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.

Here are a few things to know about the available software

- Docker is not available on compute cluster but Apptainer (formerly 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`

AVX2

Installed software as of Sat, 16 May 2026 02:40:02 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	2017, 2018, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341, 2024-hotfix-2414, 2025-hotfix-2514	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	19.2, 2019.3, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1, 2024.2, 2025.1, 2025.2	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.

Modules	Documentation	Versions	Description
ANSYSEM		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.
ASE		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.
Advisor		2025.0.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		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.

Modules	Documentation	Versions	Description
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, 2.0	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
Bazel		3.4.1, 3.7.2, 4.2.2, 6.5.0	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.
Boost		1.71.0, 1.74.0, 1.77.0, 1.81.0, 1.83.0, 1.88.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Brunsli		0.1	Desc Brunsli is a lossless JPEG repacking library.
CFITSIO		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.

Modules	Documentation	Versions	Description
CGAL		4.14.1-Python-3.7.4, 4.14.3, 5.2, 5.6.1, 6.0.1	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.
CMake		3.15.3, 3.18.4, 3.20.1, 3.21.1, 3.22.1, 3.24.3, 3.27.6, 3.31.3, 3.31.8, 4.0.3	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-2.4	Desc
COMSOL	COMSOL	5.6, 6.1, 6.2, 6.3, 6.4	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.
CPCM-X		1.1.0	Desc This is an fully open source solvation model, based on the original conductor like screening model for realistic solvation (COSMO-RS) model by Klamt et al. in combination with the universal solvation model based on solute electron density (SMD) by Marenich, Cramer and Truhlar.
CPMD	CPMD	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.

Modules	Documentation	Versions	Description
CREST		2.11.2, 2.12, 3.0.2	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.
CUDA		10.1.243, 11.1.1, 11.4.1, 11.7.0, 11.8.0, 12.0.0, 12.4.0, 12.6.0, 12.8.0, 13.0.0	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.

Modules	Documentation	Versions	Description
Clang		16.0.4, 17.0.6	Desc C, C+ +, Objective-C compiler, based on LLVM. Does not include C+ + standard library – use libstdc+ + from GCC.
Cython		0.29.22, 3.0.10, 3.1.2	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
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.
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
Eigen		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.
FEKO	FEKO	2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering

Modules	Documentation	Versions	Description
FEniCS-Basix		0.10.0	Desc Basix is a finite element definition and tabulation runtime library - C+ + library
FEniCS-Basix-Python		0.10.0	Desc Basix is a finite element definition and tabulation runtime library - Python binding
FEniCS-DOLFINx		0.10.0	Desc DOLFINx is the computational environment of FEniCSx - C+ + library
FEniCS-DOLFINx-Python		0.10.0	Desc DOLFINx is the computational environment of FEniCSx - Python binding
FEniCS-FFCx		0.10.0	Desc FFCx is a compiler for finite element variational forms
FEniCS-UFL		2025.2.1	Desc The Unified Form Language (UFL) is a domain-specific language for defining variational forms
FEniCS-ufcx		0.10.0	Desc FFCx provides the ufcx.h interface header for generated finite element kernels, used by DOLFINx.
FFTW		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.

Modules	Documentation	Versions	Description
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, 3.4.5	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.
FriBidi		1.0.5, 1.0.10, 1.0.12, 1.0.13, 1.0.16	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		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.
GCC		8.3.0, 10.2.0, 10.3.0, 11.2.0, 12.2.0, 13.2.0, 14.3.0	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,...).

Modules	Documentation	Versions	Description
GMP		6.2.1	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers.
GROMACS		2023.5-CUDA-12.0.0, 2024.1, 2025.2	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		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.
GTK3		3.24.35, 3.24.39	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.

Modules	Documentation	Versions	Description
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g16.A03, g16.B01	Desc Gaussian is a general purpose quantum chemistry software package for ab initio electronic structure calculations.
Go		1.16.6, 1.22.1, 1.25.0	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
Graphviz		8.1.0	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.

Modules	Documentation	Versions	Description
Gurobi		9.1.2, 9.5.0, 11.0.0, 11.0.3, 12.0.1, 12.0.3	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		2.4-Python-2.7.16	Desc
HDF		4.2.14, 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		1.10.5, 1.10.7, 1.12.1, 1.14.0, 1.14.3, 1.14.6	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.
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).

Modules	Documentation	Versions	Description
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		2.3	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.

Modules	Documentation	Versions	Description
Highway		1.0.3	Desc Highway is a C++ library for SIMD (Single Instruction, Multiple Data), i.e. applying the same operation to 'lanes'.
IPython		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		7.0.9-5, 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
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_92, 1.8.0_152, 1.8, 11.0.2, 11.0.18, 11.0.20	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.

Modules	Documentation	Versions	Description
Julia		1.7.2-linux-x86_64, 1.10.4-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter on LUIS 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.
KaHIP		3.16, 3.19	Desc The graph partitioning framework KaHIP – Karlsruhe High Quality Partitioning.
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.

Modules	Documentation	Versions	Description
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.
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).

Modules	Documentation	Versions	Description
Lua		5.1.5, 5.4.2, 5.4.3, 5.4.4, 5.4.6, 5.4.8	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		2023-1, 2024-1.02, 2025-1, 2025-2.01, 2026-1	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	2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b, 2024b, 2025b	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.

Modules	Documentation	Versions	Description
METIS		5.1.0	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		4.0.2, 4.1.0, 4.2.0, 4.2.1, 4.2.2	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, 5.8.1-metis	Desc A parallel sparse direct solver
Mako		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

Modules	Documentation	Versions	Description
Maple		2021.0, 2024.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface.
Mathematica		13.2.1, 14.0.0	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields.
Meson		0.55.3, 0.58.0, 0.58.2, 0.59.1-Python-3.7.4, 0.64.0, 1.2.3, 1.6.1, 1.8.2	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
Miniconda3		22.11.1-1, 23.5.2-0, 24.7.1-0	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.
Miniforge3	Conda	23.11.0-0, 24.7.1-2, 25.3.0-3	Desc Miniforge is a free minimal installer for conda and Mamba specific to conda-forge.
Molden		7.3	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		1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.

Modules	Documentation	Versions	Description
NCCL		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, 2.20.5-CUDA-12.8.0, 2.22.3-CUDA-12.6.0	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	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, 24.9-CUDA-12.6.0, 25.3-CUDA-12.8.0	Desc C, C+ + and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
Ninja		1.9.0, 1.10.1, 1.10.2, 1.11.1, 1.12.1, 1.13.0	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1, 5.0.4, 6.0.0-avx2, 6.1.0	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		5.1.0, 9.1.0, 10.2.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations.
Octopus		11.4, 13.0, 15.0	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		0.3.7, 0.3.12, 0.3.18, 0.3.21, 0.3.24, 0.3.30	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.

Modules	Documentation	Versions	Description
OpenCV		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		2.4.0, 3.1.0, 4.0.1	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.
OpenFOAM		v2012, v2106, v2212, v2412, v2506, 8, 9, 10, 13	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.

Modules	Documentation	Versions	Description
OpenFOAM-Extend		4.1-20200408-Python-2.7.16	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		3.1.4, 4.0.5, 4.1.1, 4.1.4, 4.1.6, 5.0.8	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.
PCL		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.

Modules	Documentation	Versions	Description
PETSc		3.15.5-Python-3.7.4, 3.15.5	Desc PETSc, pronounced PET-see (the S is silent), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations.
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.
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.

Modules	Documentation	Versions	Description
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.
PNFFT		20240604	Desc PNFFT is a software library written in C for computing parallel nonequispaced fast Fourier transformations.
POV-Ray		3.7.0.10	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.

Modules	Documentation	Versions	Description
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
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.

Modules	Documentation	Versions	Description
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.
ParaView		5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi, 5.12.0, 6.0.1	Desc ParaView is a scientific parallel visualizer.
Perl		5.30.0-minimal, 5.30.0, 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, 5.38.2, 5.40.0, 5.40.2	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, 5.40.0, 5.40.2	Desc A set of common packages from CPAN
Pillow		6.2.1, 8.0.1, 8.3.2, 9.4.0, 10.2.0, 11.3.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
Pixi		0.59.0, 0.67.2	Desc Pixi is a cross-platform, multi-language package manager and workflow tool built on the foundation of the conda ecosystem. It provides developers with an exceptional experience similar to popular package managers like cargo or npm, but for any language.
PnetCDF		1.12.3	Desc Parallel netCDF: A Parallel I/O Library for NetCDF File Access
ProFit		3.3	Desc ProFit is the protein least squares fitting program

Modules	Documentation	Versions	Description
PyMOL		2.5.0	Desc PyMOL is a Python-enhanced molecular graphics tool. It excels at 3D visualization of proteins, small molecules, density, surfaces, and trajectories. It also includes molecular editing, ray tracing, and movies. Open Source PyMOL is free to everyone!
PyQt5		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		1.6.0-Python-3.7.4, 1.9.0, 1.10.0, 1.13.1-CUDA-12.0.0, 1.13.1, 2.1.2	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.
Pysam		0.22.0, 0.23.2	Desc Pysam is a python module for reading and manipulating Samfiles. It's a lightweight wrapper of the samtools C-API. Pysam also includes an interface for tabix.
Python		2.7.16, 2.7.18-bare, 2.7.18, 3.7.4, 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, 3.12.3, 3.13.1, 3.13.5	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Python-bundle-PyPI		2023.10, 2025.07	Desc Bundle of Python packages from PyPI

Modules	Documentation	Versions	Description
Qt5		5.13.1, 5.14.2, 5.15.2, 5.15.7, 5.15.13	Desc Qt is a comprehensive cross-platform C+ + application framework.
Qt6		6.6.3, 6.9.3	Desc Qt is a comprehensive cross-platform C+ + application framework.
R		4.1.0, 4.1.2, 4.2.2, 4.4.1	Desc R is a free software environment for statistical computing and graphics.
ROOT		6.26.10	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, 1.85.1, 1.88.0, 1.91.1	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAMtools		1.19.2, 1.22	Desc SAM Tools provide various utilities for manipulating alignments in the SAM format, including sorting, merging, indexing and generating alignments in a per-position format.

Modules	Documentation	Versions	Description
SCIPOptSuite		8.0.4-Gurobi-9.5.0, 8.0.4	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		6.0.9, 6.1.0, 6.1.2-no-thread, 6.1.2, 7.0.2, 7.0.4, 7.0.10	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.
SDL3		3.4.4	Desc Simple DirectMedia Layer is a cross-platform development library designed to provide low level access to audio, keyboard, mouse, joystick, and graphics hardware via OpenGL and Direct3D.
SDL3_image		3.4.2	Desc This is a simple library to load images of various formats as SDL surfaces. It can load BMP, GIF, JPEG, LBM, PCX, PNG, PNM (PPM/PGM/PBM), QOI, TGA, XCF, XPM, and simple SVG format images. It can also load AVIF, JPEG-XL, TIFF, and WebP images, depending on build options (see the note below for details.)

Modules	Documentation	Versions	Description
SDL3_ttf		3.2.2	Desc This library is a wrapper around the FreeType and Harfbuzz libraries, allowing you to use TrueType fonts to render text in SDL applications.
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, 2.1.0-fb, 2.1.0, 2.2.0-fb, 2.2.2-fb	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.
SciPy-bundle		2019.10-Python-3.7.4, 2020.11, 2021.10, 2023.02, 2023.11, 2025.07	Desc Bundle of Python packages for scientific software

Modules	Documentation	Versions	Description
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.
Spyder		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.
StdEnv		2024.10	Desc
Subversion		1.14.1	Desc Subversion is an open source version control system.
SuiteSparse		5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0, 5.13.0-METIS-5.1.0, 7.7.0, 7.11.0	Desc SuiteSparse is a collection of libraries to manipulate sparse matrices.
Tcl		8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13, 8.6.14, 8.6.16, 9.0.1	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.

Modules	Documentation	Versions	Description
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		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
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		8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13, 9.0.1	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.
VMD		1.9.4a57	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

Modules	Documentation	Versions	Description
VSCode		1.102.3	Desc Visual Studio Code is a lightweight but powerful source code editor which runs on your desktop and is available for Windows, macOS and Linux. It comes with built-in support for JavaScript, TypeScript and Node.js and has a rich ecosystem of extensions for other languages and runtimes (such as C++, C#, Java, Python, PHP, Go, .NET).
VSEARCH		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.

Modules	Documentation	Versions	Description
VTK		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		2024.3.0, 2025.4.0	Desc Intel® VTune™ Profiler optimizes application performance, system performance, and system configuration for HPC, cloud, IoT, media, storage, and more.
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools

Modules	Documentation	Versions	Description
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.

Modules	Documentation	Versions	Description
Wayland		1.22.0, 1.24.0	Desc Wayland is a project to define a protocol for a compositor to talk to its clients as well as a library implementation of the protocol. The compositor can be a standalone display server running on Linux kernel modesetting and evdev input devices, an X application, or a wayland client itself. The clients can be traditional applications, X servers (rootless or fullscreen) or other display servers.
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, 4.15.1	Desc Z3 is a theorem prover from Microsoft Research.

Modules	Documentation	Versions	Description
ZeroMQ		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.
Zoltan		3.901	Desc Zoltan Dynamic Load Balancing and Graph Algorithm Toolkit
arpack-ng		3.7.0, 3.8.0, 3.9.1	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
btop		1.4.6	Desc Resource monitor that shows usage and stats for processor, memory, disks, network and processes.

Modules	Documentation	Versions	Description
cURL		7.66.0, 7.72.0, 7.76.0, 7.78.0, 7.86.0, 8.3.0, 8.11.1, 8.14.1	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.
code-server	Code-Server (VS Code) on LUIS Cluster	4.107.0	Desc Run VS Code on any machine anywhere and access it in the browser.
cryptography		41.0.5, 45.0.5	Desc cryptography is a package designed to expose cryptographic primitives and recipes to Python developers.
cuDNN		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, 9.5.0.50-CUDA-12.4.0, 9.5.0.50-CUDA-12.6.0, 9.10.1.4-CUDA-12.8.0	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		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.

Modules	Documentation	Versions	Description
dftd4		3.7.0	Desc The dftd4 project provides an implementation of the generally applicable, charge dependent London-dispersion correction, termed DFT-D4.
foss		2019b, 2020b, 2021b, 2022b, 2023b, 2025b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
fosscuda		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.

Modules	Documentation	Versions	Description
gcccuda		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.
git		2.23.0-nodocs, 2.28.0-nodocs, 2.32.0-nodocs, 2.33.1-nodocs, 2.38.1-nodocs, 2.42.0, 2.50.1	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.
gnuplot		5.2.8, 5.4.1, 5.4.2, 5.4.6, 6.0.1, 6.0.3	Desc Portable interactive, function plotting utility
gperftools		2.17.2	Desc gperftools is a collection of a high-performance multi-threaded malloc() implementation, plus some pretty nifty performance analysis tools. Includes TCMalloc, heap-checker, heap-profiler and cpu-profiler.

Modules	Documentation	Versions	Description
h5py		2.10.0-Python-3.7.4, 3.1.0, 3.6.0, 3.11.0	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.
hypothesis		4.44.2-Python-3.7.4, 5.41.2, 5.41.5, 6.14.6, 6.68.2, 6.90.0, 6.136.6	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.
iTensor		3.1.11	Desc An efficient and flexible C+ + library for performing tensor network calculations
imkl		2021.2.0, 2022.2.1, 2023.2.0, 2024.2.0, 2025.1.0, 2025.2.0	Desc Intel oneAPI Math Kernel Library
imkl-FFTW		2022.2.1, 2023.2.0, 2024.2.0, 2025.1.0, 2025.2.0	Desc FFTW interfaces using Intel oneAPI Math Kernel Library
impi		2021.2.0, 2021.7.1, 2021.10.0, 2021.13.0, 2021.15.0, 2021.16.1	Desc Intel MPI Library, compatible with MPICH ABI
intel		2021a, 2022b, 2023b, 2024a, 2025a, 2025b	Desc Compiler toolchain including Intel compilers, Intel MPI and Intel Math Kernel Library (MKL).
intel-compilers		2021.2.0, 2022.2.1, 2023.2.1, 2024.2.0, 2025.1.1, 2025.2.0	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)

Modules	Documentation	Versions	Description
jax		0.4.34-CUDA-12.8.0	Desc Composable transformations of Python+NumPy programs: differentiate, vectorize, JIT to GPU/TPU, and more
libgpuarray		0.7.6-Python-3.7.4	Desc Library to manipulate tensors on the GPU.
likwid		5.2.2	Desc Likwid stands for Like I knew what I am doing. This project contributes easy to use command line tools for Linux to support programmers in developing high performance multi threaded programs.
lmod		lmod	Desc Lmod: An Environment Module System
magma		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		3.1.1-Python-3.7.4, 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.

Modules	Documentation	Versions	Description
maturin		1.8.3, 1.9.1	Desc This project is meant as a zero configuration replacement for setuptools-rust and milksnake. It supports building wheels for python 3.5+ on windows, linux, mac and freebsd, can upload them to pypi and has basic pypy and graalpy support.
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		3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.1.4, 3.1.5	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	0.11, 0.11.1, 0.12	Desc MPI-Based File Utilities For Distributed Systems
multicharge		0.3.0	Desc Electronegativity equilibration model for atomic partial charges.
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		4.7.1, 4.7.4, 4.8.0, 4.8.1, 4.9.0, 4.9.2, 4.9.3	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.
netCDF-Fortran		4.5.3, 4.6.0, 4.6.1, 4.6.2	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.
networkx		2.4-Python-3.7.4, 2.5, 2.6.3, 3.0, 3.2.1, 3.5	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.
numsa		0.2.0	Desc Numerical surface area integrator for molecular inputs. This project is based on routines from xtb and dftb+.

Modules	Documentation	Versions	Description
nvitop		1.4.2-CUDA-12.8.0 1.5.3-CUDA-13.0.0	Desc An interactive NVIDIA-GPU process viewer and beyond, the one-stop solution for GPU process management.
nvtop		3.2.0	Desc htop-like GPU usage monitor
parallel		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
pinentry		1.1.1	Desc Pinentry is a collection of simple PIN or passphrase entry dialogs which utilize the Assuan protocol as described by the aegypten project;
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.
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.
psutil		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
robin-map		1.4.0	Desc robin-map is a C+ + implementation of a fast and memory efficient hash table. It is based on Robin Hood hashing with backward shift deletion.

Modules	Documentation	Versions	Description
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		0.16.2-Python-3.7.4, 0.18.1	Desc scikit-image is a collection of algorithms for image processing.
scikit-learn		0.21.3-Python-3.7.4, 0.23.2, 1.4.0	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.
settarg		settarg	Desc The settarg module provides a way to connect the loaded modules with your build system by setting environment variables.
setuptools-rust		1.8.0	Desc setuptools-rust is a plugin for setuptools to build Rust Python extensions implemented with PyO3 or rust-cpython.
spin		0.14	Desc Developer tool for scientific Python libraries

Modules	Documentation	Versions	Description
sympy		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		2019_U9, 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.
TensorBoard is a suite of web applications for inspecting and understanding your TensorFlow runs and graphs.			Desc
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.

Modules	Documentation	Versions	Description
typing-extensions		3.7.4.3, 4.10.0	Desc Typing Extensions – Backported and Experimental Type Hints for Python
uv	uv – Python package manager	0.7.13, 0.9.22	Desc An extremely fast Python package installer and resolver, written in Rust.
virtualenv		20.24.6	Desc A tool for creating isolated virtual python environments.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

AVX512

Installed software as of Sat, 16 May 2026 02:40:03 [updated hourly]

Modules	Documentation	Versions	Description
ABAQUS	Abaqus	2017, 2018, 2019, 2020, 2021-hotfix-2124, 2022-hotfix-2205, 2022-hotfix-2319, 2023-hotfix-2341, 2024-hotfix-2414, 2025-hotfix-2514	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	19.2, 2019.3, 2021.1, 2021.2, 2022.1, 2022.2, 2023.1, 2023.2, 2024.1, 2024.2, 2025.1, 2025.2	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.

Modules	Documentation	Versions	Description
ANSYSEM		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.
ASE		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.
Advisor		2025.0.0	Desc Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain
AlphaFold		2.1.1	Desc AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known
Amber		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.

Modules	Documentation	Versions	Description
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, 2.0	Desc BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.
Bazel		3.4.1, 3.7.2, 4.2.2, 6.5.0	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.
Boost		1.71.0, 1.74.0, 1.77.0, 1.81.0, 1.83.0, 1.88.0	Desc Boost provides free peer-reviewed portable C+ + source libraries.
Brunsli		0.1	Desc Brunsli is a lossless JPEG repacking library.
CFITSIO		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.

Modules	Documentation	Versions	Description
CGAL		4.14.1-Python-3.7.4, 4.14.3, 5.2, 5.6.1, 6.0.1	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.
CMake		3.15.3, 3.18.4, 3.20.1, 3.21.1, 3.22.1, 3.24.3, 3.27.6, 3.31.3, 3.31.8, 4.0.3	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-2.4	Desc
COMSOL	COMSOL	5.6, 6.1, 6.2, 6.3, 6.4	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.
CPCM-X		1.1.0	Desc This is an fully open source solvation model, based on the original conductor like screening model for realistic solvation (COSMO-RS) model by Klamt et al. in combination with the universal solvation model based on solute electron density (SMD) by Marenich, Cramer and Truhlar.
CPMD	CPMD	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.

Modules	Documentation	Versions	Description
CREST		2.11.2, 2.12, 3.0.2	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.
CUDA		10.1.243, 11.1.1, 11.4.1, 11.7.0, 11.8.0, 12.0.0, 12.4.0, 12.6.0, 12.8.0, 13.0.0	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.

Modules	Documentation	Versions	Description
Clang		16.0.4, 17.0.6	Desc C, C+ +, Objective-C compiler, based on LLVM. Does not include C+ + standard library – use libstdc+ + from GCC.
Cython		0.29.22, 3.0.10, 3.1.2	Desc Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).
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.
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
Eigen		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.
FEKO	FEKO	2021_hw, 2022.1_hw, 2022.3_hw	Desc FEKO is a computational electromagnetics software product developed by Altair Engineering

Modules	Documentation	Versions	Description
FEniCS-Basix		0.10.0	Desc Basix is a finite element definition and tabulation runtime library - C+ + library
FEniCS-Basix-Python		0.10.0	Desc Basix is a finite element definition and tabulation runtime library - Python binding
FEniCS-DOLFINx		0.10.0	Desc DOLFINx is the computational environment of FEniCSx - C+ + library
FEniCS-DOLFINx-Python		0.10.0	Desc DOLFINx is the computational environment of FEniCSx - Python binding
FEniCS-FFCx		0.10.0	Desc FFCx is a compiler for finite element variational forms
FEniCS-UFL		2025.2.1	Desc The Unified Form Language (UFL) is a domain-specific language for defining variational forms
FEniCS-ufcx		0.10.0	Desc FFCx provides the ufcx.h interface header for generated finite element kernels, used by DOLFINx.
FFTW		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.

Modules	Documentation	Versions	Description
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, 3.4.5	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.
FriBidi		1.0.5, 1.0.10, 1.0.12, 1.0.13, 1.0.16	Desc The Free Implementation of the Unicode Bidirectional Algorithm.
GAMS		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.
GCC		8.3.0, 10.2.0, 10.3.0, 11.2.0, 12.2.0, 13.2.0, 14.3.0	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,...).

Modules	Documentation	Versions	Description
GMP		6.2.1	Desc GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers.
GROMACS		2023.5-CUDA-12.0.0, 2024.1, 2025.2	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		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.
GTK3		3.24.35, 3.24.39	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.

Modules	Documentation	Versions	Description
GaussView		6.0.16	Desc GaussView is a very advanced and powerful graphical user interface for Gaussian
Gaussian		g16.A03, g16.B01	Desc Gaussian is a general purpose quantum chemistry software package for ab initio electronic structure calculations.
Go		1.16.6, 1.22.1, 1.25.0	Desc Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.
Graphviz		8.1.0	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.

Modules	Documentation	Versions	Description
Gurobi		9.1.2, 9.5.0, 11.0.0, 11.0.3, 12.0.1, 12.0.3	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		2.4-Python-2.7.16	Desc
HDF		4.2.14, 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		1.10.5, 1.10.7, 1.12.1, 1.14.0, 1.14.3, 1.14.6	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.
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).

Modules	Documentation	Versions	Description
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		2.3	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.

Modules	Documentation	Versions	Description
Highway		1.0.3	Desc Highway is a C++ library for SIMD (Single Instruction, Multiple Data), i.e. applying the same operation to 'lanes'.
IPython		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		7.0.9-5, 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
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_92, 1.8.0_152, 1.8, 11.0.2, 11.0.18, 11.0.20	Desc Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.

Modules	Documentation	Versions	Description
Julia		1.7.2-linux-x86_64, 1.10.4-linux-x86_64	Desc Julia is a high-level, high-performance dynamic programming language for numerical computing
JupyterLab	Jupyter on LUIS 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.
KaHIP		3.16, 3.19	Desc The graph partitioning framework KaHIP – Karlsruhe High Quality Partitioning.
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.

Modules	Documentation	Versions	Description
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.
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).

Modules	Documentation	Versions	Description
Lua		5.1.5, 5.4.2, 5.4.3, 5.4.4, 5.4.6, 5.4.8	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		2023-1, 2024-1.02, 2025-1, 2025-2.01, 2026-1	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	2019a, 2019b, 2020a, 2020b, 2021a, 2021b, 2022a, 2022b, 2023a, 2023b, 2024b, 2025b	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.

Modules	Documentation	Versions	Description
METIS		5.1.0	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		4.0.2, 4.1.0, 4.2.0, 4.2.1, 4.2.2	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, 5.8.1-metis	Desc A parallel sparse direct solver
Mako		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

Modules	Documentation	Versions	Description
Maple		2021.0, 2024.0	Desc Maple combines the world's most powerful mathematical computation engine with an intuitive, 'clickable' user interface.
Mathematica		13.2.1, 14.0.0	Desc Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields.
Meson		0.55.3, 0.58.0, 0.58.2, 0.59.1-Python-3.7.4, 0.64.0, 1.2.3, 1.6.1, 1.8.2	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
Miniconda3		22.11.1-1, 23.5.2-0, 24.7.1-0	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.
Miniforge3	Conda	23.11.0-0, 24.7.1-2, 25.3.0-3	Desc Miniforge is a free minimal installer for conda and Mamba specific to conda-forge.
Molden		7.3	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		1.48.0	Desc Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.

Modules	Documentation	Versions	Description
NCCL		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, 2.20.5-CUDA-12.8.0, 2.22.3-CUDA-12.6.0	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	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, 24.9-CUDA-12.6.0, 25.3-CUDA-12.8.0	Desc C, C+ + and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)
Ninja		1.9.0, 1.10.1, 1.10.2, 1.11.1, 1.12.1, 1.13.0	Desc Ninja is a small build system with a focus on speed.
ORCA		4.2.1, 5.0.1, 5.0.4, 6.0.0-avx2, 6.1.0	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		5.1.0, 9.1.0, 10.2.0	Desc GNU Octave is a high-level interpreted language, primarily intended for numerical computations.
Octopus		11.4, 13.0, 15.0	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		0.3.7, 0.3.12, 0.3.18, 0.3.21, 0.3.24, 0.3.30	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.

Modules	Documentation	Versions	Description
OpenCV		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		2.4.0, 3.1.0, 4.0.1	Desc OpenFAST is a multi-physics, multi-fidelity tool for simulating the coupled dynamic response of wind turbines.
OpenFOAM		v2012, v2106, v2212, v2412, v2506, 8, 9, 10, 13	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.

Modules	Documentation	Versions	Description
OpenFOAM-Extend		4.1-20200408-Python-2.7.16	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		3.1.4, 4.0.5, 4.1.1, 4.1.4, 4.1.6, 5.0.8	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.
PCL		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.

Modules	Documentation	Versions	Description
PETSc		3.15.5-Python-3.7.4, 3.15.5	Desc PETSc, pronounced PET-see (the S is silent), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations.
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.
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.

Modules	Documentation	Versions	Description
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.
PNFFT		20240604	Desc PNFFT is a software library written in C for computing parallel nonequispaced fast Fourier transformations.
POV-Ray		3.7.0.10	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.

Modules	Documentation	Versions	Description
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
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.

Modules	Documentation	Versions	Description
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.
ParaView		5.6.2-Python-3.7.4-mpi, 5.8.1-mpi, 5.9.1-mpi, 5.12.0, 6.0.1	Desc ParaView is a scientific parallel visualizer.
Perl		5.30.0-minimal, 5.30.0, 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, 5.38.2, 5.40.0, 5.40.2	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, 5.40.0, 5.40.2	Desc A set of common packages from CPAN
Pillow		6.2.1, 8.0.1, 8.3.2, 9.4.0, 10.2.0, 11.3.0	Desc Pillow is the 'friendly PIL fork' by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.
Pixi		0.59.0, 0.67.2	Desc Pixi is a cross-platform, multi-language package manager and workflow tool built on the foundation of the conda ecosystem. It provides developers with an exceptional experience similar to popular package managers like cargo or npm, but for any language.
PnetCDF		1.12.3	Desc Parallel netCDF: A Parallel I/O Library for NetCDF File Access
ProFit		3.3	Desc ProFit is the protein least squares fitting program

Modules	Documentation	Versions	Description
PyMOL		2.5.0	Desc PyMOL is a Python-enhanced molecular graphics tool. It excels at 3D visualization of proteins, small molecules, density, surfaces, and trajectories. It also includes molecular editing, ray tracing, and movies. Open Source PyMOL is free to everyone!
PyQt5		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		1.6.0-Python-3.7.4, 1.9.0, 1.10.0, 1.13.1-CUDA-12.0.0, 1.13.1, 2.1.2	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.
Pysam		0.22.0, 0.23.2	Desc Pysam is a python module for reading and manipulating Samfiles. It's a lightweight wrapper of the samtools C-API. Pysam also includes an interface for tabix.
Python		2.7.16, 2.7.18-bare, 2.7.18, 3.7.4, 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, 3.12.3, 3.13.1, 3.13.5	Desc Python is a programming language that lets you work more quickly and integrate your systems more effectively.
Python-bundle-PyPI		2023.10, 2025.07	Desc Bundle of Python packages from PyPI

Modules	Documentation	Versions	Description
Qt5		5.13.1, 5.14.2, 5.15.2, 5.15.7, 5.15.13	Desc Qt is a comprehensive cross-platform C+ + application framework.
Qt6		6.6.3, 6.9.3	Desc Qt is a comprehensive cross-platform C+ + application framework.
R		4.1.0, 4.1.2, 4.2.2, 4.4.1	Desc R is a free software environment for statistical computing and graphics.
ROOT		6.26.10	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, 1.85.1, 1.88.0, 1.91.1	Desc Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.
SAMtools		1.19.2, 1.22	Desc SAM Tools provide various utilities for manipulating alignments in the SAM format, including sorting, merging, indexing and generating alignments in a per-position format.

Modules	Documentation	Versions	Description
SCIPOptSuite		8.0.4-Gurobi-9.5.0, 8.0.4	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		6.0.9, 6.1.0, 6.1.2-no-thread, 6.1.2, 7.0.2, 7.0.4, 7.0.10	Desc Software package and libraries for sequential and parallel graph partitioning, static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.
SDL3		3.4.4	Desc Simple DirectMedia Layer is a cross-platform development library designed to provide low level access to audio, keyboard, mouse, joystick, and graphics hardware via OpenGL and Direct3D.
SDL3_image		3.4.2	Desc This is a simple library to load images of various formats as SDL surfaces. It can load BMP, GIF, JPEG, LBM, PCX, PNG, PNM (PPM/PGM/PBM), QOI, TGA, XCF, XPM, and simple SVG format images. It can also load AVIF, JPEG-XL, TIFF, and WebP images, depending on build options (see the note below for details.)

Modules	Documentation	Versions	Description
SDL3_ttf		3.2.2	Desc This library is a wrapper around the FreeType and Harfbuzz libraries, allowing you to use TrueType fonts to render text in SDL applications.
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, 2.1.0-fb, 2.1.0, 2.2.0-fb, 2.2.2-fb	Desc The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.
SciPy-bundle		2019.10-Python-3.7.4, 2020.11, 2021.10, 2023.02, 2023.11, 2025.07	Desc Bundle of Python packages for scientific software

Modules	Documentation	Versions	Description
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.
Spyder		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.
StdEnv		2024.10	Desc
Subversion		1.14.1	Desc Subversion is an open source version control system.
SuiteSparse		5.6.0-METIS-5.1.0, 5.8.1-METIS-5.1.0, 5.13.0-METIS-5.1.0, 7.7.0, 7.11.0	Desc SuiteSparse is a collection of libraries to manipulate sparse matrices.
Tcl		8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13, 8.6.14, 8.6.16, 9.0.1	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.

Modules	Documentation	Versions	Description
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		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
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		8.6.9, 8.6.10, 8.6.11, 8.6.12, 8.6.13, 9.0.1	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.
VMD		1.9.4a57	Desc VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

Modules	Documentation	Versions	Description
VSCode		1.102.3	Desc Visual Studio Code is a lightweight but powerful source code editor which runs on your desktop and is available for Windows, macOS and Linux. It comes with built-in support for JavaScript, TypeScript and Node.js and has a rich ecosystem of extensions for other languages and runtimes (such as C++, C#, Java, Python, PHP, Go, .NET).
VSEARCH		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.

Modules	Documentation	Versions	Description
VTK		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		2024.3.0, 2025.4.0	Desc Intel® VTune™ Profiler optimizes application performance, system performance, and system configuration for HPC, cloud, IoT, media, storage, and more.
Valgrind		3.16.1	Desc Valgrind: Debugging and profiling tools

Modules	Documentation	Versions	Description
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.

Modules	Documentation	Versions	Description
Wayland		1.22.0, 1.24.0	Desc Wayland is a project to define a protocol for a compositor to talk to its clients as well as a library implementation of the protocol. The compositor can be a standalone display server running on Linux kernel modesetting and evdev input devices, an X application, or a wayland client itself. The clients can be traditional applications, X servers (rootless or fullscreen) or other display servers.
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, 4.15.1	Desc Z3 is a theorem prover from Microsoft Research.

Modules	Documentation	Versions	Description
ZeroMQ		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.
Zoltan		3.901	Desc Zoltan Dynamic Load Balancing and Graph Algorithm Toolkit
arpack-ng		3.7.0, 3.8.0, 3.9.1	Desc ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
btop		1.4.6	Desc Resource monitor that shows usage and stats for processor, memory, disks, network and processes.

Modules	Documentation	Versions	Description
cURL		7.66.0, 7.72.0, 7.76.0, 7.78.0, 7.86.0, 8.3.0, 8.11.1, 8.14.1	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.
code-server	Code-Server (VS Code) on LUIS Cluster	4.107.0	Desc Run VS Code on any machine anywhere and access it in the browser.
cryptography		41.0.5, 45.0.5	Desc cryptography is a package designed to expose cryptographic primitives and recipes to Python developers.
cuDNN		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, 9.5.0.50-CUDA-12.4.0, 9.5.0.50-CUDA-12.6.0, 9.10.1.4-CUDA-12.8.0	Desc The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.
dask		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.

Modules	Documentation	Versions	Description
dftd4		3.7.0	Desc The dftd4 project provides an implementation of the generally applicable, charge dependent London-dispersion correction, termed DFT-D4.
foss		2019b, 2020b, 2021b, 2022b, 2023b, 2025b	Desc GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.
fosscuda		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.

Modules	Documentation	Versions	Description
gcccuda		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.
git		2.23.0-nodocs, 2.28.0-nodocs, 2.32.0-nodocs, 2.33.1-nodocs, 2.38.1-nodocs, 2.42.0, 2.50.1	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.
gnuplot		5.2.8, 5.4.1, 5.4.2, 5.4.6, 6.0.1, 6.0.3	Desc Portable interactive, function plotting utility
gperftools		2.17.2	Desc gperftools is a collection of a high-performance multi-threaded malloc() implementation, plus some pretty nifty performance analysis tools. Includes TCMalloc, heap-checker, heap-profiler and cpu-profiler.

Modules	Documentation	Versions	Description
h5py		2.10.0-Python-3.7.4, 3.1.0, 3.6.0, 3.11.0	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.
hypothesis		4.44.2-Python-3.7.4, 5.41.2, 5.41.5, 6.14.6, 6.68.2, 6.90.0, 6.136.6	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.
iTensor		3.1.11	Desc An efficient and flexible C+ + library for performing tensor network calculations
imkl		2021.2.0, 2022.2.1, 2023.2.0, 2024.2.0, 2025.1.0, 2025.2.0	Desc Intel oneAPI Math Kernel Library
imkl-FFTW		2022.2.1, 2023.2.0, 2024.2.0, 2025.1.0, 2025.2.0	Desc FFTW interfaces using Intel oneAPI Math Kernel Library
impi		2021.2.0, 2021.7.1, 2021.10.0, 2021.13.0, 2021.15.0, 2021.16.1	Desc Intel MPI Library, compatible with MPICH ABI
intel		2021a, 2022b, 2023b, 2024a, 2025a, 2025b	Desc Compiler toolchain including Intel compilers, Intel MPI and Intel Math Kernel Library (MKL).
intel-compilers		2021.2.0, 2022.2.1, 2023.2.1, 2024.2.0, 2025.1.1, 2025.2.0	Desc Intel C, C+ + & Fortran compilers (classic and oneAPI)

Modules	Documentation	Versions	Description
jax		0.4.34-CUDA-12.8.0	Desc Composable transformations of Python+NumPy programs: differentiate, vectorize, JIT to GPU/TPU, and more
libgpuarray		0.7.6-Python-3.7.4	Desc Library to manipulate tensors on the GPU.
likwid		5.2.2	Desc Likwid stands for Like I knew what I am doing. This project contributes easy to use command line tools for Linux to support programmers in developing high performance multi threaded programs.
lmod		lmod	Desc Lmod: An Environment Module System
magma		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		3.1.1-Python-3.7.4, 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.

Modules	Documentation	Versions	Description
maturin		1.8.3, 1.9.1	Desc This project is meant as a zero configuration replacement for setuptools-rust and milksnake. It supports building wheels for python 3.5+ on windows, linux, mac and freebsd, can upload them to pypi and has basic pypy and graalpy support.
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		3.0.3-Python-2.7.16, 3.0.3-Python-3.7.4, 3.1.4, 3.1.5	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	0.11, 0.11.1, 0.12	Desc MPI-Based File Utilities For Distributed Systems
multicharge		0.3.0	Desc Electronegativity equilibration model for atomic partial charges.
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		4.7.1, 4.7.4, 4.8.0, 4.8.1, 4.9.0, 4.9.2, 4.9.3	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.
netCDF-Fortran		4.5.3, 4.6.0, 4.6.1, 4.6.2	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.
networkx		2.4-Python-3.7.4, 2.5, 2.6.3, 3.0, 3.2.1, 3.5	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.
numsa		0.2.0	Desc Numerical surface area integrator for molecular inputs. This project is based on routines from xtb and dftb+.

Modules	Documentation	Versions	Description
nvitop		1.4.2-CUDA-12.8.0 1.5.3-CUDA-13.0.0	Desc An interactive NVIDIA-GPU process viewer and beyond, the one-stop solution for GPU process management.
nvtop		3.2.0	Desc htop-like GPU usage monitor
parallel		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
pinentry		1.1.1	Desc Pinentry is a collection of simple PIN or passphrase entry dialogs which utilize the Assuan protocol as described by the aegypten project;
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.
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.
psutil		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
robin-map		1.4.0	Desc robin-map is a C+ + implementation of a fast and memory efficient hash table. It is based on Robin Hood hashing with backward shift deletion.

Modules	Documentation	Versions	Description
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		0.16.2-Python-3.7.4, 0.18.1	Desc scikit-image is a collection of algorithms for image processing.
scikit-learn		0.21.3-Python-3.7.4, 0.23.2, 1.4.0	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.
settarg		settarg	Desc The settarg module provides a way to connect the loaded modules with your build system by setting environment variables.
setuptools-rust		1.8.0	Desc setuptools-rust is a plugin for setuptools to build Rust Python extensions implemented with PyO3 or rust-cpython.
spin		0.14	Desc Developer tool for scientific Python libraries

Modules	Documentation	Versions	Description
sympy		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		2019_U9, 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.
TensorBoard is a suite of web applications for inspecting and understanding your TensorFlow runs and graphs.			Desc
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.

Modules	Documentation	Versions	Description
typing-extensions		3.7.4.3, 4.10.0	Desc Typing Extensions – Backported and Experimental Type Hints for Python
uv	uv – Python package manager	0.7.13, 0.9.22	Desc An extremely fast Python package installer and resolver, written in Rust.
virtualenv		20.24.6	Desc A tool for creating isolated virtual python environments.
yaff		1.6.0-Python-3.7.4	Desc Yaff stands for 'Yet another force field'. It is a pythonic force-field code.