1.0, 4.5.3-METIS-5.1.0, 5.1.2-METIS-5.1.0, 5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0	Desc SuiteSparse is a collection of libraries manipulate sparse matrices.
Tcl		8.6.3, 8.6.4, 8.6.5, 8.6.6, 8.6.8, 8.6.9, 8.6.10, 8.6.11	Desc Tcl (Tool Command Language) is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. - Homepage: http://www.tcl.tk/
Tecplot360ex		2021.1	Desc Quickly plot and animate your CFD results exactly the way you want. Analyze complex solutions, arrange multiple layouts, and communicate your results with professional images and animations.
TensorFlow		1.2.0-Python-3.5.1, 1.4.0-Python-3.5.1, 1.12.0-Python-3.6.6, 2.2.0-Python-3.7.4, 2.3.1-Python-3.7.4, 2.4.1	Desc An open-source software library for Machine Intelligence
TensorRT		4.0.1.6-Python-2.7.15	Desc NVIDIA TensorRT is a platform for high-performance deep learning inference
Tk		8.6.4-no-X11, 8.6.5, 8.6.8, 8.6.9, 8.6.10, 8.6.11	Desc Tk is an open source, cross-platform widget toolchain that provides a library of basic elements for building a graphical user interface (GUI) in many different programming languages. - Homepage: http://www.tcl.tk/
TurboVNC		2.1.2, 2.2.1	Desc TurboVNC is a derivative of VNC (Virtual Network Computing) that is tuned to provide peak performance for 3D and video workloads.
VMD		1.9.3-Python-2.7.11, 1.9.3-Python-2.7.15	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.
VSEARCH		2.8.0, 2.9.1, 2.22.1	Desc VSEARCH supports de novo and reference based chimera detection, clustering, full-length and prefix dereplication, rereplication, reverse complementation, masking, all-vs-all pairwise global alignment, exact and global alignment searching, shuffling, subsampling and sorting. It also supports FASTQ file analysis, filtering, conversion and merging of paired-end reads.
VTK		5.4.2, 6.3.0-Python-2.7.11, 7.0.0-Python-2.7.11, 8.1.1-Python-2.7.15, 9.0.1, 9.1.0	Desc The Visualization Toolkit (VTK) is an open-source, freely available software system for 3D computer graphics, image processing and visualization. VTK consists of a C+ + class library and several interpreted interface layers including Tcl/Tk, Java, and Python. VTK supports a wide variety of visualization algorithms including: scalar, vector, tensor, texture, and volumetric methods; and advanced modeling techniques such as: implicit modeling, polygon reduction, mesh smoothing, cutting, contouring, and Delaunay triangulation.
VTune		2016_update3, 2019_update3, 2022.3.0, 2023.2.0	Desc Intel VTune Amplifier XE is the premier performance profiler for C, C+ +, C#, Fortran, Assembly and Java. - Homepage: http://software.intel.com/en-us/intel-vtune-amplifier-xe
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools
VirtualGL		2.5.2, 2.6.2, 2.6.4	Desc VirtualGL is an open source toolkit that gives any Linux or Unix remote display software the ability to run OpenGL applications with full hardware acceleration.
Voro+ +		Voro+ 0.4.6	Desc Voro+ + is a software library for carrying out three-dimensional computations of the Voronoi tessellation. A distinguishing feature of the Voro+ + library is that it carries out cell-based calculations, computing the Voronoi cell for each particle individually. It is particularly well-suited for applications that rely on cell-based statistics, where features of Voronoi cells (eg. volume, centroid, number of faces) can be used to analyze a system of particles.
X11		20200222	Desc The X Window System (X11) is a windowing system for bitmap displays
Xvfb		1.20.8	Desc Xvfb is an X server that can run on machines with no display hardware and no physical input devices. It emulates a dumb framebuffer using virtual memory.
ZeroMQ		4.1.4, 4.2.2, 4.2.5, 4.3.2, 4.3.3	Desc ZeroMQ looks like an embeddable networking library but acts like a concurrency framework. It gives you sockets that carry atomic messages across various transports like in-process, inter-process, TCP, and multicast. You can connect sockets N-to-N with patterns like fanout, pub-sub, task distribution, and request-reply. It's fast enough to be the fabric for clustered products. Its asynchronous I/O model gives you scalable multicore applications, built as asynchronous message-processing tasks. It has a score of language APIs and runs on most operating systems.
arpack-ng		3.3.0, 3.5.0, 3.7.0	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
at-spi2-atk		2.34.1, 2.38.0	Desc AT-SPI 2 toolkit bridge
at-spi2-core		2.34.0, 2.38.0	Desc Assistive Technology Service Provider Interface.

Modules	Documentation	Versions	Description
cURL		7.47.0, 7.49.1, 7.55.1, 7.60.0, 7.66.0, 7.69.1, 7.72.0, 7.78.0	Desc libcurl is a free and easy-to-use client-side URL transfer library, supporting DICT, FILE, FTP, FTPS, Gopher, HTTP, HTTPS, IMAP, IMAPS, LDAP, LDAPS, POP3, POP3S, RTMP, RTSP, SCP, SFTP, SMTP, SMTPS, Telnet and TFTP. libcurl supports SSL certificates, HTTP POST, HTTP PUT, FTP uploading, HTTP form based upload, proxies, cookies, user+password authentication (Basic, Digest, NTLM, Negotiate, Kerberos), file transfer resume, http proxy tunneling and more.
ccpnmr		2.4.2-Python-2.7.11	Desc CcpNmr Analysis is a graphics-based interactive NMR spectrum visualisation, resonance assignment and data analysis program
cuDNN		7.1.4.18	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		0.19.4-Python-3.6.6	Desc Dask provides multi-core execution on larger-than-memory datasets using blocked algorithms and task scheduling.
flatbuffers		1.12.0	Desc FlatBuffers: Memory Efficient Serialization Library
foss		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK. - Homepage: (none)
fosscuda		2018b	Desc GCC based compiler toolchain with CUDA support, and including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
futile		1.8.3	Desc The FUTILE project (Fortran Utilities for the Treatment of Innermost Level of Executables) is a set of modules and wrapper that encapsulate the most common low-level operations of a Fortran code.
gcccuda		2018b	Desc GNU Compiler Collection (GCC) based compiler toolchain, along with CUDA toolkit.
geopandas		0.7.0-Python-3.7.4, 0.8.2	Desc GeoPandas is a project to add support for geographic data to pandas objects. It currently implements GeoSeries and GeoDataFrame types which are subclasses of pandas.Series and pandas.DataFrame respectively. GeoPandas objects can act on shapely geometry objects and perform geometric operations.
gettext		0.19.8	Desc GNU 'gettext' is an important step for the GNU Translation Project, as it is an asset on which we may build many other steps. This package offers to programmers, translators, and even users, a well integrated set of tools and documentation - Homepage: http://www.gnu.org/software/gettext/
git		2.8.0, 2.16.1, 2.23.0-nodocs, 2.28.0-nodocs, 2.33.1-nodocs	Desc Git is a free and open source distributed version control system designed to handle everything from small to very large projects with speed and efficiency.
gmsh		2.9.1	Desc Gmsh is a 3D finite element grid generator with a build-in CAD engine and post-processor. - Homepage: http://geuz.org/gmsh
gnuplot		4.6.0, 5.0.3, 5.2.5, 5.2.8, 5.4.1, 5.4.2	Desc Portable interactive, function plotting utility
gompi		2014b, 2015b, 2016a, 2016b, 2016.04, 2017a, 2017b, 2018b, 2019b, 2020a, 2020b, 2021a, 2021b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support. - Homepage: (none)
gompic		2018b	Desc GNU Compiler Collection (GCC) based compiler toolchain along with CUDA toolkit, including OpenMPI for MPI support with CUDA features enabled.
graph-tool		2.22-Python-3.5.2	Desc Graph-tool is an efficient Python module for manipulation and statistical analysis of graphs (a.k.a. networks). Contrary to most other python modules with similar functionality, the core data structures and algorithms are implemented in C+ +, making extensive use of template metaprogramming, based heavily on the Boost Graph Library. This confers it a level of performance that is comparable (both in memory usage and computation time) to that of a pure C/C+ + library. - Homepage: https://graph-tool.skewed.de/
h5py		2.6.0-Python-2.7.11, 2.8.0-Python-2.7.15, 2.8.0-Python-3.6.6, 2.10.0-Python-3.7.4, 3.6.0	Desc HDF5 for Python (h5py) is a general-purpose Python interface to the Hierarchical Data Format library, version 5. HDF5 is a versatile, mature scientific software library designed for the fast, flexible storage of enormous amounts of data.
help2man		1.47.4	Desc help2man produces simple manual pages from the '–help' and '–version' output of other commands.
horton		2.0.0-Python-2.7.11	Desc Horton is a development platform for electronic structure methods. - Homepage: http://theochem.github.io/horton
hypothesis		4.5.0-Python-3.6.6, 5.41.2, 6.14.6	Desc Hypothesis is an advanced testing library for Python. It lets you write tests which are parametrized by a source of examples, and then generates simple and comprehensible examples that make your tests fail. This lets you find more bugs in your code with less work.
icc		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc C and C+ + compiler from Intel
iccifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32, 2019.5.281, 2020.1.217	Desc Intel C, C+ + and Fortran compilers
ifort		2015.1.133-GCC-4.9.2, 2016.1.150-GCC-4.9.3-2.25, 2016.3.210-GCC-5.4.0-2.26, 2018.3.222-GCC-7.3.0-2.30, 2019.3.199-GCC-8.3.0-2.32	Desc Fortran compiler from Intel
iimpi		7.2.3-GCC-4.9.2, 8.1.5-GCC-4.9.3-2.25, 2016b, 2016.01-GCC-4.9.3-2.25, 2018b, 2019b, 2019.03, 2020a, 2021a	Desc Intel C/C+ + and Fortran compilers, alongside Intel MPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
imkl		11.2.1.133, 11.3.1.150, 11.3.3.210, 2018.3.222, 2019.3.199, 2019.5.281, 2020.1.217, 2021.2.0	Desc Intel Math Kernel Library is a library of highly optimized, extensively threaded math routines for science, engineering, and financial applications that require maximum performance. Core math functions include BLAS, LAPACK, ScaLAPACK, Sparse Solvers, Fast Fourier Transforms, Vector Math, and more.
impi		5.0.2.044, 5.1.2.150, 5.1.3.181, 2018.3.222, 2018.5.288, 2019.3.199, 2019.7.217, 2021.2.0	Desc The Intel(R) MPI Library for Linux* OS is a multi-fabric message passing library based on ANL MPICH2 and OSU MVAPICH2. The Intel MPI Library for Linux OS implements the Message Passing Interface, version 3.0 (MPI-3) specification.
intel		2015a, 2016a, 2016b, 2018b, 2019b, 2019.03, 2020a, 2021a	Desc Intel Cluster Toolkit Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MPI & Intel MKL.
intel-compilers		2021.2.0	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)
iomkl		2016b	Desc Intel Cluster Toolchain Compiler Edition provides Intel C/C+ + and Fortran compilers, Intel MKL & OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
iompi		2016b	Desc Toolchain with Intel C, C+ + and Fortran compilers, alongside OpenMPI. - Homepage: http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
ipp		9.0.4.258, 2019.3.199	Desc Intel Integrated Performance Primitives (Intel IPP) is an extensive library of multicore-ready, highly optimized software functions for multimedia, data processing, and communications applications. Intel IPP offers thousands of optimized functions covering frequently used fundamental algorithms.
itac		9.1.2.024, 2019.3.032, 2021.10.0	Desc The Intel Trace Collector is a low-overhead tracing library that performs event-based tracing in applications. The Intel Trace Analyzer provides a convenient way to monitor application activities gathered by the Intel Trace Collector through graphical displays.

Modules	Documentation	Versions	Description
lammps		11Aug17-Python-2.7.11-mpi, 11Aug17-Python-2.7.11, 14May16-Python-2.7.11-mpi, 14May16-Python-2.7.11	Desc LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers.
libAfterImage		1.20	Desc libAfterImage is a generic image manipulation library - Homepage: http://www.afterstep.org/
libsigc+ +		libsigc+ 2.4.1	Desc The libsigc+ + package implements a typesafe callback system for standard C+ +. - Homepage: http://www.gtk.org/
libsodium		1.0.8, 1.0.13, 1.0.16	Desc Sodium is a modern, easy-to-use software library for encryption, decryption, signatures, password hashing and more.
libxml2		2.9.4-Python-2.7.12	Desc Libxml2 is the XML C parser and toolchain developed for the Gnome project (but usable outside of the Gnome platform). - Homepage: http://xmlsoft.org/
lmod		lmod	Desc Lmod: An Environment Module System
ls-dyna		8.1.105897_mpp_d, 9.0.1.109912_mpp_d, 9.1.113698_mpp_d, 9.2.119543_mpp_d, 10_0_118302_mpp_d	Desc LS-DYNA is a general-purpose finite element program capable of simulating complex real world problems. It is used by the automobile, aerospace, construction, military, manufacturing, and bioengineering industries. - Homepage: http://www.lstc.com/products/ls-dyna
magma		2.5.0	Desc The MAGMA project aims to develop a dense linear algebra library similar to LAPACK but for heterogeneous/hybrid architectures, starting with current Multicore+GPU systems.
matplotlib		1.4.3-Python-2.7.11, 1.5.1-Python-2.7.11, 1.5.1-Python-3.4.3, 1.5.1-Python-3.5.1, 1.5.1-Python-3.5.2, 2.0.2-Python-3.5.1, 2.0.2-Python-3.6.1, 3.0.0-Python-3.6.6, 3.1.1-Python-3.7.4, 3.2.1-Python-3.8.2, 3.3.3, 3.4.3	Desc matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell, web application servers, and six graphical user interface toolkits.
molmod		1.4.5-Python-3.7.4	Desc MolMod is a Python library with many compoments that are useful to write molecular modeling programs.
mpi4py		2.0.0-Python-2.7.11, 3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.0.3-Python-3.8.2	Desc MPI for Python (mpi4py) provides bindings of the Message Passing Interface (MPI) standard for the Python programming language, allowing any Python program to exploit multiple processors. - Homepage: https://bitbucket.org/mpi4py/mpi4py
mpifileutils	mpiFileUtils	0.10.1, 0.11, 0.11.1	Desc MPI-Based File Utilities For Distributed Systems
mpmath		0.19-Python-2.7.11, 0.19-Python-3.4.3	Desc mpmath can be used as an arbitrary-precision substitute for Python's float/complex types and math/cmath modules, but also does much more advanced mathematics. Almost any calculation can be performed just as well at 10-digit or 1000-digit precision, with either real or complex numbers, and in many cases mpmath implements efficient algorithms that scale well for extremely high precision work. - Homepage: http://mpmath.org/
msindo		3.6	Desc Semiempirical SCF MO program for systems with first-, second-, third-, and fourth-row elements - Homepage: http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=MSINDO&lang=english
netCDF		4.4.0, 4.4.1, 4.6.1, 4.7.1, 4.7.4, 4.8.1	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
netCDF-Fortran		4.4.3, 4.4.4, 4.5.3	Desc NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
nettle		3.2	Desc Nettle is a cryptographic library that is designed to fit easily in more or less any context: In crypto toolkits for object-oriented languages (C+ +, Python, Pike, ...), in applications like LSH or GNUPG, or even in kernel space. - Homepage: http://www.lysator.liu.se/~nisse/nettle/
networkx		1.10-Python-2.7.11, 2.2-Python-3.5.1, 2.4-Python-3.7.4, 2.5	Desc NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.
nsync		1.24.0	Desc nsync is a C library that exports various synchronization primitives, such as mutexes
numba		0.29.0-Python-2.7.11	Desc Numba is an Open Source NumPy-aware optimizing compiler for Python sponsored by Continuum Analytics, Inc. It uses the remarkable LLVM compiler infrastructure to compile Python syntax to machine code. - Homepage: http://numba.pydata.org/
numpy		1.8.2-Python-2.7.11, 1.9.2-Python-2.7.11, 1.10.1-Python-2.7.11, 1.10.1-Python-3.4.3, 1.10.1-Python-3.5.1, 1.13.0-Python-3.5.1, 1.18.5-Python-3.7.4, 1.18.5-Python-3.8.2	Desc NumPy is the fundamental package for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C+ + and Fortran code, useful linear algebra, Fourier transform, and random number capabilities. Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases. - Homepage: http://www.numpy.org
pandas		0.18.0-Python-2.7.11, 0.18.0-Python-3.5.1	Desc pandas is an open source, BSD-licensed library providing high-performance, easy-to-use data structures and data analysis tools for the Python programming language. - Homepage: https://pypi.python.org/pypi/pandas/
parallel		20190922, 20210322	Desc parallel: Build and execute shell commands in parallel
pcp		2.0.0_39-Python-2.7.16	Desc A parallel copy program for lustre
phenix		1.10.1-2155	Desc PHENIX is a software suite for the automated determination of molecular structures using X-ray crystallography and other methods. - Homepage: http://www.phenix-online.org
pigz		2.6	Desc pigz, which stands for parallel implementation of gzip, is a fully functional replacement for gzip that exploits multiple processors and multiple cores to the hilt when compressing data. pigz was written by Mark Adler, and uses the zlib and pthread libraries.
pkgconf		1.8.0	Desc pkgconf is a program which helps to configure compiler and linker flags for development libraries. It is similar to pkg-config from freedesktop.org.
protobuf		3.2.0	Desc Google Protocol Buffers - Homepage: https://github.com/google/protobuf/
protobuf-python		3.2.0-Python-3.4.3, 3.2.0-Python-3.5.1, 3.10.0-Python-3.7.4	Desc Python Protocol Buffers runtime library. - Homepage: https://github.com/google/protobuf/
psutil		5.6.3-Python-3.6.6	Desc A cross-platform process and system utilities module for Python
qutip		2.2.0-Python-2.7.11, 3.1.0-Python-2.7.11, 4.0.2-Python-3.4.3	Desc QuTiP : Quantum Toolbox in Python - Homepage: http://qutip.org/
scikit-image		0.12.3-Python-3.5.1, 0.14.1-Python-3.6.6	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-learn		0.18.1-Python-3.5.1, 0.20.0-Python-3.6.6, 0.20.3-Python-3.6.6, 0.21.3-Python-3.7.4, 0.23.2	Desc Scikit-learn integrates machine learning algorithms in the tightly-knit scientific Python world, building upon numpy, scipy, and matplotlib. As a machine-learning module, it provides versatile tools for data mining and analysis in any field of science and engineering. It strives to be simple and efficient, accessible to everybody, and reusable in various contexts.
scikit-umfpack		0.2.1-Python-2.7.11	Desc scikit-umfpack provides a wrapper of UMFPACK sparse direct solver to SciPy. - Homepage: http://rc.github.io/scikit-umfpack/
scipy		0.16.1-Python-2.7.11, 0.17.1-Python-2.7.11, 0.17.1-Python-3.4.3, 0.19.1-Python-3.5.1	Desc SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension for Python. - Homepage: http://www.scipy.org
settarg		settarg	Desc

Modules	Documentation	Versions	Description
sparsehash		2.0.2	Desc An extremely memory-efficient hash_map implementation. 2 bits/entry overhead! The SparseHash library contains several hash-map implementations, including implementations that optimize for space or speed. - Homepage: https://code.google.com/p/sparsehash/
sympy		1.0-Python-2.7.11, 1.0-Python-3.4.3	Desc SymPy is a Python library for symbolic mathematics. It aims to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries. - Homepage: http://sympy.org/
tbb		4.4.6.258, 2019_U9, 2019.2.187, 2020.3	Desc Intel(R) Threading Building Blocks (Intel(R) TBB) lets you easily write parallel C+ + programs that take full advantage of multicore performance, that are portable, composable and have future-proof scalability.
texlive		20200406, 20210324	Desc TeX is a typesetting language. Instead of visually formatting your text, you enter your manuscript text intertwined with TeX commands in a plain text file. You then run TeX to produce formatted output, such as a PDF file. Thus, in contrast to standard word processors, your document is a separate file that does not pretend to be a representation of the final typeset output, and so can be easily edited and manipulated.
typing-extensions		3.7.4.3	Desc Typing Extensions – Backported and Experimental Type Hints for Python
utf8proc		2.2.0	Desc utf8proc is a small, clean C library that provides Unicode normalization, case-folding, and other operations for data in the UTF-8 encoding.
wheel		0.29.0-Python-3.4.3, 0.29.0-Python-3.5.1, 0.31.1-Python-2.7.15, 0.31.1-Python-3.6.6	Desc A built-package format for Python.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

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