
arc-module-list

Release 0.1

The ARC Team

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This is a list of the currently installed applications/libraries on the Oxford University ARC/HTC clusters.
For information on how to load modules and other important information see the following documents:

[ARC User Guide](#)

[ARC Software Guide](#)

CONTENTS

1.1 ABINIT

Description

ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave or wavelet basis.

More Information

<https://www.abinit.org/>

Available Versions:

<code>9.4.2-foss-2021a</code> <code>9.2.1-intel-2020a</code> <code>9.6.2-intel-2021b</code>

1.2 ABySS

Description

Assembly By Short Sequences - a de novo, parallel, paired-end sequence assembler

More Information

<https://www.bcgsc.ca/platform/bioinfo/software/abyss>

Available Versions:

<code>2.1.5-foss-2019b</code>

1.3 ACTC

Description

ACTC converts independent triangles into triangle strips or fans.

More Information

<https://sourceforge.net/projects/actc>

Available Versions:

1.1-GCCcore-10.2.0
1.1-GCCcore-8.3.0

1.4 ADMIXTURE

Description

ADMIXTURE is a software tool for maximum likelihood estimation of individual ancestries from multilocus SNP genotype datasets. It uses the same statistical model as STRUCTURE but calculates estimates much more rapidly using a fast numerical optimization algorithm.

More Information

<https://dalexander.github.io/admixture>

Available Versions:

1.3.0

1.5 ADOL-C

Description

The package ADOL-C (Automatic Differentiation by OverLoading in C++) facilitates the evaluation of first and higher derivatives of vector functions that are defined by computer programs written in C or C++. The resulting derivative evaluation routines may be called from C/C++, Fortran, or any other language that can be linked with C.

More Information

<https://projects.coin-or.org/ADOL-C>

Available Versions:

2.7.2-gompi-2020a

1.6 AMOS

Description

The AMOS consortium is committed to the development of open-source whole genome assembly software

More Information

<http://amos.sourceforge.net>

Available Versions:

3.1.0-foss-2018b

1.7 ANSYS

Available Versions:

2022R1

2023R1

2021R2

1.8 ANTLR

Description

ANTLR, ANother Tool for Language Recognition, (formerly PCCTS) is a language tool that provides a framework for constructing recognizers, compilers, and translators from grammatical descriptions containing Java, C#, C++, or Python actions.

More Information

<https://www.antlr2.org/>

Available Versions:

2.7.7-GCCcore-10.3.0-Java-11

2.7.7-GCCcore-10.2.0-Java-11

1.9 APR

Description

Apache Portable Runtime (APR) libraries.

More Information

<https://apr.apache.org/>

Available Versions:

1.7.0-GCCcore-10.2.0

1.10 APR-util

Description

Apache Portable Runtime (APR) util libraries.

More Information

<https://apr.apache.org/>

Available Versions:

1.6.1-GCCcore-10.2.0

1.11 ASE

Description

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.

More Information

<https://wiki.fysik.dtu.dk/ase>

Available Versions:

3.20.1-foss-2020b
3.22.1-foss-2022a
3.22.0-foss-2021a
3.22.1-intel-2022a

1.12 ATK

Description

ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications.

More Information

<https://developer.gnome.org/ATK/stable/>

Available Versions:

2.32.0-GCCcore-8.2.0
2.34.1-GCCcore-8.3.0
2.38.0-GCCcore-11.3.0
2.28.1-foss-2018b
2.36.0-GCCcore-11.2.0
2.36.0-GCCcore-9.3.0
2.36.0-GCCcore-10.2.0

1.13 AUGUSTUS

Description

AUGUSTUS is a program that predicts genes in eukaryotic genomic sequences

More Information

<http://bioinf.uni-greifswald.de/augustus/>

Available Versions:

3.3.3-foss-2019b
3.4.0-foss-2020b

1.14 Abaqus

Description

Finite Element Analysis software for modeling, visualization and best-in-class implicit and explicit dynamics FEA.

More Information

https://www.simulia.com/products/abaqus_fea.html

Available Versions:

2022

1.15 Advisor

Description

Vectorization Optimization and Thread Prototyping - Vectorize & thread code or performance “dies” - Easy workflow + data + tips = faster code faster - Prioritize, Prototype & Predict performance gain

More Information

<https://software.intel.com/intel-advisor-xe>

Available Versions:

2019_update5

1.16 AlphaFold

Description

AlphaFold can predict protein structures with atomic accuracy even where no similar structure is known

More Information

<https://deepmind.com/research/case-studies/alphafold>

Available Versions:

```
2.1.1-fosscuda-2020b
2.3.0-foss-2021b-CUDA-11.4.1
2.0.0-fosscuda-2020b
2.2.2-foss-2021a-CUDA-11.3.1
```

1.17 Amber

Description

Amber (originally Assisted Model Building with Energy Refinement) is software for performing molecular dynamics and structure prediction.

More Information

<https://ambermd.org>

Available Versions:

```
18-foss-2019b-AmberTools-19-patchlevel-12-17-Python-2.7.16
18-foss-2018b-AmberTools-18-patchlevel-10-8
18-fosscuda-2019b-AmberTools-19-patchlevel-12-17-Python-2.7.16
18-fosscuda-2018b-AmberTools-18-patchlevel-10-8
```

1.18 AmberTools

Description

AmberTools consists of several independently developed packages that work well by themselves, and with Amber itself. The suite can also be used to carry out complete molecular dynamics simulations, with either explicit water or generalized Born solvent models.

More Information

<https://ambermd.org/>

Available Versions:

```
20-gompi-2019b-dba-Python-3.7.4
20-intel-2020a-Python-3.8.2
22.3-foss-2021b
```

1.19 Anaconda2

Description

Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.

More Information

<https://www.anaconda.com>

Available Versions:

```
4.2.0
2019.10
2019.03
```

1.20 Anaconda3

Description

Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.

More Information

<https://www.anaconda.com>

Available Versions:

```
2021.05
2022.05
2021.11
2020.11
2020.02
```

1.21 Armadillo

Description

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.

More Information

<https://arma.sourceforge.net/>

Available Versions:

```
9.900.1-foss-2020a
```

1.22 Arriba

Description

Arriba is a command-line tool for the detection of gene fusions from RNA-Seq data. It was developed for the use in a clinical research setting. Therefore, short runtimes and high sensitivity were important design criteria.

More Information

<https://github.com/suhrig/arriba>

Available Versions:

2.3.0-GCC-11.2.0

1.23 Arrow

Description

Apache Arrow (incl. PyArrow Python bindings), a cross-language development platform for in-memory data.

More Information

<https://arrow.apache.org>

Available Versions:

8.0.0-foss-2021b
0.16.0-foss-2019b-Python-3.7.4
6.0.0-foss-2021b
8.0.0-foss-2022a

1.24 Aspera-CLI

Description

IBM Aspera Command-Line Interface (the Aspera CLI) is a collection of Aspera tools for performing high-speed, secure data transfers from the command line. The Aspera CLI is for users and organizations who want to automate their transfer workflows.

More Information

<https://asperasoft.com>

Available Versions:

3.9.6.1467.159c5b1

1.25 Aspera-Connect

Description

Connect is an install-on-demand Web browser plug-in that facilitates high-speed uploads and downloads with an Aspera transfer server.

More Information

<http://downloads.asperasoft.com/connect2/>

Available Versions:

3.9.6

1.26 AutoDock

Description

AutoDock is a suite of automated docking tools. It is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure.

More Information

<http://autodock.scripps.edu/>

Available Versions:

4.2.6-GCC-9.3.0

1.27 AutoDock-Vina

Description

AutoDock Vina is an open-source program for doing molecular docking.

More Information

<https://vina.scripps.edu/>

Available Versions:

1.2.3-foss-2021b

1.28 AutoDock_Vina

Description

AutoDock Vina is an open-source program for doing molecular docking.

More Information

<http://vina.scripps.edu/index.html>

Available Versions:

1.1.2_linux_x86

1.29 Autoconf

Description

Autoconf is an extensible package of M4 macros that produce shell scripts to automatically configure software source code packages. These scripts can adapt the packages to many kinds of UNIX-like systems without manual user intervention. Autoconf creates a configuration script for a package from a template file that lists the operating system features that the package can use, in the form of M4 macro calls.

More Information

<https://www.gnu.org/software/autoconf/>

Available Versions:

```
2.71-GCCcore-10.3.0
2.69-GCCcore-9.3.0
2.69-GCCcore-7.3.0
2.69-GCCcore-10.2.0
2.71-GCCcore-11.3.0
2.71-GCCcore-11.2.0
2.69-GCCcore-8.1.0
2.69-GCCcore-8.2.0
2.69
2.71-GCCcore-12.2.0
2.69-GCCcore-8.3.0
```

1.30 Automake

Description

Automake: GNU Standards-compliant Makefile generator

More Information

<https://www.gnu.org/software/automake/automake.html>

Available Versions:

```
1.16.1-GCCcore-8.2.0
1.16.1-GCCcore-8.3.0
1.16.4-GCCcore-11.2.0
1.16.1-GCCcore-8.1.0
1.16.3-GCCcore-10.3.0
1.16.2-GCCcore-10.2.0
1.16.5-GCCcore-11.3.0
1.16.1-GCCcore-9.3.0
1.16.1-GCCcore-10.2.0
1.16.1-GCCcore-7.3.0
1.16.5-GCCcore-12.2.0
```

1.31 Autotools

Description

This bundle collect the standard GNU build tools: Autoconf, Automake and libtool

More Information

<http://autotools.io>

Available Versions:

```
20180311-GCCcore-10.2.0
20180311-GCCcore-7.3.0
20180311-GCCcore-8.1.0
```

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```
20220317-GCCcore-12.2.0
20220317-GCCcore-11.3.0
20180311-GCCcore-8.2.0
20180311-GCCcore-8.3.0
20210726-GCCcore-11.2.0
20210128-GCCcore-10.3.0
20200321-GCCcore-10.2.0
20180311-GCCcore-9.3.0
```

1.32 BAGEL

Description

BAGEL (Brilliantly Advanced General Electronic-structure Library) is a parallel electronic-structure program.

More Information

<http://www.nubakery.org>

Available Versions:

```
1.2.2-foss-2019a
1.2.2-intel-2020a
```

1.33 BCFtools

Description

Samtools is a suite of programs for interacting with high-throughput sequencing data. BCFtools - Reading/writing BCF2/VCF/gVCF files and calling/filtering/summarising SNP and short indel sequence variants

More Information

<https://www.htslib.org/>

Available Versions:

```
1.11-GCC-10.2.0
1.14-GCC-11.2.0
1.10.2-GCC-8.3.0
1.9-foss-2018b
1.10.2-GCC-9.3.0
```

1.34 BEDTools

Description

BEDTools: a powerful toolset for genome arithmetic. The BEDTools utilities allow one to address common genomics tasks such as finding feature overlaps and computing coverage. The utilities are largely based on four widely-used file formats: BED, GFF/GTF, VCF, and SAM/BAM.

More Information

<https://bedtools.readthedocs.io/>

Available Versions:

```
2.29.2-GCC-8.3.0
2.29.2-GCC-9.3.0
2.30.0-GCC-11.2.0
```

1.35 BLAST

Description

Basic Local Alignment Search Tool, or BLAST, is an algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences.

More Information

<https://blast.ncbi.nlm.nih.gov/>

Available Versions:

```
2.11.0-Linux_x86_64
2.10.1-Linux_x86_64
```

1.36 BLAST+

Description

Basic Local Alignment Search Tool, or BLAST, is an algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences.

More Information

<https://blast.ncbi.nlm.nih.gov/>

Available Versions:

```
2.13.0-gompi-2022a
2.9.0-gompi-2019b
2.7.1-foss-2018b
2.12.0-gompi-2021b
2.11.0-gompi-2021a
2.11.0-gompi-2020b
2.10.1-impi-2020a
```

1.37 BLAT

Description

BLAT on DNA is designed to quickly find sequences of 95% and greater similarity of length 25 bases or more.

More Information

<https://genome.ucsc.edu/FAQ/FAQblat.html>

Available Versions:

3.5-GCC-9.3.0

1.38 BLIS

Description

BLIS is a portable software framework for instantiating high-performance BLAS-like dense linear algebra libraries.

More Information

<https://github.com/flame/blis/>

Available Versions:

0.8.1-GCC-11.2.0

0.9.0-GCC-12.2.0

0.9.0-GCC-11.3.0

1.39 BRAKER

Description

BRAKER is a pipeline for fully automated prediction of protein coding genes with GeneMark-ES/ET and AUGUSTUS in novel eukaryotic genomes.

More Information

<https://github.com/Gaius-Augustus/BRAKER>

Available Versions:

2.1.6-foss-2019b-Python-3.7.4

1.40 BWA

Description

Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome.

More Information

<http://bio-bwa.sourceforge.net/>

Available Versions:

```
0.7.17-GCC-9.3.0
0.7.17-GCCcore-11.2.0
0.7.17-foss-2018b
```

1.41 BamTools

Description

BamTools provides both a programmer's API and an end-user's toolkit for handling BAM files.

More Information

<https://github.com/pezmaster31/bamtools>

Available Versions:

```
2.5.1-GCC-9.3.0
2.5.2-GCC-11.2.0
2.5.1-GCC-10.2.0
2.5.1-GCC-8.3.0
```

1.42 BayeScEnv

Description

BayeScEnv is a Fst-based, genome-scan method that uses environmental variables to detect local adaptation.

More Information

<https://github.com/devillemereuil/bayescenv>

Available Versions:

```
1.1-GCC-8.3.0
```

1.43 BayesTraits

Description

BayesTraits is a computer package for performing analyses of trait evolution among groups of species for which a phylogeny or sample of phylogenies is available. This new package incorporates our earlier and separate programmes Multistate, Discrete and Continuous. BayesTraits can be applied to the analysis of traits that adopt a finite number of discrete states, or to the analysis of continuously varying traits. Hypotheses can be tested about models of evolution, about ancestral states and about correlations among pairs of traits.

More Information

<http://www.evolution.reading.ac.uk/BayesTraitsV1.html>

Available Versions:

2.0-Beta-Linux64

1.44 Bazel

Description

Bazel is a build tool that builds code quickly and reliably. It is used to build the majority of Google's software.

More Information

<https://bazel.io/>

Available Versions:

4.2.2-GCCcore-11.2.0
0.26.1-GCCcore-8.3.0
0.29.1-GCCcore-8.3.0
3.7.2-GCCcore-10.2.0
3.6.0-GCCcore-9.3.0
3.7.2-GCCcore-10.3.0
3.7.2-GCCcore-11.2.0

1.45 Beagle

Description

Beagle is a software package for phasing genotypes and for imputing ungenotyped markers.

More Information

<https://faculty.washington.edu/browning/beagle/beagle.html>

Available Versions:

5.4.22Jul22.46e-Java-11

1.46 Beast

Description

BEAST is a cross-platform program for Bayesian MCMC analysis of molecular sequences. It is entirely orientated towards rooted, time-measured phylogenies inferred using strict or relaxed molecular clock models. It can be used as a method of reconstructing phylogenies but is also a framework for testing evolutionary hypotheses without conditioning on a single tree topology. BEAST uses MCMC to average over tree space, so that each tree is weighted proportional to its posterior probability.

More Information

<http://beast2.org/>

Available Versions:

2.5.2-GCC-8.2.0-2.31.1 2.5.2-GCC-7.3.0-2.30
--

1.47 BeautifulSoup

Description

Beautiful Soup is a Python library designed for quick turnaround projects like screen-scraping.

More Information

<https://www.crummy.com/software/BeautifulSoup>

Available Versions:

4.10.0-GCCcore-11.3.0

1.48 Bio-SearchIO-hmmer

Description

Code to parse output from hmmsearch, hmmscan, phmmer and nhmmer, compatible with both version 2 and version 3 of the HMMER package from <http://hmmer.org>.

More Information

<https://metacpan.org/pod/Bio::SearchIO::hmmer3>

Available Versions:

1.7.3-GCC-10.3.0

1.49 BioPerl

Description

BioPerl is the product of a community effort to produce Perl code which is useful in biology. Examples include Sequence objects, Alignment objects and database searching objects.

More Information

<https://bioperl.org/>

Available Versions:

```
1.7.8-GCCcore-11.3.0
1.7.7-GCCcore-9.3.0
1.7.8-GCCcore-11.2.0
1.7.8-GCCcore-10.3.0
```

1.50 Biopython

Description

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.

More Information

<https://www.biopython.org>

Available Versions:

```
1.79-foss-2022a
1.72-foss-2018b-Python-2.7.15
1.75-foss-2019b-Python-3.7.4
1.78-intel-2020a-Python-3.8.2
1.78-fosscuda-2020b
1.79-foss-2021b
1.79-foss-2021a
```

1.51 Bismark

Description

A tool to map bisulfite converted sequence reads and determine cytosine methylation states

More Information

<https://www.bioinformatics.babraham.ac.uk/projects/bismark/>

Available Versions:

```
0.23.1-foss-2021b
```

1.52 Bison

Description

Bison is a general-purpose parser generator that converts an annotated context-free grammar into a deterministic LR or generalized LR (GLR) parser employing LALR(1) parser tables.

More Information

<http://www.gnu.org/software/bison>

Available Versions:

3.3.2-GCCcore-8.3.0
3.0.5-GCCcore-8.1.0
3.8.2-GCCcore-12.2.0
3.3.2
3.0.5-GCCcore-8.2.0
3.7.6
3.0.5
3.5.3-GCCcore-9.3.0
3.0.4
3.7.6-GCCcore-10.3.0
3.8.2
3.0.5-GCCcore-8.3.0
3.5.3
3.8.2-GCCcore-11.3.0
3.3.2-GCCcore-9.3.0
3.0.5-GCCcore-7.3.0
3.7.1-GCCcore-10.2.0
3.7.6-GCCcore-11.2.0
3.0.4-GCCcore-7.3.0
3.7.1
3.0.4-GCCcore-8.1.0

1.53 Blender

Description

Blender is the free and open source 3D creation suite. It supports the entirety of the 3D pipeline-modeling, rigging, animation, simulation, rendering, compositing and motion tracking, even video editing and game creation.

More Information

<https://www.blender.org/>

Available Versions:

2.81-foss-2019b-Python-3.7.4

1.54 Blosc

Description

Blosc, an extremely fast, multi-threaded, meta-compressor library

More Information

<https://www.blosc.org/>

Available Versions:

1.21.0-GCCcore-10.3.0

1.55 Bonnie++

Description

Enhanced performance Test of Filesystem I/O

More Information

<https://www.coker.com.au/bonnie++>

Available Versions:

2.00a-GCC-10.3.0

1.56 Boost

Description

Boost provides free peer-reviewed portable C++ source libraries.

More Information

<https://www.boost.org/>

Available Versions:

1.79.0-GCC-11.3.0
1.72.0-iimpi-2021b
1.72.0-iimpi-2020a
1.74.0-GCC-10.2.0
1.71.0-gompi-2019b
1.67.0-foss-2018b
1.67.0-fosscuda-2018b
1.76.0-GCC-10.3.0
1.79.0-GCC-11.2.0
1.71.0-gompic-2019b
1.70.0-gompi-2019a
1.77.0-GCC-11.2.0
1.72.0-gompi-2020a
1.74.0-iccifort-2020.4.304

1.57 Boost.Python

Description

Boost.Python is a C++ library which enables seamless interoperability between C++ and the Python programming language.

More Information

<http://boostorg.github.io/python>

Available Versions:

```
1.67.0-foss-2018b-Python-2.7.15
1.71.0-gompic-2019b
1.71.0-gompi-2019b
1.67.0-fosscuda-2018b-Python-2.7.15
1.72.0-gompi-2020a
1.70.0-gompi-2019a
```

1.58 Bowtie

Description

Bowtie is an ultrafast, memory-efficient short read aligner. It aligns short DNA sequences (reads) to the human genome.

More Information

<http://bowtie-bio.sourceforge.net/index.shtml>

Available Versions:

```
1.3.1-GCC-11.2.0
1.2.3-GCC-9.3.0
```

1.59 Bowtie2

Description

Bowtie 2 is an ultrafast and memory-efficient tool for aligning sequencing reads to long reference sequences. It is particularly good at aligning reads of about 50 up to 100s or 1,000s of characters, and particularly good at aligning to relatively long (e.g. mammalian) genomes. Bowtie 2 indexes the genome with an FM Index to keep its memory footprint small: for the human genome, its memory footprint is typically around 3.2 GB. Bowtie 2 supports gapped, local, and paired-end alignment modes.

More Information

<http://bowtie-bio.sourceforge.net/bowtie2/index.shtml>

Available Versions:

```
2.3.5.1-GCC-8.3.0
2.4.5-GCC-11.2.0
2.3.4.2-foss-2018b
```

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```
2.4.1-GCC-9.3.0
2.4.4-GCC-11.2.0
```

1.60 Brotli

Description

Brotli is a generic-purpose lossless compression algorithm that compresses data using a combination of a modern variant of the LZ77 algorithm, Huffman coding and 2nd order context modeling, with a compression ratio comparable to the best currently available general-purpose compression methods. It is similar in speed with deflate but offers more dense compression. The specification of the Brotli Compressed Data Format is defined in RFC 7932.

More Information

<https://github.com/google/brotli>

Available Versions:

```
1.0.9-GCCcore-11.3.0
1.0.9-GCCcore-11.2.0
1.0.9-GCCcore-12.2.0
```

1.61 CASTEP

Description

CASTEP is a leading code for calculating the properties of materials from first principles. Using density functional theory, it can simulate a wide range of properties of materials including energetics, structure at the atomic level, vibrational properties, electronic response properties etc. In particular it has a wide range of spectroscopic features that link directly to experiment, such as infra-red and Raman spectroscopies, NMR, and core level spectra.

More Information

<http://www.castep.org>

Available Versions:

```
21.11-info
16.11-intel-2020a
16.11-info
```

1.62 CD-HIT

Description

CD-HIT is a very widely used program for clustering and comparing protein or nucleotide sequences.

More Information

<http://weizhongli-lab.org/cd-hit/>

Available Versions:

```
4.8.1-GCC-10.2.0
4.8.1-GCC-11.2.0
4.8.1-GCC-10.3.0
```

1.63 CDO

Description

CDO is a collection of command line Operators to manipulate and analyse Climate and NWP model Data.

More Information

<https://code.zmaw.de/projects/cdo>

Available Versions:

```
1.9.10-gompi-2020b
```

1.64 CFITSIO

Description

CFITSIO is a library of C and Fortran subroutines for reading and writing data files inFITS (Flexible Image Transport System) data format.

More Information

<https://heasarc.gsfc.nasa.gov/fitsio/>

Available Versions:

```
3.49-GCCcore-11.2.0
3.47-GCCcore-8.3.0
```

1.65 CGAL

Description

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.

More Information

<https://www.cgal.org/>

Available Versions:

```
4.14.3-iimpi-2020a-Python-3.8.2
4.14.3-gompi-2020a-Python-3.8.2
5.2-gompi-2020b
4.14.3-gompi-2022a
4.14.3-gompi-2021a
4.14.1-foss-2019b-Python-3.7.4
```

1.66 CIF2Cell

Description

CIF2Cell is a tool to generate the geometrical setup for various electronic structure codes from a CIF (Crystallographic Information Framework) file. The program currently supports output for a number of popular electronic structure programs, including ABINIT, ASE, CASTEP, CP2K, CPMD, CRYSTAL09, Elk, EMTO, Exciting, Fleur, FHI-aims, Hutsepot, MOPAC, Quantum Espresso, RSPt, Siesta, SPR-KKR, VASP. Also exports some related formats like .coo, .cfg and .xyz-files.

More Information

<https://sourceforge.net/projects/cif2cell>

Available Versions:

2.0.0a3-GCCcore-9.3.0-Python-3.8.2

1.67 CLHEP

Description

The CLHEP project is intended to be a set of HEP-specific foundation and utility classes such as random generators, physics vectors, geometry and linear algebra. CLHEP is structured in a set of packages independent of any external package.

More Information

<https://proj-clhep.web.cern.ch/proj-clhep/>

Available Versions:

2.4.5.1-GCC-11.2.0
2.4.4.0-GCC-10.2.0

1.68 CMake

Description

CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

More Information

<https://www.cmake.org>

Available Versions:

3.21.1-GCCcore-11.2.0
3.24.3-GCCcore-11.3.0
3.18.4-GCCcore-10.2.0
3.15.3-GCCcore-8.3.0
3.13.3-GCCcore-8.2.0
3.12.1-GCCcore-10.2.0
3.24.3-GCCcore-12.2.0

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```
3.15.3-GCCcore-7.3.0
3.12.1
3.11.4-GCCcore-7.3.0
3.12.1-GCCcore-7.3.0
3.23.1-GCCcore-11.3.0
3.22.1-GCCcore-11.2.0
3.20.1-GCCcore-10.3.0
3.16.4-GCCcore-9.3.0
3.9.4-GCCcore-9.3.0
```

1.69 CP2K

Description

CP2K is a freely available (GPL) program, written in Fortran 95, to perform atomistic and molecular simulations of solid state, liquid, molecular and biological systems. It provides a general framework for different methods such as e.g. density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW), and classical pair and many-body potentials.

More Information

<https://www.cp2k.org/>

Available Versions:

```
6.1-intel-2020a
7.1-intel-2020a
6.1-foss-2019b
8.2-foss-2021a
8.1-foss-2020a
6.1-foss-2019a
6.1-foss-2020a
7.1-intel-2020b
```

1.70 CPLEX

Description

IBM ILOG CPLEX Optimizer's mathematical programming technology enables analytical decision support for improving efficiency, reducing costs, and increasing profitability.

More Information

<https://www.ibm.com/analytics/cplex-optimizer>

Available Versions:

```
20.1.0-GCCcore-8.3.0
12.9.0
```

1.71 CREST

Description

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 analysis of structure ensembles.

More Information

<https://xtb-docs.readthedocs.io/en/latest/crest.html>

Available Versions:

2.11-intel-2021a

1.72 CUDA

Description

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.

More Information

<https://developer.nvidia.com/cuda-toolkit>

Available Versions:

11.1.1-GCC-10.2.0
 11.3.1-GCC-10.3.0
 11.3.1
 11.1.1-iccifort-2020.4.304
 11.5.1
 11.2.2
 11.0.2-GCC-9.3.0
 11.2.2-GCC-10.3.0
 11.7.0
 11.5.0
 11.4.1
 10.1.243-GCC-8.3.0
 11.8.0
 9.2.88-GCC-7.3.0-2.30
 11.4.1-GCC-10.3.0
 11.6.0

1.73 CUDAcore

Description

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.

More Information

<https://developer.nvidia.com/cuda-toolkit>

Available Versions:

11.0.2
11.1.1
11.2.2

1.74 CUnit

Description

Automated testing framework for C.

More Information

<https://sourceforge.net/projects/cunit/>

Available Versions:

2.1-3-GCCcore-11.2.0
2.1-3-GCCcore-11.3.0

1.75 CVXOPT

Description

CVXOPT is a free software package for convex optimization based on the Python programming language. Its main purpose is to make the development of software for convex optimization applications straightforward by building on Python's extensive standard library and on the strengths of Python as a high-level programming language.

More Information

<https://cvxopt.org>

Available Versions:

1.2.6-foss-2021a
1.2.4-foss-2020a
1.2.4-foss-2020a-Python-3.8.2
1.2.3-foss-2019a

1.76 Cactus

Description

Cactus is a reference-free whole-genome alignment program, as well as a pagenome graph construction toolkit.

More Information

<https://github.com/ComparativeGenomicsToolkit/cactus>

Available Versions:

2.4.0

1.77 CapnProto

Description

Cap'n Proto is an insanely fast data interchange format and capability-based RPC system.

More Information

<https://capnproto.org>

Available Versions:

0.7.0-GCCcore-7.3.0

1.78 Cartopy

Description

Cartopy is a Python package designed to make drawing maps for data analysis and visualisation easy.

More Information

<https://scitools.org.uk/cartopy/docs/latest/>

Available Versions:

0.20.3-foss-2021b

1.79 CellRanger

Description

Cell Ranger is a set of analysis pipelines that process Chromium single-cell RNA-seq output to align reads, generate gene-cell matrices and perform clustering and gene expression analysis.

More Information

<https://support.10xgenomics.com/single-cell-gene-expression/software/pipelines/latest/what-is-cell-ranger>

Available Versions:

6.0.2
7.0.0
5.0.0
7.0.1

1.80 CellRank

Description

CellRank is a toolkit to uncover cellular dynamics based on Markov state modeling of single-cell data. It contains two main modules: kernels compute cell-cell transition probabilities and estimators generate hypothesis based on these.

More Information

<https://cellrank.readthedocs.io/en/stable/>

Available Versions:

1.4.0-foss-2021a

1.81 CheMPS2

Description

CheMPS2 is a scientific library which contains a spin-adapted implementation of the density matrix renormalization group (DMRG) for ab initio quantum chemistry.

More Information

<https://github.com/SebWouters/CheMPS2>

Available Versions:

1.8.11-foss-2021b
1.8.11-intel-2021a
1.8.9-foss-2019a

1.82 Check

Description

Check is a unit testing framework for C. It features a simple interface for defining unit tests, putting little in the way of the developer. Tests are run in a separate address space, so both assertion failures and code errors that cause segmentation faults or other signals can be caught. Test results are reportable in the following: Subunit, TAP, XML, and a generic logging format.

More Information

<https://libcheck.github.io/check/>

Available Versions:

```
0.15.2-GCCcore-11.2.0
0.15.2-GCCcore-9.3.0
0.15.2-GCCcore-10.3.0
0.15.2-GCCcore-10.2.0
```

1.83 Clang

Description

C, C++, Objective-C compiler, based on LLVM. Does not include C++ standard library – use libstdc++ from GCC.

More Information

<https://clang.llvm.org/>

Available Versions:

```
11.0.1-gcccuda-2020b
11.0.1-GCCcore-10.2.0
```

1.84 ClonalFrameML

Description

Efficient Inference of Recombination in Whole Bacterial Genomes

More Information

<https://github.com/xavierdidelot/ClonalFrameML>

Available Versions:

```
1.12-foss-2022a
```

1.85 ClustalW2

Description

ClustalW2 is a general purpose multiple sequence alignment program for DNA or proteins.

More Information

<https://www.ebi.ac.uk/Tools/msa/clustalw2/>

Available Versions:

```
2.1-intel-2020a
```

1.86 ConnectomeWorkbench

Description

Connectome Workbench is an open source, freely available visualization and discovery tool used to map neuroimaging data, especially data generated by the Human Connectome Project.

More Information

<https://www.humanconnectome.org/software/connectome-workbench>

Available Versions:

1.5.0-GCCcore-10.3.0

1.87 CppUnit

Description

CppUnit is the C++ port of the famous JUnit framework for unit testing.

More Information

<https://freedesktop.org/wiki/Software/cppunit/>

Available Versions:

1.15.1-GCCcore-10.3.0

1.88 CubeGUI

Description

Cube, which is used as performance report explorer for Scalasca and Score-P, is a generic tool for displaying a multi-dimensional performance space consisting of the dimensions (i) performance metric, (ii) call path, and (iii) system resource. Each dimension can be represented as a tree, where non-leaf nodes of the tree can be collapsed or expanded to achieve the desired level of granularity. This module provides the Cube graphical report explorer.

More Information

<https://www.scalasca.org/software/cube-4.x/download.html>

Available Versions:

4.4.4-GCCcore-9.3.0

4.8-GCCcore-11.3.0

1.89 CubeLib

Description

Cube, which is used as performance report explorer for Scalasca and Score-P, is a generic tool for displaying a multi-dimensional performance space consisting of the dimensions (i) performance metric, (ii) call path, and (iii) system resource. Each dimension can be represented as a tree, where non-leaf nodes of the tree can be collapsed or expanded to achieve the desired level of granularity. This module provides the Cube general purpose C++ library component and command-line tools.

More Information

<https://www.scalasca.org/software/cube-4.x/download.html>

Available Versions:

```
4.8-GCCcore-11.3.0
4.4.4-GCCcore-9.3.0
```

1.90 CubeWriter

Description

Cube, which is used as performance report explorer for Scalasca and Score-P, is a generic tool for displaying a multi-dimensional performance space consisting of the dimensions (i) performance metric, (ii) call path, and (iii) system resource. Each dimension can be represented as a tree, where non-leaf nodes of the tree can be collapsed or expanded to achieve the desired level of granularity. This module provides the Cube high-performance C writer library component.

More Information

<https://www.scalasca.org/software/cube-4.x/download.html>

Available Versions:

```
4.8-GCCcore-11.3.0
4.4.3-GCCcore-9.3.0
```

1.91 Cufflinks

Description

Transcript assembly, differential expression, and differential regulation for RNA-Seq

More Information

<http://cole-trapnell-lab.github.io/cufflinks/>

Available Versions:

```
2.2.1-foss-2020a
```

1.92 Cython

Description

Cython is an optimising static compiler for both the Python programming language and the extended Cython programming language (based on Pyrex).

More Information

<https://cython.org/>

Available Versions:

0.29.22-GCCcore-10.2.0

1.93 DB

Description

Berkeley DB enables the development of custom data management solutions, without the overhead traditionally associated with such custom projects.

More Information

<https://www.oracle.com/technetwork/products/berkeleydb>

Available Versions:

18.1.32-GCCcore-8.2.0
18.1.32-GCCcore-9.3.0
18.1.32-GCCcore-7.3.0
18.1.40-GCCcore-10.2.0
18.1.40-GCCcore-11.2.0
18.1.40-GCCcore-12.2.0
18.1.32-GCCcore-8.3.0
18.1.40-GCCcore-11.3.0
18.1.40-GCCcore-10.3.0

1.94 DB_File

Description

Perl5 access to Berkeley DB version 1.x.

More Information

https://perldoc.perl.org/DB_File.html

Available Versions:

1.856-GCCcore-10.3.0
1.835-GCCcore-9.3.0
1.857-GCCcore-11.2.0
1.858-GCCcore-11.3.0

1.95 DBus

Description

D-Bus is a message bus system, a simple way for applications to talk to one another. In addition to interprocess communication, D-Bus helps coordinate process lifecycle; it makes it simple and reliable to code a “single instance” application or daemon, and to launch applications and daemons on demand when their services are needed.

More Information

<https://dbus.freedesktop.org/>

Available Versions:

```
1.13.12-GCCcore-9.3.0
1.13.18-GCCcore-10.3.0
1.13.18-GCCcore-10.2.0
1.13.18-GCCcore-11.2.0
1.14.0-GCCcore-11.3.0
1.13.12-GCCcore-8.3.0
1.13.8-GCCcore-8.2.0
1.13.6-GCCcore-7.3.0
```

1.96 DFT-D3

Description

DFT-D3 implements a dispersion correction for density functionals, Hartree-Fock and semi-empirical quantum chemical methods.

More Information

<http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=DFT-D3&lang=english>

Available Versions:

```
3.2.0-intel-compilers-2021.2.0
```

1.97 DFT-D4

Description

Generally Applicable Atomic-Charge Dependent London Dispersion Correction.

More Information

<https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/dftd4>

Available Versions:

```
3.4.0-foss-2020a-Python-3.8.2
```

1.98 DIALS

Description

X-ray crystallography for structural biology has benefited greatly from a number of advances in recent years including high performance pixel array detectors, new beamlines capable of delivering micron and sub-micron focus and new light sources such as XFELs. The DIALS project is a collaborative endeavour to develop new diffraction integration software to meet the data analysis requirements presented by these recent advances. There are three end goals: to develop an extensible framework for the development of algorithms to analyse X-ray diffraction data; the implementation of algorithms within this framework and finally a set of user facing tools using these algorithms to allow integration of data from diffraction experiments on synchrotron and free electron sources.

More Information

<https://dials.github.io>

Available Versions:

3.11.2

1.99 DIAMOND

Description

Accelerated BLAST compatible local sequence aligner

More Information

<https://github.com/bbuchfink/diamond>

Available Versions:

2.0.15-GCC-11.3.0
0.9.30-iccifort-2019.5.281
0.9.30-GCC-8.3.0

1.100 DL_POLY_4

Description

DL_POLY is a general purpose classical molecular dynamics (MD) simulation software

More Information

https://www.scd.stfc.ac.uk/Pages/DL_POLY.aspx

Available Versions:

5.0.0-intel-2020b

1.101 DL_POLY_Classic

Description

DL_POLY Classic is a general purpose (parallel and serial)molecular dynamics simulation package.

More Information

https://gitlab.com/DL_POLY_Classic/dl_poly

Available Versions:

1.10-foss-2019b

1.102 DOLFIN

Description

DOLFIN is the C++/Python interface of FEniCS, providing a consistent PSE (Problem Solving Environment) for ordinary and partial differential equations.

More Information

<https://bitbucket.org/fenics-project/dolfin>

Available Versions:

2019.1.0.post0-foss-2019b-Python-3.7.4

1.103 Doxygen

Description

Doxygen is a documentation system for C++, C, Java, Objective-C, Python, IDL (Corba and Microsoft flavors), Fortran, VHDL, PHP, C#, and to some extent D.

More Information

<https://www.doxygen.org>

Available Versions:

1.9.4-GCCcore-11.3.0
 1.8.15-GCCcore-8.2.0
 1.8.17-GCCcore-9.3.0
 1.8.16-GCCcore-8.3.0
 1.8.14-GCCcore-7.3.0
 1.9.1-GCCcore-11.2.0
 1.9.1-GCCcore-10.3.0
 1.8.20-GCCcore-10.2.0

1.104 EIGENSOFT

Description

The EIGENSOFT package combines functionality from our population genetics methods (Patterson et al. 2006) and our EIGENSTRAT stratification correction method (Price et al. 2006). The EIGENSTRAT method uses principal components analysis to explicitly model ancestry differences between cases and controls along continuous axes of variation; the resulting correction is specific to a candidate marker's variation in frequency across ancestral populations, minimizing spurious associations while maximizing power to detect true associations. The EIGENSOFT package has a built-in plotting script and supports multiple file formats and quantitative phenotypes.

More Information

<https://www.hsph.harvard.edu/alkes-price/software/>

Available Versions:

7.2.1-foss-2019b

1.105 ELPA

Description

Eigenvalue SoLvers for Petaflop-Applications .

More Information

<https://elpa.rzg.mpg.de>

Available Versions:

2021.05.001-intel-2021a
2020.11.001-intel-2020b
2021.11.001-intel-2022a
2019.11.001-intel-2020a
2020.11.001-foss-2020b
2019.11.001-foss-2020a
2021.11.001-foss-2022a

1.106 ESM-2

Description

ESM-2 outperforms all tested single-sequence protein language models across a range of structure prediction tasks. ESMFold harnesses the ESM-2 language model to generate accurate structure predictions end to end directly from the sequence of a protein.

More Information

<https://github.com/facebookresearch/esm>

Available Versions:

2.0.0-foss-2021a

1.107 ESMF

Description

The Earth System Modeling Framework (ESMF) is a suite of software tools for developing high-performance, multi-component Earth science modeling applications.

More Information

<https://www.earthsystemcog.org/projects/esmf/>

Available Versions:

8.1.1-foss-2021a
8.0.1-foss-2020b

1.108 EasyBuild

Description

EasyBuild is a software build and installation framework written in Python that allows you to install software in a structured, repeatable and robust way.

More Information

<https://easybuilders.github.io/easybuild>

Available Versions:

4.5.3
4.4.1
4.5.5
4.5.1
4.7.1
4.3.1
4.4.2
4.6.1
4.3.3
4.3.2
4.4.0
4.6.2
4.5.4
4.6.0
4.7.0
4.5.2
4.5.0
4.3.4

1.109 Eigen

Description

Eigen is a C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.

More Information

<https://eigen.tuxfamily.org>

Available Versions:

```
3.3.9-GCCcore-10.3.0
3.3.7
3.3.7-GCCcore-9.3.0
3.4.0-GCCcore-9.3.0
3.3.8-GCCcore-10.2.0
3.3.4
3.4.0-GCCcore-10.3.0
3.4.0-GCCcore-10.2.0
3.4.0-GCCcore-11.3.0
3.3.9-GCCcore-11.2.0
3.4.0-GCCcore-11.2.0
```

1.110 Elk

Description

An all-electron full-potential linearised augmented-plane wave (FP-LAPW) code with many advanced features. Written originally at Karl-Franzens-Universität Graz as a milestone of the EXCITING EU Research and Training Network, the code is designed to be as simple as possible so that new developments in the field of density functional theory (DFT) can be added quickly and reliably.

More Information

<http://elk.sourceforge.net/>

Available Versions:

```
7.0.12-foss-2020b
```

1.111 Emacs

Description

GNU Emacs is an extensible, customizable text editor—and more. At its core is an interpreter for Emacs Lisp, a dialect of the Lisp programming language with extensions to support text editing.

More Information

<https://www.gnu.org/software/emacs/>

Available Versions:

27.1-GCCcore-10.2.0

1.112 Exonerate

Description

Exonerate is a generic tool for pairwise sequence comparison. It allows you to align sequences using a many alignment models, using either exhaustive dynamic programming, or a variety of heuristics.

More Information

<https://www.ebi.ac.uk/about/vertebrate-genomics/software/exonerate>

Available Versions:

2.4.0-GCC-8.3.0

1.113 Extrae

Description

Extrae is the core instrumentation package developed by the Performance Tools group at BSC. Extrae is capable of instrumenting applications based on MPI, OpenMP, pthreads, CUDA1, OpenCL1, and StarSs1 using different instrumentation approaches. The information gathered by Extrae typically includes timestamped events of runtime calls, performance counters and source code references. Besides, Extrae provides its own API to allow the user to manually instrument his or her application.

More Information

<https://www.bsc.es/computer-sciences/performance-tools>

Available Versions:

3.8.0-gompi-2020b

1.114 FCM

Description

FCM is a set of tools for managing and building source code.

More Information

<http://www.metoffice.gov.uk/research/collaboration/fcm>

Available Versions:

2.3.1
2019.09.0

1.115 FEniCS

Description

FEniCS is a computing platform for solving partial differential equations (PDEs).

More Information

<https://fenicsproject.org/>

Available Versions:

2019.1.0-foss-2019b-Python-3.7.4

1.116 FFC

Description

The FEniCS Form Compiler (FFC) is a compiler for finite element variational forms.

More Information

<https://bitbucket.org/fenics-project/ffc>

Available Versions:

2019.1.0.post0-foss-2019b-Python-3.7.4

1.117 FFTW

Description

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.

More Information

<http://www.fftw.org>

Available Versions:

3.3.8-gompi-2018b
3.3.10-GCC-12.2.0
3.3.8-gompic-2018b
3.3.8-intel-2020a
3.3.8-gompi-2019a
3.3.8-gompi-2020a
3.3.8-gompic-2020b
3.3.8-gompi-2020b
3.3.8-gompic-2019b
3.3.10-GCC-11.3.0
3.3.9-gompi-2021a
3.3.8-intel-2020b
3.3.8-gompic-2020a
3.3.10-gompi-2021b

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```
3.3.9-intel-2021a
3.3.8-gompi-2019b
```

1.118 FFTW.MPI

Description

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.

More Information

<https://www.fftw.org>

Available Versions:

```
3.3.10-gompi-2022b
3.3.10-gompi-2022a
```

1.119 FFmpeg

Description

A complete, cross-platform solution to record, convert and stream audio and video.

More Information

<https://www.ffmpeg.org/>

Available Versions:

```
4.2.2-GCCcore-9.3.0
4.3.1-GCCcore-10.2.0
4.3.2-GCCcore-11.2.0
4.1.3-GCCcore-8.2.0
4.3.2-GCCcore-10.3.0
4.4.2-GCCcore-11.3.0
4.2.1-GCCcore-8.3.0
```

1.120 FIAT

Description

The Finite element Automatic Tabulator (FIAT) supports generation of arbitrary order instances of the Lagrange elements on lines, triangles, and tetrahedra. It is also capable of generating arbitrary order instances of Jacobi-type quadrature rules on the same element shapes.

More Information

<https://bitbucket.org/fenics-project/flat>

Available Versions:

2019.1.0-foss-2019b-Python-3.7.4

1.121 FLAC

Description

FLAC stands for Free Lossless Audio Codec, an audio format similar to MP3, but lossless, meaning that audio is compressed in FLAC without any loss in quality.

More Information

<https://xiph.org/flac/>

Available Versions:

1.3.3-GCCcore-10.3.0
1.4.2-GCCcore-12.2.0
1.3.3-GCCcore-11.2.0
1.3.4-GCCcore-11.3.0
1.3.3-GCCcore-10.2.0

1.122 FLAIR

Description

FLAIR (Full-Length Alternative Isoform analysis of RNA) for the correction, isoform definition, and alternative splicing analysis of noisy reads. FLAIR has primarily been used for nanopore cDNA, native RNA, and PacBio sequencing reads.

More Information

<https://github.com/BrooksLabUCSC/flair>

Available Versions:

1.5.1-20200630-foss-2019b-Python-3.7.4

1.123 FLASH

Description

FLASH (Fast Length Adjustment of SHort reads) is a very fast and accurate software tool to merge paired-end reads from next-generation sequencing experiments. FLASH is designed to merge pairs of reads when the original DNA fragments are shorter than twice the length of reads. The resulting longer reads can significantly improve genome assemblies. They can also improve transcriptome assembly when FLASH is used to merge RNA-seq data.

More Information

<https://ccb.jhu.edu/software/FLASH/>

Available Versions:

1.2.11-foss-2018b
2.2.00-foss-2018b

1.124 FLINT

Description

FLINT (Fast Library for Number Theory) is a C library in support of computations in number theory. Operations that can be performed include conversions, arithmetic, computing GCDs, factoring, solving linear systems, and evaluating special functions. In addition, FLINT provides various low-level routines for fast arithmetic. FLINT is extensively documented and tested.

More Information

<https://www.flintlib.org/>

Available Versions:

2.7.1-GCC-10.3.0

1.125 FLTK

Description

FLTK is a cross-platform C++ GUI toolkit for UNIX/Linux (X11), Microsoft Windows, and MacOS X. FLTK provides modern GUI functionality without the bloat and supports 3D graphics via OpenGL and its built-in GLUT emulation.

More Information

<https://www.fltk.org>

Available Versions:

1.3.5-GCCcore-10.2.0
1.3.7-GCCcore-11.2.0
1.3.5-GCC-8.3.0

1.126 FSL

Description

FSL is a comprehensive library of analysis tools for FMRI, MRI and DTI brain imaging data.

More Information

<https://www.fmrib.ox.ac.uk/fsl/>

Available Versions:

6.0.5.1-foss-2021a
6.0.3-foss-2019b-Python-3.7.4
6.0.5.2-ARC

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6.0.6.4-ARC
6.0.4-foss-2019b-Python-3.7.4

1.127 FastFold

Description

Optimizing Protein Structure Prediction Model Training and Inference on GPU Clusters

More Information

<https://github.com/hpcaitech/FastFold>

Available Versions:

20220729-foss-2021a-CUDA-11.3.1

1.128 FastME

Description

FastME: a comprehensive, accurate and fast distance-based phylogeny inference program.

More Information

<http://www.atgc-montpellier.fr/fastme/>

Available Versions:

2.1.6.2-GCC-8.3.0

1.129 FastQC

Description

FastQC is a quality control application for high throughput sequence data. It reads in sequence data in a variety of formats and can either provide an interactive application to review the results of several different QC checks, or create an HTML based report which can be integrated into a pipeline.

More Information

<https://www.bioinformatics.babraham.ac.uk/projects/fastqc/>

Available Versions:

0.11.9-Java-11
0.11.8-Java-1.8

1.130 FastTree

Description

FastTree infers approximately-maximum-likelihood phylogenetic trees from alignments of nucleotide or protein sequences. FastTree can handle alignments with up to a million of sequences in a reasonable amount of time and memory.

More Information

<http://www.microbesonline.org/fasttree/>

Available Versions:

2.1.11-GCCcore-11.3.0
2.1.11-GCCcore-9.3.0

1.131 Fiji

Description

Fiji is an image processing package—a ‘batteries-included’ distribution of ImageJ, bundling a lot of plugins which facilitate scientific image analysis. This release is based on ImageJ-2.1.0 and Fiji-2.1.1

More Information

<https://fiji.sc/>

Available Versions:

20201104-1356

1.132 FineSTRUCTURE

Available Versions:

4.1.1

1.133 Fiona

Description

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.

More Information

<https://github.com/Toblerity/Fiona>

Available Versions:

1.8.16-foss-2020a-Python-3.8.2
1.8.21-foss-2021b

1.134 Flask

Description

” Flask is a lightweight WSGI web application framework. It is designed to make getting started quick and easy, with the ability to scale up to complex applications.

More Information

<https://www.palletsprojects.com/p/flask/>

Available Versions:

1.1.2-GCCcore-8.3.0-Python-3.7.4
1.1.2-GCCcore-10.2.0
2.2.2-GCCcore-11.3.0
1.1.4-GCCcore-10.3.0

1.135 FlexiBLAS

Description

FlexiBLAS is a wrapper library that enables the exchange of the BLAS and LAPACK implementation used by a program without recompiling or relinking it.

More Information

<https://gitlab.mpi-magdeburg.mpg.de/software/flexiblas-release>

Available Versions:

3.0.4-GCC-11.2.0
3.2.1-GCC-12.2.0
3.0.4-GCC-10.3.0
3.2.0-GCC-11.3.0

1.136 FreeSurfer

Description

FreeSurfer is a set of tools for analysis and visualization of structural and functional brain imaging data. FreeSurfer contains a fully automatic structural imaging stream for processing cross sectional and longitudinal data.

More Information

<https://surfer.nmr.mgh.harvard.edu/>

Available Versions:

7.3.2-centos8_x86_64

1.137 FreeXL

Description

FreeXL is an open source library to extract valid data from within an Excel (.xls) spreadsheet.

More Information

<https://www.gaia-gis.it/fossil/freexl/index>

Available Versions:

1.0.5-GCCcore-8.3.0
1.0.6-GCCcore-11.2.0

1.138 FriBidi

Description

The Free Implementation of the Unicode Bidirectional Algorithm.

More Information

<https://github.com/fribidi/fribidi>

Available Versions:

1.0.10-GCCcore-10.2.0
1.0.5-GCCcore-7.3.0
1.0.5-GCCcore-8.2.0
1.0.10-GCCcore-10.3.0
1.0.12-GCCcore-11.3.0
1.0.5-GCCcore-8.3.0
1.0.9-GCCcore-9.3.0
1.0.10-GCCcore-11.2.0

1.139 GATK

Description

The Genome Analysis Toolkit or GATK is a software package developed at the Broad Institute to analyse next-generation resequencing data. The toolkit offers a wide variety of tools, with a primary focus on variant discovery and genotyping as well as strong emphasis on data quality assurance. Its robust architecture, powerful processing engine and high-performance computing features make it capable of taking on projects of any size.

More Information

<https://www.broadinstitute.org/gatk/>

Available Versions:

```
4.1.5.0-GCCcore-9.3.0-Java-1.8
3.8-1-Java-1.8.0_241
4.1.8.1-GCCcore-9.3.0-Java-1.8
```

1.140 GCC

Description

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,...).

More Information

<http://gcc.gnu.org/>

Available Versions:

```
8.2.0-2.31.1
9.3.0
7.3.0-2.30
11.2.0
10.3.0
10.2.0
8.3.0
11.3.0
8.1.0-2.30
12.2.0
```

1.141 GCCcore

Description

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,...).

More Information

<https://gcc.gnu.org/>

Available Versions:

```
8.3.0
10.3.0
11.3.0
12.1.0
8.1.0
11.2.0
12.2.0
11.2.0-multilib
9.3.0
7.3.0
10.2.0
8.2.0
```

1.142 GConf

Description

GConf is a system for storing application preferences. It is intended for user preferences; not configuration of something like Apache, or arbitrary data storage.

More Information

<https://developer.gnome.org/gconf/>

Available Versions:

```
3.2.6-GCCcore-8.3.0
3.2.6-GCCcore-11.2.0
```

1.143 GDAL

Description

GDAL is a translator library for raster geospatial data formats that is released under an X/MIT style Open Source license by the Open Source Geospatial Foundation. As a library, it presents a single abstract data model to the calling application for all supported formats. It also comes with a variety of useful commandline utilities for data translation and processing.

More Information

<https://www.gdal.org>

Available Versions:

```
3.0.4-foss-2020a-Python-3.8.2
3.3.2-foss-2021b
3.0.0-foss-2019a-Python-2.7.15
3.5.0-foss-2022a
3.3.0-foss-2021a
3.2.1-fosscuda-2020b
3.0.4-intel-2020a-Python-3.8.2
```

1.144 GDRCopy

Description

A low-latency GPU memory copy library based on NVIDIA GPUDirect RDMA technology.

More Information

<https://github.com/NVIDIA/gdrcopy>

Available Versions:

```
2.1-GCCcore-10.3.0-CUDA-11.1.1
2.1-GCCcore-9.3.0-CUDA-11.0.2
2.3-GCCcore-11.2.0
2.3-GCCcore-11.3.0
```

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```
2.2-GCCcore-10.3.0
2.1-GCCcore-10.2.0-CUDA-11.1.1
```

1.145 GEOS

Description

GEOS (Geometry Engine - Open Source) is a C++ port of the Java Topology Suite (JTS)

More Information

<https://trac.osgeo.org/geos>

Available Versions:

```
3.10.3-GCC-11.3.0
3.9.1-GCC-10.2.0
3.9.1-GCC-11.2.0
3.8.1-GCC-9.3.0-Python-3.8.2
3.6.2-foss-2018b-Python-2.7.15
3.7.2-foss-2019a-Python-2.7.15
3.8.1-iccifort-2020.1.217-Python-3.8.2
3.8.0-GCC-8.3.0-Python-3.7.4
3.9.1-GCC-10.3.0
```

1.146 GL2PS

Description

GL2PS: an OpenGL to PostScript printing library

More Information

<https://www.geuz.org/gl2ps/>

Available Versions:

```
1.4.2-GCCcore-11.2.0
1.4.0-GCCcore-8.3.0
```

1.147 GLM

Description

OpenGL Mathematics (GLM) is a header only C++ mathematics library for graphics software based on the OpenGL Shading Language (GLSL) specifications.

More Information

<https://github.com/g-truc/glm>

Available Versions:


```
0.9.9.8-GCCcore-9.3.0
0.9.9.8-GCCcore-8.3.0
```

1.148 GLPK

Description

The GLPK (GNU Linear Programming Kit) package is intended for solving large-scale linear programming (LP), mixed integer programming (MIP), and other related problems. It is a set of routines written in ANSI C and organized in the form of a callable library.

More Information

<https://www.gnu.org/software/glpk/>

Available Versions:

```
4.65-GCCcore-8.3.0
5.0-GCCcore-12.2.0
5.0-GCCcore-11.3.0
5.0-GCCcore-11.2.0
4.65-GCCcore-9.3.0
4.65-GCCcore-10.2.0
5.0-GCCcore-10.3.0
```

1.149 GLib

Description

GLib is one of the base libraries of the GTK+ project

More Information

<https://www.gtk.org/>

Available Versions:

```
2.72.1-GCCcore-11.3.0
2.60.1-GCCcore-8.2.0
2.75.0-GCCcore-12.2.0
2.69.1-GCCcore-11.2.0
2.68.2-GCCcore-10.3.0
2.62.0-GCCcore-8.3.0
2.66.1-GCCcore-10.2.0
2.64.1-GCCcore-9.3.0
2.54.3-GCCcore-7.3.0
```

1.150 GLibmm

Description

C++ bindings for Glib

More Information

<https://www.gtk.org/>

Available Versions:

2.49.7-GCCcore-8.3.0
2.66.4-GCCcore-10.3.0

1.151 GMAP-GSNAP

Description

GMAP: A Genomic Mapping and Alignment Program for mRNA and EST Sequences GSNAP: Genomic Short-read Nucleotide Alignment Program

More Information

<http://research-pub.gene.com/gmap/>

Available Versions:

2019-09-12-GCC-8.3.0

1.152 GMP

Description

GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers.

More Information

<https://gmplib.org/>

Available Versions:

6.2.1-GCCcore-11.2.0
6.2.1-GCCcore-11.3.0
6.2.0-GCCcore-9.3.0
6.2.1-GCCcore-10.3.0
6.1.2-GCCcore-10.2.0
6.1.2-GCCcore-8.2.0
6.1.2-GCCcore-8.3.0
6.2.0-GCCcore-10.2.0
6.1.2-GCCcore-9.3.0
6.1.2-GCCcore-7.3.0
6.2.1-GCCcore-12.2.0

1.153 GObject-Introspection

Description

GObject introspection is a middleware layer between C libraries (using GObject) and language bindings. The C library can be scanned at compile time and generate a metadata file, in addition to the actual native C library. Then at runtime, language bindings can read this metadata and automatically provide bindings to call into the C library.

More Information

<https://wiki.gnome.org/GObjectIntrospection/>

Available Versions:

```
1.54.1-foss-2018b-Python-2.7.15
1.68.0-GCCcore-11.2.0
1.64.0-GCCcore-9.3.0-Python-3.8.2
1.66.1-GCCcore-10.2.0
1.63.1-GCCcore-8.3.0-Python-3.7.4
1.68.0-GCCcore-10.3.0
1.72.0-GCCcore-11.3.0
1.60.1-GCCcore-8.2.0-Python-3.7.2
```

1.154 GPAW

Description

GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.

More Information

<https://wiki.fysik.dtu.dk/gpaw/>

Available Versions:

```
22.8.0-foss-2022a
21.6.0-foss-2021a
22.8.0-intel-2022a
20.10.0-foss-2020b
```

1.155 GPAW-setups

Description

PAW setup for the GPAW Density Functional Theory package. Users can install setups manually using 'gpaw install-data' or use setups from this package. The versions of GPAW and GPAW-setups can be intermixed.

More Information

<https://wiki.fysik.dtu.dk/gpaw/>

Available Versions:

0.9.20000

1.156 GRASS

Description

The Geographic Resources Analysis Support System - used for geospatial data management and analysis, image processing, graphics and maps production, spatial modeling, and visualization

More Information

<https://grass.osgeo.org>

Available Versions:

8.2.0-foss-2021b

1.157 GROMACS

Description

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.

More Information

<http://www.gromacs.org>

Available Versions:

2020-fosscuda-2019b
2021.5-foss-2021b
2021-foss-2021a-PLUMED-2.7.2
2020.4-foss-2020a-PLUMED-2.6.2
2022.2-foss-2021a
2021.5-foss-2021b-CUDA-11.4.1
2021.5-foss-2021b-CUDA-11.4.1-PLUMED-2.8.0
2021.3-foss-2021a-CUDA-11.3.1
2021-foss-2020b
2020.4-foss-2020a
2021.3-foss-2021a
2021.5-foss-2021b-PLUMED-2.8.0

1.158 GSL

Description

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.

More Information

<https://www.gnu.org/software/gsl/>

Available Versions:

```
2.6-GCC-8.3.0
2.5-GCC-8.2.0-2.31.1
2.7-GCC-11.3.0
2.5-GCC-7.3.0-2.30
2.6-GCC-9.3.0
2.7-GCC-10.3.0
2.7-GCC-11.2.0
2.6-iccifort-2020.1.217
2.6-iccifort-2020.4.304
2.7-GCC-12.2.0
2.6-GCC-10.2.0
```

1.159 GST-plugins-bad

Description

GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing.

More Information

<https://gstreamer.freedesktop.org/>

Available Versions:

```
1.20.2-GCC-11.3.0
```

1.160 GST-plugins-base

Description

GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing.

More Information

<https://gstreamer.freedesktop.org/>

Available Versions:

1.20.2-GCC-11.3.0
1.18.5-GCC-11.2.0
1.16.2-GCC-8.3.0

1.161 GStreamer

Description

GStreamer is a library for constructing graphs of media-handling components. The applications it supports range from simple Ogg/Vorbis playback, audio/video streaming to complex audio (mixing) and video (non-linear editing) processing.

More Information

<https://gstreamer.freedesktop.org/>

Available Versions:

1.20.2-GCC-11.3.0
1.16.2-GCC-8.3.0
1.18.5-GCC-11.2.0

1.162 GTK+

Description

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.

More Information

<https://developer.gnome.org/gtk3/stable/>

Available Versions:

3.24.23-GCCcore-10.2.0
3.24.8-GCCcore-8.2.0
2.24.32-foss-2018b
3.24.13-GCCcore-8.3.0

1.163 GTK2

Description

The GTK+ 2 package contains libraries used for creating graphical user interfaces for applications.

More Information

<https://www.gtk.org>

Available Versions:

`2.24.33-GCCcore-11.3.0`

1.164 GTK3

Description

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.

More Information

<https://developer.gnome.org/gtk3/stable/>

Available Versions:

`3.24.31-GCCcore-11.2.0`

1.165 GTK4

Description

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.

More Information

<https://docs.gtk.org/gtk4/>

Available Versions:

`4.7.0-GCC-11.3.0`

1.166 GTS

Description

GTS stands for the GNU Triangulated Surface Library. It is an Open Source Free Software Library intended to provide a set of useful functions to deal with 3D surfaces meshed with interconnected triangles.

More Information

<http://gts.sourceforge.net/>

Available Versions:

`0.7.6-GCCcore-10.3.0`

1.167 Gaussian

Description

Gaussian provides state-of-the-art capabilities for electronic structure modeling. Gaussian 09 is licensed for a wide variety of computersystems. All versions of Gaussian 09 contain every scientific/modelingfeature, and none imposes any artificial limitations on calculations other than your computing resources and patience. This is the build from the legacy ARCUS-B system, using PGI 12.5 compiler and Atlas.

More Information

<https://www.gaussian.com/>

Available Versions:

09.D.01-ARCUS-B
16.C.01
03.E.01-ARCUS-B
16.A.03-ARCUS-B

1.168 Gaussview

Available Versions:

5.0.9

1.169 Gdk-Pixbuf

Description

The Gdk Pixbuf is a toolkit for image loading and pixel buffer manipulation. It is used by GTK+ 2 and GTK+ 3 to load and manipulate images. In the past it was distributed as part of GTK+ 2 but it was split off into a separate package in preparation for the change to GTK+ 3.

More Information

<https://developer.gnome.org/gdk-pixbuf/stable/>

Available Versions:

2.36.12-foss-2018b
2.42.6-GCCcore-11.2.0
2.40.0-GCCcore-10.2.0
2.42.8-GCCcore-11.3.0
2.38.1-GCCcore-8.2.0
2.38.2-GCCcore-8.3.0
2.42.6-GCCcore-10.3.0

1.170 Geant4

Description

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science.

More Information

<https://geant4.cern.ch/>

Available Versions:

```
10.7.1-GCC-10.2.0
11.0.0-GCC-11.2.0
11.0.0-foss-2021b-G4MPI
```

1.171 Geant4-data

Description

Datasets for Geant4.

More Information

<https://geant4.cern.ch/>

Available Versions:

```
20210510
```

1.172 GeneMark-ET

Description

Eukaryotic gene prediction suite with automatic training

More Information

<http://exon.gatech.edu/GeneMark>

Available Versions:

```
4.69-GCCcore-8.3.0
```

1.173 GenomeThreader

Description

GenomeThreader is a software tool to compute gene structure predictions.

More Information

<http://genomethreader.org>

Available Versions:

1.7.3-Linux_x86_64-64bit

1.174 GenomeTools

Description

A comprehensive software library for efficient processing of structured genome annotations.

More Information

<http://genometools.org>

Available Versions:

1.6.1-GCC-10.2.0
1.6.2-GCC-10.3.0

1.175 GeoMxNGSPipeline

Available Versions:

2022

1.176 Ghostscript

Description

Ghostscript is a versatile processor for PostScript data with the ability to render PostScript to different targets. It used to be part of the cups printing stack, but is no longer used for that.

More Information

<https://ghostscript.com>

Available Versions:

9.50-GCCcore-8.3.0
9.54.0-GCCcore-11.2.0
9.52-GCCcore-9.3.0
9.56.1-GCCcore-11.3.0

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```
9.53.3-GCCcore-10.2.0
9.54.0-GCCcore-10.3.0
```

1.177 GitPython

Description

GitPython is a python library used to interact with Git repositories

More Information

<https://gitpython.readthedocs.org>

Available Versions:

```
3.1.24-GCCcore-11.2.0
3.1.0-GCCcore-8.3.0-Python-3.7.4
3.1.14-GCCcore-10.2.0
```

1.178 GlobalArrays

Description

Global Arrays (GA) is a Partitioned Global Address Space (PGAS) programming model

More Information

<https://hpc.pnl.gov/globalarrays>

Available Versions:

```
5.8-intel-2021a
5.7-intel-2020b
5.7.2-foss-2019b-peigs
5.8-intel-2020a
```

1.179 Globus-CLI

Description

A Command Line Wrapper over the Globus SDK for Python, which provides an interface to Globus services from the shell, and is suited to both interactive and simple scripting use cases.

More Information

<https://docs.globus.org/cli/>

Available Versions:

```
3.6.0-GCCcore-11.2.0
```

1.180 GlobusConnectPersonal

Description

Globus Connect Personal turns your laptop or other personal computer into a Globus endpoint with a just a few clicks. With Globus Connect Personal you can share and transfer files to/from a local machine—campus server, desktop computer or laptop—even if it's behind a firewall and you don't have administrator privileges.

More Information

<https://www.globus.org/globus-connect-personal>

Available Versions:

2.3.6

1.181 Glucose

Description

Glucose is based on a new scoring scheme (well, not so new now, it was introduced in 2009) for the clause learning mechanism of so called Modern SATsolvers (it is based on our IJCAI'09 paper). It is designed to be parallel, since v4.0.

More Information

<https://www.labri.fr/perso/lisimon/glucose/>

Available Versions:

4.1-GCC-9.3.0

1.182 GnuTLS

Description

GnuTLS is a secure communications library implementing the SSL, TLS and DTLS protocols and technologies around them. It provides a simple C language application programming interface (API) to access the secure communications protocols as well as APIs to parse and write X.509, PKCS #12, OpenPGP and other required structures. It is aimed to be portable and efficient with focus on security and interoperability.

More Information

<https://www.gnutls.org>

Available Versions:

3.7.3-GCCcore-11.2.0

1.183 Go

Description

Go is an open source programming language that makes it easy to build simple, reliable, and efficient software.

More Information

<https://www.golang.org>

Available Versions:

```
1.17.6
1.14.1
```

1.184 Grace

Description

Grace is a WYSIWYG tool to make two-dimensional plots of numerical data.

More Information

<https://plasma-gate.weizmann.ac.il/Grace/>

Available Versions:

```
5.1.25-foss-2021b
5.1.25-foss-2019b-5build1
5.1.25-intel-2021b
```

1.185 Graphene

Description

Graphene is a thin layer of types for graphic libraries

More Information

<https://ebassi.github.io/graphene/>

Available Versions:

```
1.10.8-GCCcore-11.3.0
```

1.186 GraphicsMagick

Description

GraphicsMagick is the swiss army knife of image processing.

More Information

<http://www.graphicsmagick.org/>

Available Versions:

1.3.36-GCCcore-11.2.0
1.3.34-foss-2019b

1.187 Graphviz

Description

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.

More Information

<https://www.graphviz.org/>

Available Versions:

2.47.2-GCCcore-10.3.0

1.188 Guile

Description

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.

More Information

<https://www.gnu.org/software/guile/>

Available Versions:

1.8.8-GCCcore-9.3.0
1.8.8-GCCcore-8.2.0
3.0.7-GCCcore-11.2.0
3.0.8-GCCcore-11.3.0
1.8.8-GCCcore-8.3.0

1.189 Guppy

Available Versions:

```
5.0.11
6.4.2
6.4.2-CPU
3.6.0
```

1.190 Gurobi

Description

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.

More Information

<https://www.gurobi.com>

Available Versions:

```
9.5.2-GCCcore-11.3.0
9.1.2-GCCcore-10.3.0
```

1.191 HDF

Description

HDF (also known as HDF4) is a library and multi-object file format for storing and managing data between machines.

More Information

<https://www.hdfgroup.org/products/hdf4/>

Available Versions:

```
4.2.14-GCCcore-8.3.0
4.2.15-GCCcore-11.3.0
4.2.15-GCCcore-10.2.0
4.2.15-GCCcore-11.2.0
4.2.15-GCCcore-10.3.0
```

1.192 HDF5

Description

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.

More Information

<https://portal.hdfgroup.org/display/support>

Available Versions:

```
1.10.7-iimpi-2021a
1.10.6-iimpi-2020a
1.10.2-fosscuda-2018b
1.10.5-iimpi-2020a
1.10.7-gompi-2021a
1.12.2-gompi-2022a
1.12.1-gompi-2021b
1.10.2-foss-2018b
1.12.2-iimpi-2022a
1.12.1-iimpi-2021b
1.10.5-gompic-2019b
1.10.6-gompi-2020a
1.10.7-gompi-2020b
1.13.1-iimpi-2022a
1.13.1-gompi-2022a
1.10.5-gompi-2019b-dba
1.10.6-gompic-2020a
1.10.7-gompic-2020b
1.12.0-gompi-2020a
1.12.1-gompi-2021a
1.10.7-iimpi-2020b
1.10.5-gompi-2019b
1.14.0-gompi-2022b
1.10.2-intel-2020b
1.10.5-gompi-2019a
```

1.193 HH-suite

Description

The HH-suite is an open-source software package for sensitive protein sequence searching based on the pairwise alignment of hidden Markov models (HMMs).

More Information

<https://github.com/soedinglab/hh-suite>

Available Versions:

```
3.3.0-gompi-2021b
3.3.0-gompic-2020b
3.3.0-gompi-2021a
```


1.194 HISAT2

Description

HISAT2 is a fast and sensitive alignment program for mapping next-generation sequencing reads (both DNA and RNA) against the general human population (as well as against a single reference genome).

More Information

<https://daehwankimlab.github.io/hisat2>

Available Versions:

2.2.1-gompi-2020b

1.195 HMMER

Description

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.

More Information

<http://hmmer.org/>

Available Versions:

3.3.2-gompi-2021a
3.3.1-iimpi-2020a
3.3.2-gompic-2020b
3.3.2-gompi-2020b
3.3.2-gompi-2021b

1.196 HMMER2

Description

HMMER is used for searching sequence databases for sequence homologs, and for making sequence alignments.

More Information

<http://hmmer.org>

Available Versions:

2.3.2-GCC-8.3.0

1.197 HTSlib

Description

A C library for reading/writing high-throughput sequencing data. This package includes the utilities bgzip and tabix

More Information

<https://www.htslib.org/>

Available Versions:

```
1.14-GCC-11.2.0
1.10.2-GCC-8.3.0
1.10.2-GCC-9.3.0
1.12-GCC-10.2.0
1.9-foss-2018b
1.11-GCC-10.2.0
```

1.198 HarfBuzz

Description

HarfBuzz is an OpenType text shaping engine.

More Information

<https://www.freedesktop.org/wiki/Software/HarfBuzz>

Available Versions:

```
4.2.1-GCCcore-11.3.0
2.2.0-foss-2018b
2.4.0-GCCcore-8.2.0
2.8.1-GCCcore-10.3.0
2.6.4-GCCcore-8.3.0
2.6.4-GCCcore-9.3.0
2.6.7-GCCcore-10.2.0
2.8.2-GCCcore-11.2.0
```

1.199 HemeLB

Description

HemeLB is a high performance lattice-Boltzmann solver optimized for simulating blood flow through sparse geometries, such as those found in the human vasculature. It is routinely deployed on powerful supercomputers, scaling to hundreds of thousands of cores even for complex geometries. HemeLB has traditionally been used to model cerebral bloodflow and vascular remodelling in retinas, but is now being applied to simulating the fully coupled human arterial and venous trees.

More Information

<http://hemelb.org.s3-website.eu-west-2.amazonaws.com/>

Available Versions:

0.8

1.200 HyPhy

Description

HyPhy (Hypothesis Testing using Phylogenies) is an open-source software package for the analysis of genetic sequences (in particular the inference of natural selection) using techniques in phylogenetics, molecular evolution, and machine learning

More Information

<https://veg.github.io/hyphy-site/>

Available Versions:

2.5.1-gompi-2019a

1.201 Hypre

Description

Hypre is a library for solving large, sparse linear systems of equations on massively parallel computers. The problems of interest arise in the simulation codes being developed at LLNL and elsewhere to study physical phenomena in the defense, environmental, energy, and biological sciences.

More Information

<https://computation.llnl.gov/projects/hypre-scalable-linear-solvers-multigrid-methods>

Available Versions:

2.20.0-foss-2020b
2.18.2-foss-2019b
2.25.0-foss-2022a
2.18.2-intel-2020a
2.21.0-foss-2021a
2.18.2-foss-2020a

1.202 ICU

Description

ICU is a mature, widely used set of C/C++ and Java libraries providing Unicode and Globalization support for software applications.

More Information

<http://site.icu-project.org/home>

Available Versions:

64.2-GCCcore-8.2.0
64.2-GCCcore-8.3.0
66.1-GCCcore-9.3.0
69.1-GCCcore-10.3.0
69.1-GCCcore-11.2.0
72.1-GCCcore-12.2.0
67.1-GCCcore-10.2.0
61.1-GCCcore-7.3.0
71.1-GCCcore-11.3.0

1.203 IDBA-UD

Description

IDBA-UD is a iterative De Bruijn Graph De Novo Assembler for Short Reads Sequencing data with Highly Uneven Sequencing Depth. It is an extension of IDBA algorithm. IDBA-UD also iterates from small k to a large k. In each iteration, short and low-depth contigs are removed iteratively with cutoff threshold from low to high to reduce the errors in low-depth and high-depth regions. Paired-end reads are aligned to contigs and assembled locally to generate some missing k-mers in low-depth regions. With these technologies, IDBA-UD can iterate k value of de Bruijn graph to a very large value with less gaps and less branches to form long contigs in both low-depth and high-depth regions.

More Information

https://i.cs.hku.hk/~alse/hkubrg/projects/idba_ud/

Available Versions:

1.1.3-GCC-8.3.0

1.204 IGV

Description

This package contains command line utilities for preprocessing, computing feature count density (coverage), sorting, and indexing data files.

More Information

<https://www.broadinstitute.org/software/igv/>

Available Versions:

2.8.0-Java-11

1.205 IMPUTE2

Description

IMPUTE version 2 (also known as IMPUTE2) is a genotype imputation and haplotype phasing program based on ideas from Howie et al. 2009

More Information

http://mathgen.stats.ox.ac.uk/impute/impute_v2.html

Available Versions:

```
2.3.2_x86_64_dynamic
2.3.2_x86_64_static
```

1.206 IOR

Description

The IOR software is used for benchmarking parallel file systems using POSIX, MPIIO, or HDF5 interfaces.

More Information

<https://github.com/IOR-LANL/ior>

Available Versions:

```
3.3.0-gompi-2020b
3.2.1-gompi-2019b
```

1.207 IPython

Description

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.

More Information

<https://ipython.org/index.html>

Available Versions:

```
7.9.0-foss-2019b-Python-3.7.4
8.5.0-GCCcore-11.3.0
7.18.1-GCCcore-10.2.0
7.26.0-GCCcore-11.2.0
7.15.0-foss-2020a-Python-3.8.2
```

1.208 IQ-TREE

Description

Efficient phylogenomic software by maximum likelihood

More Information

<http://www.iqtree.org/>

Available Versions:

1.6.12-foss-2018b

1.209 ISA-L

Description

Intelligent Storage Acceleration Library

More Information

<https://github.com/intel/isa-l>

Available Versions:

2.30.0-GCCcore-11.3.0

2.30.0-GCCcore-11.2.0

1.210 ImageMagick

Description

ImageMagick is a software suite to create, edit, compose, or convert bitmap images

More Information

<https://www.imagemagick.org/>

Available Versions:

7.0.11-14-GCCcore-10.3.0

7.1.0-4-GCCcore-11.2.0

7.0.10-1-GCCcore-9.3.0

7.0.9-5-GCCcore-8.3.0

7.0.10-35-GCCcore-10.2.0

7.1.0-37-GCCcore-11.3.0

1.211 Imath

Description

Imath is a C++ and python library of 2D and 3D vector, matrix, and math operations for computer graphics

More Information

<https://imath.readthedocs.io/en/latest/>

Available Versions:

3.1.5-GCCcore-11.3.0

1.212 Infernal

Description

Infernal (“INFERence of RNA ALignment”) is for searching DNA sequence databases for RNA structure and sequence similarities.

More Information

<http://eddylab.org/infernal/>

Available Versions:

1.1.2-foss-2018b

1.213 Ipopt

Description

Ipopt (Interior Point OPTimizer, pronounced eye-pea-Opt) is a software package for large-scale nonlinear optimization.

More Information

<https://coin-or.github.io/Ipopt>

Available Versions:

3.12.13-intel-2020b

1.214 JAGS

Description

JAGS is Just Another Gibbs Sampler. It is a program for analysis of Bayesian hierarchical models using Markov Chain Monte Carlo (MCMC) simulation

More Information

<http://mcmc-jags.sourceforge.net/>

Available Versions:

```
4.3.0-foss-2022a
4.3.0-foss-2021b
4.3.0-foss-2020a
4.3.0-foss-2019b
4.3.0-foss-2021a
```

1.215 Jansson

Description

Jansson is a C library for encoding, decoding and manipulating JSON data. Its main features and design principles are:
* Simple and intuitive API and data model * Comprehensive documentation * No dependencies on other libraries * Full Unicode support (UTF-8) * Extensive test suite

More Information

<https://www.digip.org/jansson/>

Available Versions:

```
2.13.1-GCC-11.2.0
2.14-GCC-11.3.0
```

1.216 JasPer

Description

The JasPer Project is an open-source initiative to provide a free software-based reference implementation of the codec specified in the JPEG-2000 Part-1 standard.

More Information

<http://www.ece.uvic.ca/~frodo/jasper/>

Available Versions:

```
2.0.14-GCCcore-7.3.0
2.0.24-GCCcore-10.2.0
2.0.28-GCCcore-10.3.0
2.0.14-GCCcore-10.2.0
2.0.14-GCCcore-8.2.0
2.0.33-GCCcore-11.2.0
2.0.14-GCCcore-8.3.0
2.0.33-GCCcore-11.3.0
1.900.1-intel-2020b
2.0.14-GCCcore-9.3.0
```


1.217 Java

Description

Java Platform, Standard Edition (Java SE) lets you develop and deploy Java applications on desktops and servers.

More Information

<https://openjdk.java.net>

Available Versions:

```
16.0.1
1.8.0_131
1.8.0_241
11.0.2
1.7.0_60
```

1.218 Jellyfish

Description

Jellyfish is a tool for fast, memory-efficient counting of k-mers in DNA.

More Information

<http://www.genome.umd.edu/jellyfish.html>

Available Versions:

```
2.3.0-GCC-11.2.0
2.3.0-GCC-8.3.0
```

1.219 JsonCpp

Description

JsonCpp is a C++ library that allows manipulating JSON values, including serialization and deserialization to and from strings. It can also preserve existing comment in unserialization/serialization steps, making it a convenient format to store user input files.

More Information

<https://open-source-parsers.github.io/jsoncpp-docs/doxygen/index.html>

Available Versions:

```
1.9.4-GCCcore-10.3.0
1.9.4-GCCcore-10.2.0
1.9.4-GCCcore-9.3.0
1.9.3-GCCcore-8.3.0
1.9.4-GCCcore-11.2.0
```

1.220 Judy

Description

A C library that implements a dynamic array.

More Information

<http://judy.sourceforge.net/>

Available Versions:

```
1.0.5-GCCcore-8.3.0
1.0.5-GCCcore-10.3.0
1.0.5-GCCcore-10.2.0
```

1.221 Julia

Description

Julia is a high-level, high-performance dynamic programming language for numerical computing

More Information

<https://julialang.org>

Available Versions:

```
1.5.3-linux-x86_64
1.8.5-linux-x86_64
1.6.2-linux-x86_64
1.8.2-linux-x86_64
1.5.1-linux-x86_64
```

1.222 JupyterHub

Description

JupyterHub is a multiuser version of the Jupyter (IPython) notebook designed for centralized deployments in companies, university classrooms and research labs.

More Information

<https://jupyter.org>

Available Versions:

```
1.1.0-GCCcore-10.2.0
```

1.223 JupyterLab

Description

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.

More Information

<https://jupyter.org/>

Available Versions:

```
3.5.0-GCCcore-11.3.0
2.2.8-GCCcore-10.2.0
```

1.224 KMC

Description

KMC is a disk-based program for counting k-mers from (possibly gzipped) FASTQ/FASTA files.

More Information

<http://sun.aei.polsl.pl/kmc>

Available Versions:

```
3.1.0-foss-2018b
```

1.225 Kalign

Description

Kalign is a fast multiple sequence alignment program for biological sequences.

More Information

<https://github.com/TimoLassmann/kalign>

Available Versions:

```
3.3.1-GCCcore-10.3.0
3.3.2-GCCcore-11.2.0
3.3.1-GCCcore-10.2.0
```

1.226 Kent_tools

Description

Kent utilities: collection of tools used by the UCSC genome browser.

More Information

<https://genome.cse.ucsc.edu/>

Available Versions:

```
401-gompi-2019b
411-GCC-10.2.0
418-GCC-10.3.0
```

1.227 Keras

Description

Keras is a minimalist, highly modular neural networks library, written in Python and capable of running on top of either TensorFlow or Theano.

More Information

<https://keras.io/>

Available Versions:

```
2.3.1-foss-2019b-Python-3.7.4
2.4.3-foss-cuda-2020b
```

1.228 Kraken2

Description

Kraken is a system for assigning taxonomic labels to short DNA sequences, usually obtained through metagenomic studies. Previous attempts by other bioinformatics software to accomplish this task have often used sequence alignment or machine learning techniques that were quite slow, leading to the development of less sensitive but much faster abundance estimation programs. Kraken aims to achieve high sensitivity and high speed by utilizing exact alignments of k-mers and a novel classification algorithm.

More Information

<https://github.com/DerrickWood/kraken2/wiki>

Available Versions:

```
2.1.1-gompi-2020b
2.1.2-gompi-2021b
```

1.229 LAME

Description

LAME is a high quality MPEG Audio Layer III (MP3) encoder licensed under the LGPL.

More Information

<http://lame.sourceforge.net/>

Available Versions:

```
3.100-GCCcore-11.3.0
3.100-GCCcore-10.3.0
3.100-GCCcore-10.2.0
3.100-GCCcore-8.3.0
3.100-GCCcore-11.2.0
3.100-GCCcore-8.2.0
3.100-GCCcore-12.2.0
3.100-GCCcore-9.3.0
```

1.230 LAMMPS

Description

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.

More Information

<https://lammps.sandia.gov/>

Available Versions:

```
3Mar2020-foss-2020a-Python-3.8.2-kokkos
23Jun2022-foss-2021b-kokkos-CUDA-11.4.1
23Jun2022-foss-2021b-kokkos
3Mar2020-foss-2020a-Python-3.8.2-kokkos-QUIP
```

1.231 LAPACK

Description

LAPACK is written in Fortran90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems.

More Information

<https://www.netlib.org/lapack/>

Available Versions:

```
3.9.1-GCC-9.3.0
3.9.1-GCC-10.2.0
3.9.1-GCC-11.2.0
3.9.1-GCC-10.3.0
```

1.232 LDC

Description

The LLVM-based D Compiler

More Information

<https://wiki.dlang.org/LDC>

Available Versions:

```
1.26.0-GCCcore-10.3.0
1.25.1-GCCcore-10.2.0
0.17.6-x86_64
1.28.1-GCCcore-8.3.0
```

1.233 LIBSVM

Description

LIBSVM is an integrated software for support vector classification, (C-SVC, nu-SVC), regression (epsilon-SVR, nu-SVR) and distribution estimation (one-class SVM). It supports multi-class classification.

More Information

<https://www.csie.ntu.edu.tw/~cjlin/libsvm/>

Available Versions:

```
3.25-GCCcore-11.2.0
```

1.234 LLVM

Description

The LLVM Core libraries provide a modern source- and target-independent optimizer, along with code generation support for many popular CPUs (as well as some less common ones!) These libraries are built around a well specified code representation known as the LLVM intermediate representation (“LLVM IR”). The LLVM Core libraries are well documented, and it is particularly easy to invent your own language (or port an existing compiler) to use LLVM as an optimizer and code generator.

More Information

<https://llvm.org/>

Available Versions:

```
14.0.3-GCCcore-11.3.0
9.0.0-GCCcore-8.3.0
11.1.0-GCCcore-10.3.0
7.0.1-GCCcore-8.2.0
9.0.1-GCCcore-9.3.0
8.0.1-GCCcore-8.3.0
11.0.0-GCCcore-10.2.0
12.0.1-GCCcore-11.2.0
15.0.5-GCCcore-12.2.0
6.0.0-GCCcore-7.3.0
```

1.235 LMDB

Description

LMDB is a fast, memory-efficient database. With memory-mapped files, it has the read performance of a pure in-memory database while retaining the persistence of standard disk-based databases.

More Information

<https://symas.com/lmdb>

Available Versions:

```
0.9.22-GCCcore-7.3.0
0.9.29-GCCcore-11.2.0
0.9.24-GCCcore-8.3.0
0.9.28-GCCcore-10.3.0
0.9.29-GCCcore-11.3.0
0.9.24-GCCcore-10.2.0
0.9.24-GCCcore-9.3.0
```

1.236 LTR_retriever

Description

LTR_retriever is a highly accurate and sensitive program for identification of LTR retrotransposons; The LTR Assembly Index (LAI) is also included in this package.

More Information

https://github.com/oushujun/LTR_retriever

Available Versions:

```
2.9.0-foss-2021a
2.9.0-foss-2020b
```

1.237 LZO

Description

Portable lossless data compression library

More Information

<https://www.oberhumer.com/opensource/lzo/>

Available Versions:

```
2.10-GCCcore-10.3.0
2.10-GCCcore-8.3.0
2.10-GCCcore-10.2.0
```

1.238 Leptonica

Description

Leptonica is a collection of pedagogically-oriented open source software that is broadly useful for image processing and image analysis applications.

More Information

<http://www.leptonica.org>

Available Versions:

```
1.78.0-GCCcore-8.2.0
1.83.0-GCCcore-11.3.0
```

1.239 LibSoup

Description

libsoup is an HTTP client/server library for GNOME. It uses GObject and the glib main loop, to integrate well with GNOME applications, and also has a synchronous API, for use in threaded applications.

More Information

<https://wiki.gnome.org/Projects/libsoup>

Available Versions:

```
3.0.7-GCC-11.2.0
```


1.240 LibTIFF

Description

tiff: Library and tools for reading and writing TIFF data files

More Information

<https://libtiff.maptools.org/>

Available Versions:

```
4.1.0-GCCcore-9.3.0
4.0.9-GCCcore-7.3.0
4.3.0-GCCcore-11.3.0
4.3.0-GCCcore-11.2.0
4.0.10-GCCcore-8.3.0
4.0.10-GCCcore-8.2.0
4.2.0-GCCcore-10.3.0
4.1.0-GCCcore-10.2.0
4.4.0-GCCcore-12.2.0
```

1.241 Libint

Description

Libint library is used to evaluate the traditional (electron repulsion) and certain novel two-body matrix elements (integrals) over Cartesian Gaussian functions used in modern atomic and molecular theory.

More Information

<https://sourceforge.net/p/libint/>

Available Versions:

```
1.1.6-foss-2020a
2.6.0-GCC-10.2.0-lmax-6-cp2k
2.6.0-iccifort-2020.4.304-lmax-6-cp2k
1.1.6-GCC-8.2.0-2.31.1
2.6.0-GCC-10.3.0-lmax-6-cp2k
2.6.0-gompi-2020a-lmax-6-cp2k
1.1.6-foss-2019b
2.6.0-iimpi-2020a-lmax-6-cp2k
1.1.6-intel-2020a
```

1.242 Lighter

Description

Fast and memory-efficient sequencing error corrector

More Information

<https://github.com/mourisl/Lighter>

Available Versions:

1.1.2-foss-2018b

1.243 LinkTest

Description

The mpilinktest program is a parallel ping-pong test between all connections of a machine. Output of this program is a fullcommunication matrix which shows the bandwidth between each processorpair and a report including the minimum bandwidth. The linktest runsfor n processors in n steps where in each step n/2 pairs of processorswill perform the MPI pingpong test (3 iterations, 128 kBmessages). The selection of the pairs is random but after running allsteps all possible pairs are covered.

More Information

http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/LinkTest/linktest-download_node.html

Available Versions:

1.2p1-foss-2019b

1.2p1-foss-2020a

1.244 LittleCMS

Description

Little CMS intends to be an OPEN SOURCE small-footprint color management engine, with special focus on accuracy and performance.

More Information

<http://www.littlecms.com/>

Available Versions:

2.9-GCCcore-8.3.0

2.13.1-GCCcore-11.3.0

2.12-GCCcore-10.3.0

2.12-GCCcore-11.2.0

2.11-GCCcore-10.2.0

2.9-GCCcore-9.3.0

1.245 Lua

Description

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.

More Information

<https://www.lua.org/>

Available Versions:

```
5.4.4-GCCcore-11.3.0
5.4.3-GCCcore-11.2.0
5.4.2-GCCcore-10.2.0
5.4.3-GCCcore-10.3.0
5.1.5-GCCcore-8.3.0
5.3.5-GCCcore-9.3.0
```

1.246 M4

Description

GNU M4 is an implementation of the traditional Unix macro processor. It is mostly SVR4 compatible although it has some extensions (for example, handling more than 9 positional parameters to macros). GNU M4 also has built-in functions for including files, running shell commands, doing arithmetic, etc.

More Information

<https://www.gnu.org/software/m4/m4.html>

Available Versions:

```
1.4.18-GCCcore-8.1.0
1.4.18-GCCcore-8.2.0
1.4.17
1.4.18-GCCcore-8.3.0
1.4.19
1.4.18-GCCcore-10.2.0
1.4.19-GCCcore-12.2.0
1.4.18-GCCcore-7.3.0
1.4.18-GCCcore-10.3.0
1.4.18-GCCcore-9.3.0
1.4.18
1.4.19-GCCcore-11.2.0
1.4.19-GCCcore-11.3.0
```

1.247 MACS2

Description

Model Based Analysis for ChIP-Seq data

More Information

<https://github.com/taoliu/MACS/>

Available Versions:

2.2.5-foss-2018b-Python-3.6.6

1.248 MAFFT

Description

MAFFT is a multiple sequence alignment program for unix-like operating systems. It offers a range of multiple alignment methods, L-INS-i (accurate; for alignment of <200 sequences), FFT-NS-2 (fast; for alignment of <30,000 sequences), etc.

More Information

<https://mafft.cbrc.jp/alignment/software/source.html>

Available Versions:

7.453-GCC-9.3.0-with-extensions
7.490-GCC-11.2.0-with-extensions
7.470-gompi-2020a-with-extensions
7.475-gompi-2020b-with-extensions
7.453-iimpi-2020a-with-extensions
7.487-gompi-2021a-with-extensions

1.249 MALT

Available Versions:

0.5.3

1.250 MATIO

Description

matio is an C library for reading and writing Matlab MAT files.

More Information

<https://sourceforge.net/projects/matio/>

Available Versions:

1.5.17-GCCcore-8.3.0

1.251 MATLAB

Available Versions:

R2020b
R2020a
R2022a
R2022b
R2019b
R2021b

1.252 MCL

Description

The MCL algorithm is short for the Markov Cluster Algorithm, a fast and scalable unsupervised cluster algorithm for graphs (also known as networks) based on simulation of (stochastic) flow in graphs.

More Information

<https://micans.org/mcl/>

Available Versions:

14.137-GCCcore-8.3.0
14.137-GCCcore-9.3.0

1.253 MDAnalysis

Description

MDAnalysis is an object-oriented Python library to analyze trajectories from molecular dynamics (MD) simulations in many popular formats.

More Information

<https://www.mdanalysis.org/>

Available Versions:

0.20.1-foss-2019b-Python-3.7.4

1.254 MEGAHIT

Description

An ultra-fast single-node solution for large and complex metagenomics assembly via succinct de Bruijn graph

More Information

<https://github.com/voutcn/megahit>

Available Versions:

1.2.9-GCCcore-9.3.0
1.1.4-foss-2018b-Python-2.7.15

1.255 MEME

Description

The MEME Suite allows you to: * discover motifs using MEME, DREME (DNA only) or GLAM2 on groups of related DNA or protein sequences, * search sequence databases with motifs using MAST, FIMO, MCAST or GLAM2SCAN, * compare a motif to all motifs in a database of motifs, * associate motifs with Gene Ontology terms via their putative target genes, and * analyse motif enrichment using SpaMo or CentriMo.

More Information

<https://meme-suite.org/meme/index.html>

Available Versions:

5.4.1-GCC-10.3.0

1.256 METIS

Description

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.

More Information

<http://glaros.dtc.umn.edu/gkhome/metis/metis/overview>

Available Versions:

5.1.0-GCCcore-10.3.0
5.1.0-GCCcore-9.3.0
5.1.0-GCCcore-11.3.0
5.1.0-GCCcore-10.2.0
5.1.0-foss-2018b
5.1.0-GCCcore-8.2.0
5.1.0-GCCcore-8.3.0
5.1.0-GCCcore-11.2.0

1.257 MGLTools

Available Versions:

```
1.5.7
1.5.7.old
```

1.258 MIRA

Description

MIRA is a whole genome shotgun and EST sequence assembler for Sanger, 454, Solexa (Illumina), IonTorrent data and PacBio (the latter at the moment only CCS and error-corrected CLR reads).

More Information

<https://sourceforge.net/p/mira-assembler/wiki/Home/>

Available Versions:

```
4.0.2-gompi-2019b
```

1.259 MMseqs2

Description

MMseqs2: ultra fast and sensitive search and clustering suite

More Information

<https://mmseqs.com>

Available Versions:

```
13-45111-gompi-2020b
10-6d92c-gompi-2019b
```

1.260 MOOSE

Description

The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a finite-element, multiphysicsframework primarily developed by Idaho National Laboratory

More Information

<https://mooseframework.inl.gov>

Available Versions:

```
2021-05-18-foss-2019b-Python-3.7.4
```

1.261 MPC

Description

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.

More Information

<http://www.multiprecision.org/>

Available Versions:

```
1.1.0-GCC-9.3.0
1.1.0-GCC-8.3.0
1.2.1-GCCcore-10.3.0
```

1.262 MPFR

Description

The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.

More Information

<https://www.mpfr.org>

Available Versions:

```
4.0.1-GCCcore-7.3.0
4.1.0-GCCcore-10.2.0
4.1.0-GCCcore-10.3.0
4.1.0-GCCcore-11.3.0
4.0.2-GCCcore-8.3.0
4.1.0-GCCcore-11.2.0
4.0.2-GCCcore-9.3.0
4.0.2-GCCcore-8.2.0
```

1.263 MPICH2

Description

MPICH v3.x is an open source high-performance MPI 3.0 implementation. It does not support InfiniBand (use MVA-PICH2 with InfiniBand devices).

More Information

<http://www.mpich.org/>

Available Versions:

```
1.5rc3-GCC-7.3.0-2.30
```


1.264 MUMPS

Description

A parallel sparse direct solver

More Information

<https://graal.ens-lyon.fr/MUMPS/>

Available Versions:

```
5.2.1-intel-2020a-metis
5.4.0-foss-2021a-metis
5.2.1-foss-2020a-metis
5.2.1-foss-2019b-metis
5.3.5-foss-2020b-metis
5.5.1-foss-2022a-metis
5.2.1-foss-2019a-metis-seq
```

1.265 MUMmer

Description

MUMmer is a system for rapidly aligning entire genomes, whether in complete or draft form. AMOS makes use of it.

More Information

<http://mummer.sourceforge.net/>

Available Versions:

```
4.0.0rc1-GCCcore-11.2.0
4.0.0beta2-foss-2018b
4.0.0beta2-GCCcore-10.2.0
```

1.266 MUSCLE

Description

MUSCLE is one of the best-performing multiple alignment programs according to published benchmark tests, with accuracy and speed that are consistently better than CLUSTALW. MUSCLE can align hundreds of sequences in seconds. Most users learn everything they need to know about MUSCLE in a few minutes-only a handful of command-line options are needed to perform common alignment tasks.

More Information

<https://drive5.com/muscle/>

Available Versions:

```
3.8.31-foss-2018b
```

1.267 MaSuRCA

Description

MaSuRCA is whole genome assembly software. It combines the efficiency of the de Bruijn graph and Overlap-Layout-Consensus (OLC) approaches. MaSuRCA can assemble data sets containing only short reads from Illumina sequencing or a mixture of short reads and long reads (Sanger, 454, Pacbio and Nanopore).

More Information

<https://www.genome.umd.edu/masurca.html>

Available Versions:

4.0.9-foss-2021a-Perl-5.32.1

1.268 Mako

Description

A super-fast templating language that borrows the best ideas from the existing templating languages

More Information

<https://www.makotemplates.org>

Available Versions:

1.0.7-foss-2018b-Python-2.7.15
1.1.4-GCCcore-10.3.0
1.0.8-GCCcore-8.2.0
1.1.0-GCCcore-8.3.0
1.2.0-GCCcore-11.3.0
1.1.2-GCCcore-9.3.0
1.1.4-GCCcore-11.2.0
1.2.4-GCCcore-12.2.0
1.1.3-GCCcore-10.2.0

1.269 Mamba

Description

Mamba is a fast, robust, and cross-platform package manager. It runs on Windows, OS X and Linux (ARM64 and PPC64LE included) and is fully compatible with conda packages and supports most of conda's commands.

More Information

<https://mamba.readthedocs.io/>

Available Versions:

4.14.0-0

1.270 MariaDB

Description

MariaDB is an enhanced, drop-in replacement for MySQL. Included engines: myISAM, Aria, InnoDB, RocksDB, TokuDB, OQGraph, Mroonga.

More Information

<https://mariadb.org/>

Available Versions:

```
10.4.13-gompi-2019b
10.6.4-GCC-10.3.0
10.5.8-GCC-10.2.0
```

1.271 MariaDB-connector-c

Description

MariaDB Connector/C is used to connect applications developed in C/C++ to MariaDB and MySQL databases.

More Information

<https://downloads.mariadb.org/connector-c/>

Available Versions:

```
2.3.7-GCCcore-8.3.0
```

1.272 Mash

Description

Fast genome and metagenome distance estimation using MinHash

More Information

<http://mash.readthedocs.org>

Available Versions:

```
2.1-foss-2018b
```

1.273 Mathematica

Available Versions:

12.2.0
11.3.0
13.0.0

1.274 MaxQuant

Description

MaxQuant is a quantitative proteomics software package designed for analyzing large mass-spectrometric data sets. It is specifically aimed at high-resolution MS data. Several labeling techniques as well as label-free quantification are supported.

More Information

<https://maxquant.org/maxquant>

Available Versions:

2.3.0.0-GCCcore-11.2.0

1.275 Mellanox

Available Versions:

ib_mgmt-5.8.1-1.e18

1.276 Mercurial

Description

Mercurial is a free, distributed source control management tool. It efficiently handles projects of any size and offers an easy and intuitive interface.

More Information

<https://www.mercurial-scm.org>

Available Versions:

5.7.1-GCCcore-10.2.0
6.2-GCCcore-11.3.0

1.277 Mesa

Description

Mesa is an open-source implementation of the OpenGL specification - a system for rendering interactive 3D graphics.

More Information

<https://www.mesa3d.org/>

Available Versions:

```
21.1.1-GCCcore-10.3.0
20.0.2-GCCcore-9.3.0
20.2.1-GCCcore-10.2.0
21.1.7-GCCcore-11.2.0
22.0.3-GCCcore-11.3.0
22.2.4-GCCcore-12.2.0
18.1.1-foss-2018b
19.1.7-GCCcore-8.3.0
19.0.1-GCCcore-8.2.0
```

1.278 Meson

Description

Meson is a cross-platform build system designed to be both as fast and as user friendly as possible.

More Information

<https://mesonbuild.com>

Available Versions:

```
0.51.2-GCCcore-8.3.0-Python-3.7.4
0.50.0-GCCcore-8.2.0-Python-3.7.2
0.59.1-GCCcore-8.3.0-Python-3.7.4
0.58.0-GCCcore-10.3.0
0.64.0-GCCcore-12.2.0
0.62.1-GCCcore-11.3.0
0.58.2-GCCcore-11.2.0
0.55.3-GCCcore-10.2.0
0.55.1-GCCcore-9.3.0-Python-3.8.2
```

1.279 MetaPhlAn2

Description

MetaPhlAn is a computational tool for profiling the composition of microbial communities (Bacteria, Archaea, Eukaryotes and Viruses) from metagenomic shotgun sequencing data (i.e. not 16S) with species-level. With the newly added StrainPhlAn module, it is now possible to perform accurate strain-level microbial profiling.

More Information

<https://bitbucket.org/biobakery/metaphlan2/>

Available Versions:

2.7.8-foss-2018b-Python-3.6.6

1.280 MiniSat

Description

MiniSat is a minimalistic, open-source SAT solver, developed to help researchers and developers alike to get started on SAT.

More Information

<http://minisat.se/>

Available Versions:

2.2.0-GCC-9.3.0

1.281 Miniconda3

Description

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.

More Information

<https://docs.conda.io/en/latest/miniconda.html>

Available Versions:

23.1.0-1
22.11.1-1
4.9.2
4.7.10
4.12.0
4.5.12

1.282 Molden

Description

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

More Information

<http://www.cmbi.ru.nl/molden/>

Available Versions:

5.7-foss-2018b

1.283 Mono

Description

An open source, cross-platform, implementation of C# and the CLR that is binary compatible with Microsoft.NET.

More Information

<https://www.mono-project.com/>

Available Versions:

```
6.8.0.105-GCCcore-8.3.0
6.4.0.198-foss-2018b
6.12.0.122-GCCcore-11.2.0
```

1.284 Mothur

Description

Mothur is a single piece of open-source, expandable software to fill the bioinformatics needs of the microbial ecology community.

More Information

<https://www.mothur.org/>

Available Versions:

```
1.43.0-foss-2019a-Python-3.7.2
```

1.285 MrBayes

Description

MrBayes is a program for Bayesian inference and model choice across a wide range of phylogenetic and evolutionary models.

More Information

<https://nbisweden.github.io/MrBayes/>

Available Versions:

```
3.2.7-gompi-2020b
```

1.286 MultiQC

Description

Aggregate results from bioinformatics analyses across many samples into a single report. MultiQC searches a given directory for analysis logs and compiles a HTML report. It's a general use tool, perfect for summarising the output from numerous bioinformatics tools.

More Information

<https://multiqc.info>

Available Versions:

1.9-foss-2020a-Python-3.8.2

1.287 Multiwfn

Description

Multiwfn is an extremely powerful program for realizing electronic wavefunction analysis, which is a key ingredient of quantum chemistry. Multiwfn is free, open-source, high-efficient, very user-friendly and flexible, it supports almost all of the most important wavefunction analysis methods.

More Information

<http://sobereva.com/multiwfn/>

Available Versions:

3.8-intel-2021b-dev

1.288 MySQL

Description

MySQL is one of the world's most widely used open-source relational database management system (RDBMS).

More Information

<http://www.mysql.com/>

Available Versions:

5.7.21-GCCcore-9.3.0-clientonly

1.289 NAMD

Description

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.

More Information

<https://www.ks.uiuc.edu/Research/namd/>

Available Versions:

```
2.14-intel-2020a-mpi
2.14-fosscuda-2019b
```

1.290 NASM

Description

NASM: General-purpose x86 assembler

More Information

<https://www.nasm.us/>

Available Versions:

```
2.15.05-GCCcore-12.2.0
2.14.02-GCCcore-8.2.0
2.14.02-GCCcore-9.3.0
2.15.05-GCCcore-11.3.0
2.14.02-GCCcore-8.3.0
2.15.05-GCCcore-10.2.0
2.15.05-GCCcore-10.3.0
2.13.03-GCCcore-7.3.0
2.15.05-GCCcore-11.2.0
```

1.291 NCCL

Description

The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.

More Information

<https://developer.nvidia.com/nccl>

Available Versions:

```
2.4.8-gccuda-2019b
2.12.12-GCCcore-11.3.0-CUDA-11.7.0
2.8.3-CUDA-11.1.1
2.10.3-GCCcore-11.2.0-CUDA-11.4.1
2.10.3-GCCcore-10.3.0-CUDA-11.3.1
```

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```
2.8.3-CUDA-11.0.2
2.8.3-GCCcore-10.2.0-CUDA-11.1.1
```

1.292 NCO

Description

manipulates and analyzes data stored in netCDF-accessible formats, including DAP, HDF4, and HDF5

More Information

<https://nco.sourceforge.net>

Available Versions:

```
4.9.7-foss-2020b
5.0.1-foss-2021a
```

1.293 NEURON

Description

Empirically-based simulations of neurons and networks of neurons.

More Information

<http://www.neuron.yale.edu/neuron>

Available Versions:

```
7.7.2-foss-2020a-Python-3.7.4
7.6.5-foss-2018b-Python-2.7.15
7.6.5-foss-2019a-Python-2.7.15
7.8.2-foss-2021b
```

1.294 NGS

Description

NGS is a new, domain-specific API for accessing reads, alignments and pileups produced from Next Generation Sequencing.

More Information

<https://github.com/ncbi/ngs>

Available Versions:

```
2.10.9-GCCcore-10.2.0
2.9.3-foss-2018b-Java-1.8
```

1.295 NLOpt

Description

NLOpt is a free/open-source library for nonlinear optimization, providing a common interface for a number of different free optimization routines available online as well as original implementations of various other algorithms.

More Information

<http://ab-initio.mit.edu/wiki/index.php/NLOpt>

Available Versions:

```
2.4.2-GCCcore-7.3.0
2.6.2-GCCcore-10.2.0
2.7.1-GCCcore-12.2.0
2.6.1-GCCcore-9.3.0
2.7.0-GCCcore-11.2.0
2.6.1-GCCcore-8.3.0
2.7.1-GCCcore-11.3.0
2.7.0-GCCcore-10.3.0
```

1.296 NSPR

Description

Netscape Portable Runtime (NSPR) provides a platform-neutral API for system level and libc-like functions.

More Information

<https://developer.mozilla.org/en-US/docs/Mozilla/Projects/NSPR>

Available Versions:

```
4.25-GCCcore-9.3.0
4.30-GCCcore-10.3.0
4.29-GCCcore-10.2.0
4.20-GCCcore-7.3.0
4.32-GCCcore-11.2.0
4.34-GCCcore-11.3.0
4.21-GCCcore-8.3.0
```

1.297 NSS

Description

Network Security Services (NSS) is a set of libraries designed to support cross-platform development of security-enabled client and server applications.

More Information

<https://developer.mozilla.org/en-US/docs/Mozilla/Projects/NSS>

Available Versions:

```
3.79-GCCcore-11.3.0
3.39-GCCcore-7.3.0
3.51-GCCcore-9.3.0
3.65-GCCcore-10.3.0
3.45-GCCcore-8.3.0
3.69-GCCcore-11.2.0
3.57-GCCcore-10.2.0
```

1.298 NVHPC

Description

C, C++ and Fortran compilers included with the NVIDIA HPC SDK (previously: PGI)

More Information

<https://developer.nvidia.com/hpc-sdk/>

Available Versions:

```
21.7
21.9
20.11
21.11
```

1.299 NWChem

Description

NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters. NWChem software can handle: biomolecules, nanostructures, and solid-state; from quantum to classical, and all combinations; Gaussian basis functions or plane-waves; scaling from one to thousands of processors; properties and relativity.

More Information

<http://www.nwchem-sw.org>

Available Versions:

```
7.0.0-foss-2019b-Python-3.7.4
7.0.2-intel-2021a
```

1.300 NetLogo

Description

NetLogo is a multi-agent programmable modeling environment. It is used by tens of thousands of students, teachers and researchers worldwide. It also powers HubNet participatory simulations. It is authored by Uri Wilensky and developed at the CCL.

More Information

<https://ccl.northwestern.edu/netlogo/>

Available Versions:

6.2.0-64
6.0.4-64

1.301 NgsRelate

Available Versions:

2022

1.302 Ninja

Description

Ninja is a small build system with a focus on speed.

More Information

<https://ninja-build.org/>

Available Versions:

1.9.0-GCCcore-8.2.0
1.10.2-GCCcore-10.3.0
1.9.0-GCCcore-8.3.0
1.11.1-GCCcore-12.2.0
1.10.0-GCCcore-9.3.0
1.10.2-GCCcore-11.2.0
1.10.1-GCCcore-10.2.0
1.10.2-GCCcore-11.3.0

1.303 OPARI2

Description

OPARI2, the successor of Forschungszentrum Juelich's OPARI, is a source-to-source instrumentation tool for OpenMP and hybrid codes. It surrounds OpenMP directives and runtime library calls with calls to the POMP2 measurement interface.

More Information

<https://www.score-p.org>

Available Versions:

```
2.0.5-GCCcore-9.3.0
2.0.7-GCCcore-11.3.0
```

1.304 ORCA

Description

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. (OpenMPI –disable-builtin-atomics version)

More Information

<https://orcaforum.kofo.mpg.de>

Available Versions:

```
4.2.1-gompi-2019b-dba
5.0.1-gompi-2019b-dba
5.0.4-gompi-2021b
5.0.2-gompi-2019b-dba
5.0.0-gompi-2019b
4.2.1-gompi-2019b
5.0.4-gompi-2021b-static
5.0.3-gompi-2021b
```

1.305 OSU-Micro-Benchmarks

Description

OSU Micro-Benchmarks

More Information

<https://mvapich.cse.ohio-state.edu/benchmarks/>

Available Versions:

```
5.8-GCC-10.3.0-CUDA-11.1.1
6.2-gompi-2022b
5.8-fosscuda-2020b
```

1.306 OTF2

Description

The Open Trace Format 2 is a highly scalable, memory efficient event trace data format plus support library. It is the new standard trace format for Scalasca, Vampir, and TAU and is open for other tools.

More Information

<https://www.score-p.org>

Available Versions:

```
3.0.2-GCCcore-11.3.0
2.2-GCCcore-9.3.0
```

1.307 Octave

Description

GNU Octave is a high-level interpreted language, primarily intended for numerical computations.

More Information

<https://www.gnu.org/software/octave/>

Available Versions:

```
5.1.0-foss-2019b
7.1.0-foss-2021b
```

1.308 OpenBLAS

Description

OpenBLAS is an optimized BLAS library based on GotoBLAS2 1.13 BSD version.

More Information

<https://xianyi.github.com/OpenBLAS/>

Available Versions:

```
0.3.15-GCC-10.3.0
0.3.12-GCC-10.2.0
0.3.7-GCC-8.3.0
0.3.18-GCC-11.2.0
0.3.20-GCC-11.3.0
0.3.5-GCC-8.2.0-2.31.1
```

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```
0.3.1-GCC-7.3.0-2.30
0.3.21-GCC-12.2.0
0.3.9-GCC-9.3.0
```

1.309 OpenBabel

Description

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.

More Information

<https://openbabel.org>

Available Versions:

```
3.1.1-gompi-2019b-Python-3.7.4
```

1.310 OpenCV

Description

OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products. Includes extra modules for OpenCV from the contrib repository.

More Information

<https://opencv.org/>

Available Versions:

```
4.5.1-fosscuda-2020b-contrib
3.4.7-foss-2019a-Python-3.7.2
```

1.311 OpenColorIO

Description

OpenColorIO (OCIO) is a complete color management solution geared towards motion picture production with an emphasis on visual effects and computer animation.

More Information

<http://opencolorio.org/>

Available Versions:

```
1.1.0-foss-2018b
```


1.312 OpenEXR

Description

OpenEXR is a high dynamic-range (HDR) image file format developed by Industrial Light & Magic for use in computer imaging applications

More Information

<https://www.openexr.com/>

Available Versions:

```
2.4.0-GCCcore-8.3.0
3.1.5-GCCcore-11.3.0
2.5.5-GCCcore-10.2.0
2.4.1-GCCcore-9.3.0
```

1.313 OpenFOAM

Description

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.

More Information

<https://www.openfoam.com/>

Available Versions:

```
v2206-foss-2022a
6-foss-2018b
9-foss-2021a
v2012-foss-2020a
10-foss-2022a
10-foss-2022a
10-intel-2022a
8-foss-2020a
5.0-20180108-foss-2018b
6-foss-2019b
v2106-foss-2021a
v2006-intel-2020a
8-foss-2020b
v1912-foss-2019b
6-intel-2020a
v2006-foss-2020a
v2006-foss-2019b
```

1.314 OpenFOAM-ESI

Available Versions:

v2006-foss-2020a

1.315 OpenFold

Description

A faithful PyTorch reproduction of DeepMind's AlphaFold 2

More Information

<https://github.com/aqlaboratory/openfold>

Available Versions:

1.0.1-foss-2021a-CUDA-11.3.1
1.0.0-foss-2021a-CUDA-11.3.1

1.316 OpenImageIO

Description

OpenImageIO is a library for reading and writing images, and a bunch of related classes, utilities, and applications.

More Information

<https://openimageio.org/>

Available Versions:

2.0.12-gompi-2019b
2.1.12.0-gompi-2020a

1.317 OpenJPEG

Description

OpenJPEG is an open-source JPEG 2000 codec written in C language. It has been developed in order to promote the use of JPEG 2000, a still-image compression standard from the Joint Photographic Experts Group (JPEG). Since may 2015, it is officially recognized by ISO/IEC and ITU-T as a JPEG 2000 Reference Software.

More Information

<https://www.openjpeg.org/>

Available Versions:

2.5.0-GCCcore-11.3.0
2.4.0-GCCcore-11.2.0

1.318 OpenMM

Description

OpenMM is a toolkit for molecular simulation.

More Information

<https://openmm.org>

Available Versions:

```
7.7.0-fosscuda-2020b
7.4.2-intel-2020a-Python-3.8.2
7.5.1-foss-2021b-DeepMind-patch
7.5.1-fosscuda-2020b
7.4.1-foss-2019b-Python-3.7.4
7.5.1-foss-2021a-DeepMind-patch
7.5.0-fosscuda-2020a-Python-3.8.2
```

1.319 OpenMPI

Description

The Open MPI Project is an open source MPI-3 implementation.

More Information

<https://www.open-mpi.org/>

Available Versions:

```
4.1.1-GCC-10.3.0-CUDA-11.1.1
4.0.5-iccifort-2020.4.304
4.0.5-gcccuda-2020b
3.1.1-gcccuda-2018b
4.0.5-GCC-10.2.0
3.1.3-GCC-8.2.0-2.31.1
3.1.4-GCC-8.3.0-dba
4.1.1-GCC-11.2.0-CXX
4.1.1-intel-compilers-2021.2.0
3.1.4-gcccuda-2019b
4.1.1-GCC-11.2.0
4.1.4-GCC-12.2.0
4.0.3-GCC-9.3.0
3.1.1-GCC-7.3.0-2.30
3.1.4-GCC-8.3.0
4.1.4-GCC-11.3.0
4.1.1-GCC-10.3.0
3.1.4-PGI-19.10-GCC-8.3.0-2.32
4.0.3-gcccuda-2020a
```

1.320 OpenMolcas

Description

OpenMolcas is a quantum chemistry software package

More Information

<https://gitlab.com/Molcas/OpenMolcas>

Available Versions:

```
18.09-intel-2020b-Python-3.6.6
20.10-intel-2020a-Python-3.8.2
21.06-intel-2021a
```

1.321 OpenPGM

Description

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.

More Information

<https://code.google.com/p/openpgm/>

Available Versions:

```
5.2.122-GCCcore-11.2.0
5.2.122-GCCcore-8.3.0
5.2.122-GCCcore-10.3.0
5.2.122-GCCcore-10.2.0
5.2.122-GCCcore-9.3.0
5.2.122-GCCcore-11.3.0
```

1.322 OpenSSL

Description

The OpenSSL Project is a collaborative effort to develop a robust, commercial-grade, full-featured, and Open Source toolchain implementing the Secure Sockets Layer (SSL v2/v3) and Transport Layer Security (TLS v1) protocols as well as a full-strength general purpose cryptography library.

More Information

<https://www.openssl.org/>

Available Versions:

```
1.1.1h-GCCcore-10.2.0
1.1
```

1.323 OpenSees

Description

Open System for Earthquake Engineering Simulation

More Information

<https://opensees.berkeley.edu/index.php>

Available Versions:

3.2.0-intel-2020a-Python-3.8.2

1.324 OptaDOS

Available Versions:

v2018-foss-2018b

1.325 OrthoFinder

Description

OrthoFinder is a fast, accurate and comprehensive platform for comparative genomics

More Information

<https://github.com/davidemms/OrthoFinder>

Available Versions:

2.3.8-foss-2019b-Python-2.7.16
2.3.8-foss-2019b-Python-3.7.4

1.326 PAPI

Description

PAPI provides the tool designer and application engineer with a consistent interface and methodology for use of the performance counter hardware found in most major microprocessors. PAPI enables software engineers to see, in near real time, the relation between software performance and processor events. In addition Component PAPI provides access to a collection of components that expose performance measurement opportunities across the hardware and software stack.

More Information

<https://icl.cs.utk.edu/projects/papi/>

Available Versions:

6.0.0-GCCcore-10.2.0
6.0.0-GCCcore-9.3.0

1.327 PAUP

Description

PAUP* (Phylogenetic Analysis Using Parsimony *and other methods) is a computational phylogenetics program for inferring evolutionary trees.

More Information

<https://paup.phylosolutions.com/>

Available Versions:

4.0a168-centos64

1.328 PCMSolver

Description

An API for the Polarizable Continuum Model.

More Information

<https://pcmsolver.readthedocs.org>

Available Versions:

1.2.3-gompi-2019a-Python-3.7.2

1.329 PCRE

Description

The PCRE library is a set of functions that implement regular expression pattern matching using the same syntax and semantics as Perl 5.

More Information

<https://www.pcre.org/>

Available Versions:

8.44-GCCcore-9.3.0
8.44-GCCcore-10.2.0
8.45-GCCcore-11.3.0
8.43-GCCcore-8.3.0
8.41-GCCcore-7.3.0
8.44-GCCcore-10.3.0
8.43-GCCcore-8.2.0
8.45-GCCcore-11.2.0

1.330 PCRE2

Description

The PCRE library is a set of functions that implement regular expression pattern matching using the same syntax and semantics as Perl 5.

More Information

<https://www.pcre.org/>

Available Versions:

```
10.36-GCCcore-10.3.0
10.33-GCCcore-8.3.0
10.37-GCCcore-11.2.0
10.40-GCCcore-11.3.0
10.40-GCCcore-12.2.0
10.34-GCCcore-9.3.0
10.35-GCCcore-10.2.0
```

1.331 PDT

Description

Program Database Toolkit (PDT) is a framework for analyzing source code written in several programming languages and for making rich program knowledge accessible to developers of static and dynamic analysis tools. PDT implements a standard program representation, the program database (PDB), that can be accessed in a uniform way through a class library supporting common PDB operations.

More Information

<https://www.cs.uoregon.edu/research/pdt/>

Available Versions:

```
3.25.1-GCCcore-9.3.0
```

1.332 PEPPAN

Available Versions:

```
2023
```

1.333 PETSc

Description

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.

More Information

<https://www.mcs.anl.gov/petsc>

Available Versions:

```
3.12.4-intel-2020a-Python-3.8.2
3.15.0-foss-2020b
3.15.1-foss-2021a
3.14.4-foss-2020b
3.12.4-foss-2019b-Python-3.7.4
3.17.4-foss-2022a
3.17.4-foss-2021a
3.12.4-foss-2020a-Python-3.8.2
```

1.334 PGI

Description

C, C++ and Fortran compilers from The Portland Group - PGI

More Information

<https://www.pgroup.com/>

Available Versions:

```
18.10-GCC-7.3.0-2.30
18.10-GCC-8.1.0-2.30
19.10-GCC-8.3.0-2.32
16.5-GCC-7.3.0-2.30
```

1.335 PIRATE

Description

PIRATE clusters genes (or other annotated features) over a wide range of amino-acid or nucleotide identity thresholds, and classifies paralogous genes families into either putative gene fission/fusion events or gene duplications. Furthermore, PIRATE provides a measure of allelic variance and cluster homology, and orders the resulting pangenome on a pangenome graph. Additional scripts are provided for comparison and visualization. PIRATE provides a robust framework for analysing the pangenomes of bacteria, from largely clonal to panmictic species.

More Information

<https://github.com/SionBayliss/PIRATE>

Available Versions:

1.0.5

1.336 PLINK

Description

Whole-genome association analysis toolset

More Information

<https://www.cog-genomics.org/plink/2.0/>

Available Versions:

2.00a2.3_x86_64

1.337 PLINKSEQ

Description

PLINK/SEQ is an open-source C/C++ library for working with human genetic variation data. The specific focus is to provide a platform for analytic tool development for variation data from large-scale resequencing and genotyping projects, particularly whole-exome and whole-genome studies. It is independent of (but designed to be complementary to) the existing PLINK package.

More Information

<https://atgu.mgh.harvard.edu/plinkseq/>

Available Versions:

0.10-GCCcore-7.3.0

1.338 PLUMED

Description

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.

More Information

<https://www.plumed.org>

Available Versions:

2.6.0-intel-2020a-Python-3.8.2
 2.7.2-foss-2021a
 2.8.1-foss-2022a
 2.6.2-intel-2020b

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```
2.8.0-foss-2021b
2.5.1-foss-2019a
2.7.0-foss-2020a
2.7.3-foss-2021b
2.7.0-intel-2020b
2.6.0-foss-2020a-Python-3.8.2
2.6.2-foss-2020a-Python-3.8.2
2.7.0-foss-2020b
2.5.1-foss-2020a
2.5.1-foss-2019b
```

1.339 PLY

Description

PLY is yet another implementation of lex and yacc for Python.

More Information

<https://www.dabeaz.com/ply/>

Available Versions:

```
3.11-GCCcore-8.3.0-Python-3.7.4
```

1.340 PMIx

Description

Process Management for Exascale Environments PMI Exascale (PMIx) represents an attempt to provide an extended version of the PMI standard specifically designed to support clusters up to and including exascale sizes. The overall objective of the project is not to branch the existing pseudo-standard definitions - in fact, PMIx fully supports both of the existing PMI-1 and PMI-2 APIs - but rather to (a) augment and extend those APIs to eliminate some current restrictions that impact scalability, and (b) provide a reference implementation of the PMI-server that demonstrates the desired level of scalability.

More Information

<https://pmix.org/>

Available Versions:

```
4.1.2-GCCcore-11.3.0
4.1.0-GCCcore-11.2.0
3.1.5-GCCcore-9.3.0
4.2.2-GCCcore-12.2.0
3.2.3-GCCcore-10.3.0
3.1.5-GCCcore-10.2.0
```

1.341 POV-Ray

Description

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.

More Information

<https://www.povray.org/>

Available Versions:

3.7.0.8-GCC-10.2.0

1.342 PRANK

Description

PRANK is a probabilistic multiple alignment program for DNA, codon and amino-acid sequences. PRANK is based on a novel algorithm that treats insertions correctly and avoids over-estimation of the number of deletion events.

More Information

<http://wasabiapp.org/software/prank/>

Available Versions:

170427-GCC-9.3.0

1.343 PROJ

Description

Program proj is a standard Unix filter function which converts geographic longitude and latitude coordinates into cartesian coordinates

More Information

<https://proj.org>

Available Versions:

6.2.1-GCCcore-8.3.0
 6.0.0-GCCcore-8.2.0
 8.1.0-GCCcore-11.2.0
 7.2.1-GCCcore-10.2.0
 7.0.0-GCCcore-9.3.0
 8.0.1-GCCcore-10.3.0
 5.0.0-foss-2018b
 9.0.0-GCCcore-11.3.0

1.344 PSI4

Description

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.

More Information

<http://www.psicode.org/>

Available Versions:

1.3.1-foss-2019a-Python-3.7.2

1.345 Pango

Description

Pango is a library for laying out and rendering of text, with an emphasis on internationalization. Pango can be used anywhere that text layout is needed, though most of the work on Pango so far has been done in the context of the GTK+ widget toolkit. Pango forms the core of text and font handling for GTK+-2.x.

More Information

<https://www.pango.org/>

Available Versions:

1.44.7-GCCcore-9.3.0
1.48.5-GCCcore-10.3.0
1.47.0-GCCcore-10.2.0
1.44.7-GCCcore-8.3.0
1.42.4-foss-2018b
1.50.7-GCCcore-11.3.0
1.43.0-GCCcore-8.2.0
1.48.8-GCCcore-11.2.0

1.346 ParMETIS

Description

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.

More Information

<http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview>

Available Versions:

```
4.0.3-gompi-2019b
4.0.3-gompi-2022a
4.0.3-gompi-2019a
4.0.3-gompi-2020b
4.0.3-gompi-2020a
4.0.3-iimpi-2020a
```

1.347 ParaView

Description

ParaView is a scientific parallel visualizer.

More Information

<https://www.paraview.org>

Available Versions:

```
5.9.1-foss-2021a-mpi
5.8.0-foss-2020a-Python-3.8.2-mpi
5.8.0-intel-2020a-Python-3.8.2-mpi
5.8.1-foss-2020b-mpi
5.6.2-foss-2019b-Python-3.7.4-mpi
5.10.1-foss-2022a-mpi
```

1.348 PennCNV

Description

A free software tool for Copy Number Variation (CNV) detection from SNP genotyping arrays. Currently it can handle signal intensity data from Illumina and Affymetrix arrays. With appropriate preparation of file format, it can also handle other types of SNP arrays and oligonucleotide arrays.

More Information

<https://penncnv.openbioinformatics.org/>

Available Versions:

```
1.0.5-GCCcore-8.3.0
```

1.349 Perl

Description

Larry Wall's Practical Extraction and Report Language

More Information

<https://www.perl.org/>

Available Versions:

```
5.28.0-GCCcore-10.2.0
5.36.0-GCCcore-12.2.0
5.34.1-GCCcore-11.3.0
5.34.0-GCCcore-11.2.0
5.32.0-GCCcore-10.2.0-minimal
5.32.1-GCCcore-10.3.0-minimal
5.30.0-GCCcore-8.3.0
5.28.1-GCCcore-8.2.0
5.32.0-GCCcore-10.2.0
5.28.0-GCCcore-7.3.0
5.34.0-GCCcore-11.2.0-ARC
5.34.0-GCCcore-11.2.0-minimal
5.34.1-GCCcore-11.3.0-minimal
5.28.1-GCCcore-8.3.0
5.28.0-GCCcore-8.1.0
5.32.1-GCCcore-10.3.0
5.30.0-GCCcore-7.3.0
5.30.2-GCCcore-9.3.0
```

1.350 PhyloBayes-MPI

Description

A Bayesian software for phylogenetic reconstruction using mixture models

More Information

<https://github.com/bayesiancook/pbmpi>

Available Versions:

```
20161021-intel-2020b
```

1.351 Pillow

Description

Pillow is the ‘friendly PIL fork’ by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.

More Information

<https://pillow.readthedocs.org/>

Available Versions:

```
7.0.0-GCCcore-9.3.0-Python-3.8.2
8.0.1-GCCcore-10.2.0
6.0.0-GCCcore-8.2.0
8.2.0-GCCcore-10.3.0
9.1.1-GCCcore-11.3.0
6.2.1-GCCcore-8.3.0
8.3.2-GCCcore-11.2.0
```

1.352 Pillow-SIMD

Description

Pillow is the ‘friendly PIL fork’ by Alex Clark and Contributors. PIL is the Python Imaging Library by Fredrik Lundh and Contributors.

More Information

<https://github.com/uploadcare/pillow-simd>

Available Versions:

```
8.2.0-GCCcore-10.3.0
6.0.x.post0-GCCcore-8.2.0
```

1.353 Pilon

Description

Pilon is an automated genome assembly improvement and variant detection tool

More Information

<https://github.com/broadinstitute/pilon>

Available Versions:

```
1.23-Java-1.8
```

1.354 Platypus

Description

Platypus is a tool designed for efficient and accurate variant-detection# in high-throughput sequencing data.

More Information

<https://vcru.wisc.edu/simonlab/bioinformatics/programs/install/platypus.htm>

Available Versions:

```
latest-GCC-11.2.0-Python-2.7.18
```

1.355 Pmw

Description

Pmw is a toolkit for building high-level compound widgets in Python using the Tkinter module.

More Information

<http://pmw.sourceforge.net>

Available Versions:

2.0.1-foss-2020a-Python-3.8.2
2.0.1-foss-2019b-Python-2.7.16

1.356 PnetCDF

Description

Parallel netCDF: A Parallel I/O Library for NetCDF File Access

More Information

<https://trac.mcs.anl.gov/projects/parallel-netcdf>

Available Versions:

1.12.2-gompi-2020b
1.12.1-gompi-2020a
1.12.2-gompi-c-2020b
1.12.3-gompi-2021b

1.357 PostGis

Available Versions:

2

1.358 PostgreSQL

Description

PostgreSQL is a powerful, open source object-relational database system. It is fully ACID compliant, has full support for foreign keys, joins, views, triggers, and stored procedures (in multiple languages). It includes most SQL:2008 data types, including INTEGER, NUMERIC, BOOLEAN, CHAR, VARCHAR, DATE, INTERVAL, and TIMESTAMP. It also supports storage of binary large objects, including pictures, sounds, or video. It has native programming interfaces for C/C++, Java, .Net, Perl, Python, Ruby, Tcl, ODBC, among others, and exceptional documentation.

More Information

<https://www.postgresql.org/>

Available Versions:

13.3-GCCcore-10.3.0
13.4-GCCcore-11.2.0

1.359 ProtoMS

Available Versions:

3.4

1.360 PyCairo

Description

Python bindings for the cairo library

More Information

<https://pycairo.readthedocs.io/>

Available Versions:

1.21.0-GCCcore-11.3.0
1.18.0-foss-2018b-Python-2.7.15

1.361 PyCharm

Description

PyCharm Community Edition: Python IDE for Professional Developers

More Information

<https://www.jetbrains.com/pycharm/>

Available Versions:

2022.2.2

1.362 PyCifRW

Description

PyCIFRW provides support for reading and writing CIF(Crystallographic Information Format) files using Python.

More Information

<https://bitbucket.org/jamesrhester/pycifrw/src/development>

Available Versions:

4.4.2-GCCcore-9.3.0

1.363 PyGObject

Description

Python Bindings for GLib/GObject/GIO/GTK+

More Information

<http://www.pygtk.org/>

Available Versions:

2.28.7-foss-2018b-Python-2.7.15 3.42.1-GCCcore-11.3.0
--

1.364 PyGTK

Description

PyGTK lets you to easily create programs with a graphical user interface using the Python programming language.

More Information

<http://www.pygtk.org/>

Available Versions:

2.24.0-foss-2018b-Python-2.7.15

1.365 PyMOL

Description

PyMOL is an OpenGL based molecular visualization system

More Information

<http://sourceforge.net/projects/pymol>

Available Versions:

2.3.0-foss-2019b-Python-2.7.16 2.5.0-foss-2020a-Python-3.8.2

1.366 PyQt5

Description

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.

More Information

<https://www.riverbankcomputing.com/software/pyqt>

Available Versions:

```
5.15.1-GCCcore-9.3.0-Python-3.8.2
5.15.4-GCCcore-11.2.0
```

1.367 PySCF

Description

PySCF is an open-source collection of electronic structure modules powered by Python.

More Information

<http://www.pyscf.org>

Available Versions:

```
1.6.3-foss-2019a-Python-3.7.2
2.1.1-foss-2021a
1.7.6-foss-2021a
1.7.0-foss-2020a-Python-3.8.2
```

1.368 PyTables

Description

PyTables is a package for managing hierarchical datasets and designed to efficiently and easily cope with extremely large amounts of data. PyTables is built on top of the HDF5 library, using the Python language and the NumPy package. It features an object-oriented interface that, combined with C extensions for the performance-critical parts of the code (generated using Cython), makes it a fast, yet extremely easy to use tool for interactively browse, process and search very large amounts of data. One important feature of PyTables is that it optimizes memory and disk resources so that data takes much less space (specially if on-flight compression is used) than other solutions such as relational or object oriented databases.

More Information

<https://www.pytables.org>

Available Versions:

```
3.6.1-foss-2021a
```

1.369 PyTorch

Description

Tensors and Dynamic neural networks in Python with strong GPU acceleration. PyTorch is a deep learning framework that puts Python first.

More Information

<https://pytorch.org/>

Available Versions:

```
1.6.0-fosscuda-2019b-Python-3.7.4
1.6.0-foss-2019b-Python-3.7.4
1.7.1-fosscuda-2020b
1.10.0-foss-2021a
1.12.0-foss-2022a
1.11.0-foss-2021a-CUDA-11.3.1
1.8.1-fosscuda-2019b-Python-3.7.4
```

1.370 PyTorch-Lightning

Description

PyTorch Lightning is the lightweight PyTorch wrapper for ML researchers.

More Information

<https://pytorchlightning.ai>

Available Versions:

```
1.7.7-foss-2022a
1.5.9-foss-2021a-CUDA-11.3.1
```

1.371 PyYAML

Description

PyYAML is a YAML parser and emitter for the Python programming language.

More Information

<https://github.com/yaml/pyyaml>

Available Versions:

```
5.1.2-GCCcore-8.3.0
5.4.1-GCCcore-10.3.0
5.4.1-GCCcore-11.2.0
5.1-GCCcore-8.2.0
5.3.1-GCCcore-10.2.0
5.3-GCCcore-9.3.0
6.0-GCCcore-11.3.0
```

1.372 Pysam

Description

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.

More Information

<https://github.com/pysam-developers/pysam>

Available Versions:

```
0.16.0.1-GCC-9.3.0
0.15.3-GCC-8.3.0
0.19.1-GCC-11.3.0
0.18.0-GCC-11.2.0
```

1.373 Python

Description

Python is a programming language that lets you work more quickly and integrate your systems more effectively.

More Information

<https://python.org/>

Available Versions:

```
3.10.4-GCCcore-11.3.0
3.8.6-GCCcore-10.2.0
2.7.15-fosscuda-2018b
3.9.6-GCCcore-11.2.0-bare
2.7.15-GCCcore-7.3.0-bare
3.10.8-GCCcore-12.2.0
3.6.6-foss-2018b
3.9.6-GCCcore-11.2.0
3.9.5-GCCcore-10.3.0-bare
3.10.8-GCCcore-12.2.0-bare
2.7.18-GCCcore-10.2.0
3.9.5-GCCcore-10.3.0-SKL
3.6.6-intel-2020b
3.7.2-GCCcore-8.2.0
3.8.2-GCCcore-9.3.0
2.7.16-GCCcore-8.3.0
3.7.4-GCCcore-9.3.0
3.7.4-GCCcore-8.3.0
2.7.18-GCCcore-11.2.0
3.10.4-GCCcore-11.3.0-bare
2.7.18-GCCcore-11.3.0-bare
2.7.18-GCCcore-9.3.0
2.7.18-GCCcore-10.3.0-bare
3.9.5-GCCcore-10.3.0
2.7.15-foss-2018b
```

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2.7.18-GCCcore-11.2.0-bare
2.7.15-GCCcore-8.2.0

1.374 QCA

Description

Taking a hint from the similarly-named Java Cryptography Architecture, QCA aims to provide a straightforward and cross-platform crypto API, using Qt datatypes and conventions. QCA separates the API from the implementation, using plugins known as Providers. The advantage of this model is to allow applications to avoid linking to or explicitly depending on any particular cryptographic library. This allows one to easily change or upgrade crypto implementations without even needing to recompile the application! QCA should work everywhere Qt does, including Windows/Unix/MacOSX.

More Information

<https://userbase.kde.org/QCA>

Available Versions:

2.3.5-GCCcore-11.2.0

1.375 QGIS

Description

QGIS is a user friendly Open Source Geographic Information System (GIS)

More Information

<http://www.qgis.org/>

Available Versions:

3.28.1-foss-2021b

1.376 QIIME2

Description

QIIME is an open-source bioinformatics pipeline for performing microbiome analysis from raw DNA sequencing data.

More Information

<http://qiime2.org/>

Available Versions:

2019.7

1.377 QScintilla

Description

QScintilla is a port to Qt of Neil Hodgson's Scintilla C++ editor control

More Information

<https://www.riverbankcomputing.com/software/qscintilla>

Available Versions:

2.11.6-GCCcore-11.2.0

1.378 QUAST

Description

QUAST evaluates genome assemblies by computing various metrics. It works both with and without reference genomes. The tool accepts multiple assemblies, thus is suitable for comparison.

More Information

<https://github.com/ablab/quast>

Available Versions:

5.0.2-foss-2020a-Python-3.8.2

1.379 Qhull

Description

Qhull computes the convex hull, Delaunay triangulation, Voronoi diagram, halfspace intersection about a point, furthest-site Delaunay triangulation, and furthest-site Voronoi diagram. The source code runs in 2-d, 3-d, 4-d, and higher dimensions. Qhull implements the Quickhull algorithm for computing the convex hull.

More Information

<http://www.qhull.org>

Available Versions:

2020.2-GCCcore-10.3.0
2019.1-GCCcore-8.3.0
2020.2-GCCcore-11.2.0
2020.2-GCCcore-11.3.0

1.380 Qiskit

Description

Qiskit is an open-source framework for working with noisy quantum computers at the level of pulses, circuits, and algorithms.

More Information

<https://qiskit.org>

Available Versions:

0.23.1-foss-2020a-Python-3.8.2

1.381 Qt5

Description

Qt is a comprehensive cross-platform C++ application framework.

More Information

<https://qt.io/>

Available Versions:

5.14.1-GCCcore-9.3.0
5.13.1-GCCcore-8.3.0
5.15.2-GCCcore-11.2.0
5.15.5-GCCcore-11.3.0
5.14.2-GCCcore-10.2.0
5.15.2-GCCcore-10.3.0

1.382 Qt5Webkit

Description

Qt Port of WebKit. WebKit is an open source web browser engine.

More Information

<https://github.com/qt/qtwebkit>

Available Versions:

5.212.0-alpha4-GCCcore-11.2.0

1.383 QtKeychain

Description

Platform-independent Qt API for storing passwords securely.

More Information

<https://github.com/frankosterfeld/qtkeychain>

Available Versions:

0.13.2-GCCcore-11.2.0

1.384 Quandl

Description

A Python library for Quandl's RESTful API.

More Information

<https://pypi.python.org/pypi/Quandl>

Available Versions:

3.4.8-foss-2019a
3.5.3-foss-2020a-Python-3.8.2
3.6.1-foss-2021a

1.385 QuantumESPRESSO

Description

Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).

More Information

<https://www.quantum-espresso.org>

Available Versions:

7.1-foss-2022a
7.1-intel-2022a
6.5-intel-2020a
6.6-foss-2020b
6.7-foss-2020b
6.7-intel-2020a
6.6-intel-2020a

1.386 Qwt

Description

The Qwt library contains GUI Components and utility classes which are primarily useful for programs with a technical background.

More Information

<https://qwt.sourceforge.io/>

Available Versions:

```
6.2.0-GCCcore-11.2.0
6.2.0-GCCcore-10.3.0
6.1.4-GCCcore-8.3.0
```

1.387 R

Description

R is a free software environment for statistical computing and graphics.

More Information

<https://www.r-project.org/>

Available Versions:

```
4.1.0-foss-2021a
4.0.2-foss-2020a-ARC
4.1.2-foss-2021b
3.6.2-foss-2019b
4.1.0-foss-2021a-ARC
4.2.1-foss-2022a
4.2.1-foss-2021b-ARC
4.2.2-foss-2022a-ARC
4.2.1-foss-2022a-ARC
4.2.1-foss-2021b
4.2.2-foss-2022a
4.1.2-foss-2021b-ARC
4.0.2-foss-2020a
```

1.388 R-bundle-Bioconductor

Description

Bioconductor provides tools for the analysis and comprehension of high-throughput genomic data.

More Information

<https://bioconductor.org>

Available Versions:

```
3.13-foss-2021a-R-4.1.0
3.14-foss-2021b-R-4.1.2
3.15-foss-2022a-R-4.2.1
3.10-foss-2019b
```

1.389 RAxML

Description

RAxML search algorithm for maximum likelihood based inference of phylogenetic trees.

More Information

<https://github.com/stamatak/standard-RAxML>

Available Versions:

```
8.2.12-gompi-2020a-hybrid-avx2
8.2.12-gompi-2021b-hybrid-avx2
```

1.390 RAxML-NG

Description

RAxML-NG is a phylogenetic tree inference tool which uses maximum-likelihood (ML) optimality criterion. Its search heuristic is based on iteratively performing a series of Subtree Pruning and Regrafting (SPR) moves, which allows to quickly navigate to the best-known ML tree.

More Information

<https://github.com/amkozlov/raxml-ng>

Available Versions:

```
1.0.2-gompi-2020b
```

1.391 RDKit

Description

RDKit is a collection of cheminformatics and machine-learning software written in C++ and Python.

More Information

<https://www.rdkit.org>

Available Versions:

```
2020.03.3-foss-2020a-Python-3.8.2
```

1.392 RE2

Description

RE2 is a fast, safe, thread-friendly alternative to backtracking regular expression engines like those used in PCRE, Perl, and Python. It is a C++ library.

More Information

<https://github.com/google/re2>

Available Versions:

<code>2020-07-01-GCCcore-8.3.0</code>
<code>2022-06-01-GCCcore-11.3.0</code>
<code>2022-02-01-GCCcore-11.2.0</code>

1.393 RECON

Description

Patched version of RECON to be used with RepeatModeler.

More Information

<https://www.repeatmasker.org/RepeatModeler/>

Available Versions:

<code>1.08-GCC-10.2.0</code>
<code>1.08-GCC-10.3.0</code>

1.394 RELION

Description

RELION (for REgularised LIkelihood Optimisation, pronounce rely-on) is a stand-alone computer program that employs an empirical Bayesian approach to refinement of (multiple) 3D reconstructions or 2D class averages in electron cryo-microscopy (cryo-EM).

More Information

http://www2.mrc-lmb.cam.ac.uk/relion/index.php/Main_Page

Available Versions:

<code>3.0.4-foss-2019b</code>

1.395 RMBlast

Description

RMBlast is a RepeatMasker compatible version of the standard NCBI BLAST suite. The primary difference between this distribution and the NCBI distribution is the addition of a new program 'rmblastn' for use with RepeatMasker and RepeatModeler.

More Information

<https://www.repeatmasker.org/RMBlast.html>

Available Versions:

```
2.11.0-gompi-2020b
2.11.0-gompi-2021a
```

1.396 ROOT

Description

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.

More Information

<https://root.cern.ch/drupal/>

Available Versions:

```
6.24.06-foss-2021b
6.20.04-foss-2019b-Python-3.7.4
```

1.397 RStudio

Available Versions:

```
2022.02-R-4.2.1-ARC
```

1.398 RapidJSON

Description

A fast JSON parser/generator for C++ with both SAX/DOM style API

More Information

<https://rapidjson.org>

Available Versions:

```
1.1.0-GCCcore-8.3.0
1.1.0-GCCcore-11.3.0
1.1.0-GCCcore-11.2.0
```

1.399 Ray-assembler

Description

Parallel genome assemblies for parallel DNA sequencing

More Information

<http://denovoassembler.sourceforge.net/>

Available Versions:

```
2.3.1-iimpi-2020a
```

1.400 RepeatMasker

Description

RepeatMasker is a program that screens DNA sequences for interspersed repeats and low complexity DNA sequences.

More Information

<https://www.repeatmasker.org/>

Available Versions:

```
4.1.2-p1-foss-2020b
4.1.2-p1-foss-2021a
```

1.401 RepeatModeler

Description

RepeatModeler is a de novo transposable element (TE) family identification and modeling package.

More Information

<https://www.repeatmasker.org/>

Available Versions:

```
2.0.2a-foss-2020b
```

1.402 RepeatScout

Description

De Novo Repeat Finder, Price A.L., Jones N.C. and Pevzner P.A. Developed and tested with our multiple sequence version of RepeatScout (1.0.6)

More Information

<https://www.repeatmasker.org/>

Available Versions:

```
1.0.6-GCC-10.3.0
1.0.6-GCC-10.2.0
```

1.403 RevBayes

Description

RevBayes provides an interactive environment for statistical computation in phylogenetics. It is primarily intended for modeling, simulation, and Bayesian inference in evolutionary biology, particularly phylogenetics.

More Information

<https://revbayes.github.io/>

Available Versions:

```
1.1.1-GCC-10.2.0
```

1.404 Ruby

Description

Ruby is a dynamic, open source programming language with a focus on simplicity and productivity. It has an elegant syntax that is natural to read and easy to write.

More Information

<https://www.ruby-lang.org>

Available Versions:

```
3.0.1-GCCcore-10.3.0
3.0.1-GCCcore-11.2.0
2.6.1-GCCcore-7.3.0
```

1.405 Rust

Description

Rust is a systems programming language that runs blazingly fast, prevents segfaults, and guarantees thread safety.

More Information

<https://www.rust-lang.org>

Available Versions:

```
1.60.0-GCCcore-11.3.0
1.42.0-GCCcore-8.3.0
1.54.0-GCCcore-11.2.0
1.42.0-GCCcore-9.3.0
1.65.0-GCCcore-12.2.0
1.52.1-GCCcore-10.3.0
```

1.406 SAMtools

Description

SAM Tools provide various utilities for manipulating alignments in the SAM format, including sorting, merging, indexing and generating alignments in a per-position format.

More Information

<http://www.htslib.org/>

Available Versions:

```
0.1.20-foss-2020a
1.10-GCC-9.3.0
1.14-GCC-11.2.0
1.12-GCC-10.2.0
1.10-GCC-8.3.0
0.1.20-GCC-8.3.0
1.9-foss-2018b
1.16.1-GCC-11.3.0
1.11-GCC-10.2.0
1.15.1-GCC-11.2.0
```

1.407 SCOTCH

Description

Software package and libraries for sequential and parallel graph partitioning,static mapping, and sparse matrix block ordering, and sequential mesh and hypergraph partitioning.

More Information

<https://gforge.inria.fr/projects/scotch/>

Available Versions:


```
6.0.9-gompi-2019b
6.0.6-gompi-2019a
6.0.9-iimpi-2020a
6.1.0-gompi-2020b
7.0.1-gompi-2022a
6.0.6-foss-2018b
6.0.9-gompi-2020a
6.1.0-gompi-2021a
```

1.408 SCons

Description

SCons is a software construction tool.

More Information

<https://www.scons.org/>

Available Versions:

```
3.0.5-GCCcore-8.2.0-Python-2.7.15
3.0.1-fosscuda-2018b-Python-2.7.15
3.0.5-GCCcore-8.2.0
3.0.1-foss-2018b-Python-2.7.15
3.1.1-GCCcore-8.3.0
4.0.1-GCCcore-10.2.0
```

1.409 SDL2

Description

SDL: Simple DirectMedia Layer, a cross-platform multimedia library

More Information

<https://www.libsdl.org/>

Available Versions:

```
2.0.14-GCCcore-10.2.0
2.0.20-GCCcore-11.2.0
```

1.410 SIONlib

Description

SIONlib is a scalable I/O library for parallel access to task-local files. The library not only supports writing and reading binary data to or from several thousands of processors into a single or a small number of physical files, but also provides global open and close functions to access SIONlib files in parallel. This package provides a stripped-down installation of SIONlib for use with performance tools (e.g., Score-P), with renamed symbols to avoid conflicts when an application using SIONlib itself is linked against a tool requiring a different SIONlib version.

More Information

https://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SIONlib/_node.html

Available Versions:

```
1.7.7-GCCcore-11.3.0-tools
1.7.6-GCCcore-9.3.0-tools
1.7.6-foss-2019b
1.7.6-foss-2020a
```

1.411 SKESA

Description

SKESA is a de-novo sequence read assembler for cultured single isolate genomes based on DeBruijn graphs.

More Information

<https://github.com/ncbi/SKESA>

Available Versions:

```
2.3.0-foss-2018b
```

1.412 SLEPc

Description

SLEPc (Scalable Library for Eigenvalue Problem Computations) is a software library for the solution of large scale sparse eigenvalue problems on parallel computers. It is an extension of PETSc and can be used for either standard or generalized eigenproblems, with real or complex arithmetic. It can also be used for computing a partial SVD of a large, sparse, rectangular matrix, and to solve quadratic eigenvalue problems.

More Information

<https://slepc.upv.es/>

Available Versions:

```
3.12.2-foss-2019b-Python-3.7.4
3.15.1-foss-2021a
3.12.2-intel-2020a-Python-3.8.2
```

1.413 SNPsplit

Description

SNPsplit is an allele-specific alignment sorter which is designed to read alignment files in SAM/BAM format and determine the allelic origin of reads that cover known SNP positions. For this to work a library must have been aligned to a genome which had all SNP positions masked by the ambiguity base 'N', and aligned using aligners that are capable of using a reference genome which contains ambiguity nucleobases.

More Information

<https://felixkrueger.github.io/SNPsplit/>

Available Versions:

0.6.0-GCC-11.2.0

1.414 SNeP1

Available Versions:

1

1.415 SOAPdenovo2

Description

SOAPdenovo is a novel short-read assembly method that can build a de novo draft assembly for human-sized genomes. The program is specially designed to assemble Illumina short reads. It creates new opportunities for building reference sequences and carrying out accurate analyses of unexplored genomes in a cost effective way. SOAPdenovo2 is the successor of SOAPdenovo.

More Information

<http://soap.genomics.org.cn/index.html>

Available Versions:

r241-foss-2020a

1.416 SOCI

Description

SOCI is a database access library for C++ that makes the illusion of embedding SQL queries in the regular C++ code, staying entirely within the Standard C++.

More Information

<http://soci.sourceforge.net/>

Available Versions:

4.0.2-GCC-10.3.0

1.417 SPAdes

Description

Genome assembler for single-cell and isolates data sets

More Information

<https://cab.spbu.ru/software/spades/>

Available Versions:

3.15.2-GCC-10.2.0
3.13.0-foss-2018b

1.418 SQLite

Description

SQLite: SQL Database Engine in a C Library

More Information

<https://www.sqlite.org/>

Available Versions:

3.36-GCCcore-11.2.0
3.33.0-GCCcore-10.2.0
3.27.2-GCCcore-8.2.0
3.31.1-GCCcore-9.3.0
3.24.0-GCCcore-10.2.0
3.38.3-GCCcore-11.3.0
3.39.4-GCCcore-12.2.0
3.29.0-GCCcore-9.3.0
3.35.4-GCCcore-10.3.0
3.27.2-GCCcore-8.3.0
3.29.0-GCCcore-8.3.0
3.24.0-GCCcore-7.3.0

1.419 SRA-Toolkit

Description

The SRA Toolkit, and the source-code SRA System Development Kit (SDK), will allow you to programmatically access data housed within SRA and convert it from the SRA format

More Information

<https://github.com/ncbi/sra-tools>

Available Versions:

```
3.0.3-gompi-2022a
2.10.9-gompi-2020b
```

1.420 SSW

Description

SSW is a fast implementation of the Smith-Waterman algorithm, which uses the Single-Instruction Multiple-Data (SIMD) instructions to parallelize the algorithm at the instruction level. SSW library provides an API that can be flexibly used by programs written in C, C++ and other languages. We also provide a software that can do protein and genome alignment directly. Current version of our implementation is ~50 times faster than an ordinary Smith-Waterman. It can return the Smith-Waterman score, alignment location and traceback path (cigar) of the optimal alignment accurately; and return the sub-optimal alignment score and location heuristically.

More Information

<https://github.com/mengyao/Complete-Striped-Smith-Waterman-Library>

Available Versions:

```
1.1-GCCcore-11.2.0
```

1.421 STAR

Description

STAR aligns RNA-seq reads to a reference genome using uncompressed suffix arrays.

More Information

<https://github.com/alexdobin/STAR>

Available Versions:

```
2.7.10b-GCC-11.3.0
2.7.1a-GCC-8.2.0-2.31.1
2.7.9a-GCC-11.2.0
2.7.3a-GCC-9.3.0
```

1.422 STARCCM+

Available Versions:

```
2021.2.1
2022.1
2020.2.1
```

1.423 STEAK

Description

Detects integrations of any sort in high-throughput sequencing (HTS) data. STEAK was built for validating and discovering transposable element (TE) and retroviral integrations in a variety of HTS data. The software performs on both single-end (SE) and paired-end (PE) libraries and on a variety of HTS sequencing strategies. It can be applied to a broad range of research interests and clinical uses such as population genetic studies and detecting polymorphic integrations.

More Information

<https://omictools.com/steak-tool>

Available Versions:

2019.09.12-foss-2019b-Python-2.7.16

1.424 SUNDIALS

Description

SUNDIALS: SUite of Nonlinear and Differential/ALgebraic Equation Solvers

More Information

<https://computation.llnl.gov/projects/sundials>

Available Versions:

6.3.0-foss-2021b
5.1.0-foss-2019b

1.425 SWIG

Description

SWIG is a software development tool that connects programs written in C and C++ with a variety of high-level programming languages.

More Information

<http://www.swig.org/>

Available Versions:

4.0.1-GCCcore-8.3.0
3.0.12-GCCcore-8.2.0-Python-2.7.15
4.0.2-GCCcore-10.2.0
3.0.12-foss-2018b-Python-2.7.15
4.0.1-GCCcore-9.3.0
4.0.2-GCCcore-11.2.0
4.0.2-GCCcore-10.3.0
3.0.12-GCCcore-8.3.0

1.426 Salmon

Description

Salmon is a wicked-fast program to produce a highly-accurate, transcript-level quantification estimates from RNA-seq data.

More Information

<https://github.com/COMBINE-lab/salmon>

Available Versions:

```
1.4.0-gompi-2020b
1.1.0-gompi-2019b
1.4.0-GCC-11.2.0
```

1.427 Sambamba

Description

Sambamba is a high performance modern robust and fast tool (and library), written in the D programming language, for working with SAM and BAM files. Current functionality is an important subset of samtools functionality, including view, index, sort, markup, and depth.

More Information

<https://lomeriteir.github.io/sambamba/>

Available Versions:

```
0.7.1
0.8.2-GCC-10.3.0
```

1.428 ScaFaCoS

Description

ScaFaCoS is a library of scalable fast coulomb solvers.

More Information

<http://www.scafacos.de/>

Available Versions:

```
1.0.1-foss-2020a
1.0.1-foss-2021b
1.0.1-foss-2021a
1.0.1-intel-2020a
```

1.429 ScaLAPACK

Description

The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers.

More Information

<https://www.netlib.org/scalapack/>

Available Versions:

```
2.1.0-gompi-2020a
2.1.0-gompic-2020b
2.2.0-gompi-2022a-fb
2.0.2-gompi-2019a-OpenBLAS-0.3.5
2.0.2-gompic-2019b
2.1.0-gompi-2020b
2.0.2-gompic-2018b-OpenBLAS-0.3.1
2.0.2-gompi-2019b
2.1.0-gompi-2021b-fb
2.1.0-gompi-2021a-fb
2.1.0-gompic-2020a
2.0.2-gompi-2018b-OpenBLAS-0.3.1
2.2.0-gompi-2022b-fb
```

1.430 Scalasca

Description

Scalasca is a software tool that supports the performance optimization of parallel programs by measuring and analyzing their runtime behavior. The analysis identifies potential performance bottlenecks – in particular those concerning communication and synchronization – and offers guidance in exploring their causes.

More Information

<https://www.scalasca.org/>

Available Versions:

```
2.5-gompi-2020a
```

1.431 SciPy-bundle

Description

Bundle of Python packages for scientific software

More Information

<https://python.org/>

Available Versions:


```
2019.10-foss-2019b-Python-3.7.4
2020.11-fosscuda-2020b
2019.10-fosscuda-2019b-Python-3.7.4
2019.10-fosscuda-2019b-Python-2.7.16
2020.03-intel-2020a-Python-3.8.2
2022.05-foss-2022a
2021.05-foss-2021a
2020.11-intel-2020b
2022.05-intel-2022a
2021.05-foss-2021a-SKL
2020.03-foss-2020a-Python-3.8.2
2020.11-foss-2020b
2020.03-fosscuda-2020a-Python-3.8.2
2019.03-foss-2019a
2019.10-foss-2019b-Python-2.7.16
2021.10-foss-2021b
```

1.432 Score-P

Description

The Score-P measurement infrastructure is a highly scalable and easy-to-use tool suite for profiling, event tracing, and online analysis of HPC applications.

More Information

<https://www.score-p.org>

Available Versions:

```
6.0-gompi-2020a
```

1.433 Seaborn

Description

Seaborn is a Python visualization library based on matplotlib. It provides a high-level interface for drawing attractive statistical graphics.

More Information

<https://seaborn.pydata.org/>

Available Versions:

```
0.10.0-foss-2019b-Python-3.7.4
```

1.434 SegAlign

Available Versions:

master-feb23

1.435 SentencePiece

Description

Unsupervised text tokenizer for Neural Network-based text generation.

More Information

<https://github.com/google/sentencepiece>

Available Versions:

0.1.85-GCC-8.3.0-Python-3.7.4

1.436 SeqKit

Description

SeqKit - a cross-platform and ultrafast toolkit for FASTA/Q file manipulation

More Information

<https://bioinf.shenwei.me/seqkit/>

Available Versions:

2.2.0
0.13.2

1.437 SeqLib

Description

C++ interface to HTSlib, BWA-MEM and Fermi.

More Information

<https://github.com/walaj/SeqLib>

Available Versions:

1.2.0-GCC-11.2.0

1.438 Serf

Description

The serf library is a high performance C-based HTTP client library built upon the Apache Portable Runtime (APR) library

More Information

<https://serf.apache.org/>

Available Versions:

1.3.9-GCCcore-10.2.0

1.439 Shapely

Description

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.

More Information

<https://github.com/Toblerity/Shapely>

Available Versions:

1.7.1-GCC-9.3.0-Python-3.8.2

1.8.2-foss-2021b

1.440 Siesta

Description

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.

More Information

<http://departments.icmab.es/leem/siesta>

Available Versions:

4.1.5-intel-2022a

4.1.5-foss-2020a

4.1-b4-intel-2020a

1.441 Stacks

Description

Stacks is a software pipeline for building loci from short-read sequences, such as those generated on the Illumina platform. Stacks was developed to work with restriction enzyme-based data, such as RAD-seq, for the purpose of building genetic maps and conducting population genomics and phylogeography.

More Information

<http://catchenlab.life.illinois.edu/stacks>

Available Versions:

2.41-icciFORT-2019.5.281
2.53-foss-2019b
2.41-GCC-8.3.0

1.442 Stata

Available Versions:

14

1.443 Subversion

Description

Subversion is an open source version control system.

More Information

<https://subversion.apache.org/>

Available Versions:

1.14.0-GCCcore-10.2.0

1.444 SuiteSparse

Description

SuiteSparse is a collection of libraries manipulate sparse matrices.

More Information

<http://faculty.cse.tamu.edu/davis/suitesparse.html>

Available Versions:

```
5.4.0-foss-2019a-METIS-5.1.0
5.13.0-foss-2022a-METIS-5.1.0
5.7.1-foss-2020a-METIS-5.1.0
5.6.0-foss-2019b-METIS-5.1.0
5.8.1-foss-2020b-METIS-5.1.0
5.10.1-foss-2021a-METIS-5.1.0
5.10.1-foss-2021b-METIS-5.1.0
5.11.0-foss-2021a-METIS-5.1.0
5.7.1-intel-2020a-METIS-5.1.0
```

1.445 SuperLU

Description

SuperLU is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations on high performance machines.

More Information

<https://crd-legacy.lbl.gov/~xiaoye/SuperLU/>

Available Versions:

```
5.2.2-intel-2020a
```

1.446 SuperLU_DIST

Description

SuperLU is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations on high performance machines.

More Information

<https://crd-legacy.lbl.gov/~xiaoye/SuperLU/>

Available Versions:

```
8.1.0-foss-2022a
```

1.447 SymEngine

Description

SymEngine is a standalone fast C++ symbolic manipulation library

More Information

<https://github.com/symengine/symengine>

Available Versions:

0.7.0-GCC-10.3.0

1.448 SymEngine-python

Description

Python wrappers to the C++ library SymEngine, a fast C++ symbolic manipulation library.

More Information

<https://github.com/symengine/symengine.py>

Available Versions:

0.7.2-GCC-10.3.0

1.449 Szip

Description

Szip compression software, providing lossless compression of scientific data

More Information

http://www.hdfgroup.org/doc_resource/SZIP/

Available Versions:

2.1.1-GCCcore-7.3.0
2.1.1-GCCcore-10.2.0
2.1.1-GCCcore-10.3.0
2.1.1-GCCcore-11.3.0
2.1.1-GCCcore-9.3.0
2.1.1-GCCcore-8.2.0
2.1.1-GCCcore-8.3.0
2.1.1-GCCcore-11.2.0
2.1.1-GCCcore-12.2.0
2.1.1-intel-2020a

1.450 TCLAP

Description

TCLAP is a small, flexible library that provides a simple interface for defining and accessing command line arguments. It was initially inspired by the user friendly CLAP library.

More Information

<http://tclap.sourceforge.net/>

Available Versions:

```
1.2.5-GCCcore-11.2.0
```

1.451 Tetranscripts

Description

Tetranscripts and TEcount takes RNA-seq (and similar data) and annotates reads to both genes & transposable elements. Tetranscripts then performs differential analysis using DESeq2.

More Information

<https://github.com/mhammell-laboratory/Tetranscripts>

Available Versions:

```
2.2.0-foss-2021b
```

1.452 TRF

Description

Tandem Repeats Finder: a program to analyze DNA sequences.

More Information

<https://tandem.bu.edu/trf/trf.html>

Available Versions:

```
4.09.1-GCCcore-10.3.0  
4.09.1-GCCcore-10.2.0
```

1.453 TWL-NINJA

Description

Nearly Infinite Neighbor Joining Application.

More Information

<https://github.com/TravisWheelerLab/NINJA>

Available Versions:

```
0.97-cluster_only-GCC-10.3.0  
0.97-cluster_only-GCC-10.2.0
```

1.454 Tcl

Description

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.

More Information

<https://www.tcl.tk/>

Available Versions:

```
8.6.9-GCCcore-9.3.0
8.6.9-GCCcore-8.3.0
8.6.10-GCCcore-9.3.0
8.6.8-GCCcore-7.3.0
8.6.11-GCCcore-11.2.0
8.6.11-GCCcore-10.3.0
8.6.12-GCCcore-12.2.0
8.6.12-GCCcore-11.3.0
8.6.8-GCCcore-10.2.0
8.6.9-GCCcore-8.2.0
8.6.10-GCCcore-10.2.0
```

1.455 TensorFlow

Description

An open-source software library for Machine Intelligence

More Information

<https://www.tensorflow.org/>

Available Versions:

```
2.3.1-foss-2020a-Python-3.8.2
2.8.4-foss-2021b
2.1.0-foss-2019b-Python-3.7.4
2.6.0-foss-2021a
1.15.2-fosscuda-2019b-Python-3.7.4
2.5.0-fosscuda-2020b
2.4.1-fosscuda-2020b
2.7.1-foss-2021b-CUDA-11.4.1
2.6.0-foss-2021a-CUDA-11.3.1
2.5.3-foss-2021a-CUDA-11.3.1
```


1.456 Theano

Description

Theano is a Python library that allows you to define, optimize, and evaluate mathematical expressions involving multi-dimensional arrays efficiently.

More Information

<https://deeplearning.net/software/theano>

Available Versions:

```
1.0.4-foss-2019b-Python-3.7.4
1.1.2-foss-2020b-PyMC
1.0.4-fosscuda-2019b-Python-3.7.4
1.1.2-fosscuda-2020b-PyMC
```

1.457 Tinker9

Description

The Tinker molecular modeling software is a complete and general package for molecular mechanics and dynamics, with some special features for biopolymers.

More Information

<https://github.com/TinkerTools/tinker9>

Available Versions:

```
1.0.4-GIT-31839758
```

1.458 Tk

Description

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.

More Information

<https://www.tcl.tk/>

Available Versions:

```
8.6.11-GCCcore-10.3.0
8.6.8-GCCcore-7.3.0
8.6.9-GCCcore-8.2.0
8.6.9-GCCcore-8.3.0
8.6.10-GCCcore-9.3.0
8.6.10-GCCcore-10.2.0
8.6.9-GCCcore-9.3.0
8.6.11-GCCcore-11.2.0
```

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8.6.12-GCCcore-11.3.0
8.6.12-GCCcore-12.2.0

1.459 Tkinter

Description

Tkinter module, built with the Python buildsystem

More Information

<http://python.org/>

Available Versions:

2.7.15-foss-2018b-Python-2.7.15
3.10.4-GCCcore-11.3.0
2.7.16-GCCcore-8.3.0
3.8.6-GCCcore-10.2.0
3.8.2-GCCcore-9.3.0
3.9.5-GCCcore-10.3.0
3.7.2-GCCcore-8.2.0
3.7.4-GCCcore-8.3.0
2.7.15-fosscuda-2018b-Python-2.7.15
3.9.6-GCCcore-11.2.0

1.460 Togl

Description

A Tcl/Tk widget for OpenGL rendering.

More Information

<https://sourceforge.net/projects/togl/>

Available Versions:

2.0-GCCcore-8.3.0

1.461 TopHat

Description

TopHat is a fast splice junction mapper for RNA-Seq reads.

More Information

<http://ccb.jhu.edu/software/tophat/>

Available Versions:

2.1.2-gompi-2019b

1.462 TreeMix

Description

TreeMix is a method for inferring the patterns of population splits and mixtures in the history of a set of populations.

More Information

<http://bitbucket.org/nygcresearch/treemix>

Available Versions:

1.13-intel-2020a

1.13-GCC-10.3.0

1.463 Trilinos

Description

The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages.

More Information

<https://trilinos.org>

Available Versions:

12.12.1-foss-2019b-Python-3.7.4

1.464 Trim_Galore

Description

Trim Galore is a wrapper around Cutadapt and FastQC to consistently apply adapter and quality trimming to FastQ files, with extrafunctionality for RRBS data.

More Information

https://www.bioinformatics.babraham.ac.uk/projects/trim_galore/

Available Versions:

0.6.5-GCCcore-8.3.0-Java-11-Python-3.7.4

0.5.0-foss-2018b

1.465 Trimmomatic

Description

Trimmomatic performs a variety of useful trimming tasks for illumina paired-end and single ended data. The selection of trimming steps and their associated parameters are supplied on the command line.

More Information

<http://www.usadellab.org/cms/?page=trimmomatic>

Available Versions:

<code>0.38-Java-1.8</code>
<code>0.39-Java-1.8</code>

1.466 Trinity

Description

Trinity represents a novel method for the efficient and robust de novo reconstruction of transcriptomes from RNA-Seq data. Trinity combines three independent software modules: Inchworm, Chrysalis, and Butterfly, applied sequentially to process large volumes of RNA-Seq reads.

More Information

<https://trinityrnaseq.github.io>

Available Versions:

<code>2.10.0-foss-2019b-Python-3.7.4</code>
<code>2.12.0-foss-2019b-Python-3.7.4</code>
<code>2.14.0-foss-2019b-Python-3.7.4</code>
<code>2.13.2-foss-2019b-Python-3.7.4</code>

1.467 TwoBit

Available Versions:

<code>2022</code>

1.468 UCC

Description

UCC (Unified Collective Communication) is a collective communication operations API and library that is flexible, complete, and feature-rich for current and emerging programming models and runtimes.

More Information

<https://www.openucx.org/>

Available Versions:

```
1.1.0-GCCcore-12.2.0
1.0.0-GCCcore-11.3.0
```

1.469 UCX

Description

Unified Communication XAn open-source production grade communication framework for data centricand high-performance applications

More Information

<https://www.openucx.org/>

Available Versions:

```
1.10.0-GCCcore-10.3.0
1.8.0-GCCcore-9.3.0-CUDA-11.0.2
1.9.0-GCCcore-10.3.0-CUDA-11.1.1
1.8.0-GCCcore-9.3.0
1.11.2-GCCcore-11.2.0
1.9.0-GCCcore-10.2.0
1.13.1-GCCcore-12.2.0
1.12.1-GCCcore-11.3.0
1.9.0-GCCcore-10.2.0-CUDA-11.1.1
```

1.470 UCX-CUDA

Description

Unified Communication XAn open-source production grade communication framework for data centricand high-performance applicationsThis module adds the UCX CUDA support.

More Information

<http://www.openucx.org/>

Available Versions:

```
1.12.1-GCCcore-11.3.0-CUDA-11.7.0
1.11.2-GCCcore-11.2.0-CUDA-11.4.1
1.10.0-GCCcore-10.3.0-CUDA-11.3.1
```

1.471 UDUNITS

Description

UDUNITS supports conversion of unit specifications between formatted and binary forms, arithmetic manipulation of units, and conversion of values between compatible scales of measurement.

More Information

<https://www.unidata.ucar.edu/software/udunits/>

Available Versions:

```
2.2.26-GCCcore-8.3.0
2.2.28-GCCcore-10.3.0
2.2.28-GCCcore-11.2.0
2.2.28-GCCcore-12.2.0
2.2.26-GCCcore-10.2.0
2.2.26-foss-2020a
2.2.28-GCCcore-11.3.0
```

1.472 UFL

Description

The Unified Form Language (UFL) is a domain specific language for declaration of finite element discretizations of variational forms. More precisely, it defines a flexible interface for choosing finite element spaces and defining expressions for weak forms in a notation close to mathematical notation.

More Information

<https://bitbucket.org/fenics-project/ufl>

Available Versions:

```
2019.1.0-foss-2019b-Python-3.7.4
```

1.473 UMI-tools

Description

Tools for handling Unique Molecular Identifiers in NGS data sets

More Information

<https://umi-tools.readthedocs.io>

Available Versions:

```
1.0.1-foss-2020a-Python-3.8.2
```

1.474 UNICOR

Available Versions:

3.00

1.475 UnZip

Description

UnZip is an extraction utility for archives compressed in .zip format (also called “zipfiles”). Although highly compatible both with PKWARE’s PKZIP and PKUNZIP utilities for MS-DOS and with Info-ZIP’s own Zip program, our primary objectives have been portability and non-MSDOS functionality.

More Information

<http://www.info-zip.org/UnZip.html>

Available Versions:

6.0-GCCcore-11.2.0
6.0-GCCcore-11.3.0
6.0-GCCcore-10.2.0
6.0-GCCcore-10.3.0
6.0-GCCcore-12.2.0
6.0-GCCcore-9.3.0

1.476 V8

Description

R interface to Google’s open source JavaScript engine

More Information

<https://cran.r-project.org/web/packages/V8/>

Available Versions:

2.2-foss-2020a-R-4.0.2
3.6.0-foss-2021b-R-4.1.2
3.6.0-foss-2021b-R-4.2.1
3.6.0-foss-2022a-R-4.2.1
3.6.0-foss-2021a-R-4.1.0
3.6.0-foss-2022a-R-4.2.2

1.477 VASP

Available Versions:

1.0-info

1.478 VCF-kit

Description

VCF-kit is a command-line based collection of utilities for performing analysis on Variant Call Format (VCF) files.

More Information

<https://github.com/AndersenLab/VCF-kit>

Available Versions:

0.1.6-foss-2018b-Python-2.7.15

1.479 VCFtools

Description

The aim of VCFtools is to provide easily accessible methods for working with complex genetic variation data in the form of VCF files.

More Information

<https://vcftools.github.io>

Available Versions:

0.1.16-GCC-9.3.0
0.1.16-GCC-11.2.0

1.480 VMD

Description

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

More Information

<https://www.ks.uiuc.edu/Research/vmd>

Available Versions:

1.9.4a51-foss-2020b

1.481 VTK

Description

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.

More Information

<https://www.vtk.org>

Available Versions:

```
8.2.0-foss-2019b-Python-3.7.4
9.1.0-foss-2021b
8.2.0-intel-2020a-Python-3.8.2
8.2.0-foss-2020a-Python-3.8.2
9.0.1-foss-2021a
```

1.482 VTune

Description

Intel VTune Amplifier XE is the premier performance profiler for C, C++, C#, Fortran, Assembly and Java.

More Information

<https://software.intel.com/en-us/vtune>

Available Versions:

```
2019_update5
2021.9.0
2020_update3
```

1.483 Valgrind

Description

Valgrind: Debugging and profiling tools

More Information

<http://valgrind.org>

Available Versions:

```
3.14.0-foss-2018b
3.16.1-gompi-2020a
3.20.0-gompi-2022a
3.16.1-iimpi-2020a
3.17.0-gompi-2021a
```

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3.19.0-gompi-2022a
3.18.1-gompi-2021b

1.484 Vampire

Available Versions:

6.0
5.0

1.485 Velvet

Description

Sequence assembler for very short reads

More Information

<http://www.ebi.ac.uk/~zerbino/velvet/>

Available Versions:

1.2.10-foss-2018b-mt-kmer_191

1.486 Vim

Description

Vim is an advanced text editor that seeks to provide the power of the de-facto Unix editor 'Vi', with a more complete feature set.

More Information

<http://www.vim.org>

Available Versions:

8.1.1209-GCCcore-8.2.0-Python-3.7.2

1.487 Voro++

Description

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.

More Information

<http://math.lbl.gov/voro++/>

Available Versions:

```
0.4.6-GCCcore-9.3.0
0.4.6-GCCcore-10.3.0
0.4.6-GCCcore-11.2.0
```

1.488 WIEN2k

Description

The program package WIEN2k allows to perform electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. WIEN2k is an all-electron scheme including relativistic effects and has many features.

More Information

<http://www.wien2k.at/>

Available Versions:

```
21.1-intel-2021a
1.0-info
21.1-JP-intel-2021a
```

1.489 Wannier90

Description

A tool for obtaining maximally-localised Wannier functions

More Information

<http://www.wannier.org>

Available Versions:

```
3.1.0-intel-2021b
3.1.0-foss-2020b
3.1.0-foss-2021b
3.1.0-intel-2020a
3.1.0-foss-2021a
```

1.490 WannierTools

Description

WannierTools is an open source software that studies the physical properties of given tight-binding model.

More Information

<http://www.wanniertools.com>

Available Versions:

```
2.5.1-intel-2020b
2.5.1-intel-2021b
```

1.491 Wayland

Description

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.

More Information

<https://wayland.freedesktop.org/>

Available Versions:

```
1.21.0-GCCcore-11.2.0
1.20.0-GCCcore-11.3.0
```

1.492 Waylandpp

Description

Wayland is an object oriented display protocol, which features request and events. Requests can be seen as method calls on certain objects, whereas events can be seen as signals of an object. This makes the Wayland protocol a perfect candidate for a C++ binding. The goal of this library is to create such a C++ binding for Wayland using the most modern C++ technology currently available, providing an easy to use C++ API to Wayland.

More Information

<https://github.com/NilsBrause/waylandpp>

Available Versions:

```
1.0.0-GCCcore-11.2.0
```

1.493 WebKitGTK+

Description

WebKitGTK+ is a full-featured port of the WebKitrendering engine, suitable for projects requiring any kind of webintegration, from hybrid HTML/CSS applications to full-fledged webbrowsers. It offers WebKit's full functionality and is useful in a widerange of systems from desktop computers to embedded systems like phones,tablets, and televisions.

More Information

<https://webkitgtk.org/>

Available Versions:

2.37.1-GCC-11.2.0

1.494 X11

Description

The X Window System (X11) is a windowing system for bitmap displays

More Information

<https://www.x.org>

Available Versions:

20180604-GCCcore-7.3.0
 20220504-GCCcore-11.3.0
 20200222-GCCcore-9.3.0
 20190717-GCCcore-9.3.0
 20201008-GCCcore-10.2.0
 20190311-GCCcore-8.2.0
 20210802-GCCcore-11.2.0
 20221110-GCCcore-12.2.0
 20210518-GCCcore-10.3.0
 20190717-GCCcore-8.3.0

1.495 XCFun

Description

XCFun is a library of DFT exchange-correlation (XC) functionals. It is based on automatic differentiation and can therefore generate arbitrary order derivatives of these functionals.

More Information

<http://dftlibs.org/xcfun/>

Available Versions:

20190127-foss-2020a-Python-3.8.2
 20190127-foss-2019a-Python-3.7.2
 2.1.1-GCCcore-10.3.0

1.496 XCfun

Description

XCfun is a library of DFT exchange-correlation (XC) functionals. It is based on automatic differentiation and can therefore generate arbitrary order derivatives of these functionals.

More Information

<http://dftlibs.org/xcfun/>

Available Versions:

20190127-foss-2019a-Python-3.7.2

1.497 XCrySDen

Description

XCrySDen is a crystalline and molecular structure visualisation program aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated.

More Information

<http://www.xcrysdn.org/>

Available Versions:

1.6.2-foss-2019b

1.498 XMDS2

Description

The purpose of XMDS2 is to simplify the process of creating simulations that solve systems of initial-value first-order partial and ordinary differential equations.

More Information

<http://www.xmds.org/>

Available Versions:

2.2.3-foss-2018b-Python-2.7.15
3.1.0-foss-2020a-Python-3.8.2

1.499 XML-LibXML

Description

Perl binding for libxml2

More Information

<https://metacpan.org/pod/distribution/XML-LibXML/LibXML.pod>

Available Versions:

```
2.0207-GCCcore-11.2.0
2.0207-GCCcore-10.3.0
2.0207-GCCcore-11.3.0
2.0205-GCCcore-9.3.0
```

1.500 XML-Parser

Description

This is a Perl extension interface to James Clark's XML parser, expat.

More Information

<http://search.cpan.org/~toddr/XML-Parser-2.41/>

Available Versions:

```
2.44_01-GCCcore-7.3.0-Perl-5.28.0
```

1.501 XZ

Description

xz: XZ utilities

More Information

<https://tukaani.org/xz/>

Available Versions:

```
5.2.4-GCCcore-7.3.0
5.2.4-GCCcore-9.3.0
5.2.7-GCCcore-12.2.0
5.2.4-GCCcore-8.3.0
5.2.5-GCCcore-11.3.0
5.2.4-GCCcore-10.2.0
5.2.5-GCCcore-10.3.0
5.2.5-GCCcore-11.2.0
5.2.5-GCCcore-9.3.0
5.2.5-GCCcore-10.2.0
5.2.4-GCCcore-8.2.0
```

1.502 Xvfb

Description

Xvfb is an X server that can run on machines with no display hardware and no physical input devices. It emulates a dumb framebuffer using virtual memory.

More Information

<https://www.x.org/releases/X11R7.6/doc/man/man1/Xvfb.1.xhtml>

Available Versions:

```
1.20.13-GCCcore-11.2.0
1.20.11-GCCcore-10.3.0
21.1.3-GCCcore-11.3.0
1.20.9-GCCcore-10.2.0
21.1.6-GCCcore-12.2.0
```

1.503 YAXT

Description

Yet Another eXchange Tool

More Information

<https://www.dkrz.de/redmine/projects/yaxt>

Available Versions:

```
0.9.0-gompi-2020b
```

1.504 Yasm

Description

Yasm: Complete rewrite of the NASM assembler with BSD license

More Information

<http://www.tortall.net/projects/yasm/>

Available Versions:

```
1.3.0-GCCcore-8.2.0
1.3.0-GCCcore-10.3.0
1.3.0-GCCcore-11.2.0
1.3.0-GCCcore-8.3.0
1.3.0-GCCcore-11.3.0
1.3.0-GCCcore-10.2.0
1.3.0-GCCcore-9.3.0
```


1.505 Z3

Description

Z3 is a theorem prover from Microsoft Research.

More Information

<https://github.com/Z3Prover/z3>

Available Versions:

4.8.10-GCCcore-10.2.0

1.506 ZeroMQ

Description

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.

More Information

<https://www.zeromq.org/>

Available Versions:

4.3.2-GCCcore-8.3.0
 4.3.2-GCCcore-9.3.0
 4.3.4-GCCcore-11.3.0
 4.3.3-GCCcore-10.2.0
 4.3.4-GCCcore-11.2.0
 4.3.4-GCCcore-10.3.0

1.507 Zip

Description

Zip is a compression and file packaging/archive utility. Although highly compatible both with PKWARE's PKZIP and PKUNZIP utilities for MS-DOS and with Info-ZIP's own UnZip, our primary objectives have been portability and other-than-MSDOS functionality.

More Information

<http://www.info-zip.org/Zip.html>

Available Versions:

3.0-GCCcore-8.3.0
 3.0-GCCcore-10.2.0
 3.0-GCCcore-11.2.0

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3.0-GCCcore-10.3.0
3.0-GCCcore-9.3.0

1.508 aiohttp

Description

Asynchronous HTTP client/server framework for asyncio and Python.

More Information

<https://github.com/aio-libs/aiohttp>

Available Versions:

3.8.1-GCCcore-11.2.0

1.509 angsd

Description

Program for analysing NGS data.

More Information

<http://www.popgen.dk/angsd>

Available Versions:

0.935-GCC-10.2.0
0.933-GCC-8.3.0
0.925-foss-2018b

1.510 annovar

Description

ANNOVAR is an efficient software tool to utilize update-to-date information to functionally annotate genetic variants detected from diverse genomes (including human genome hg18, hg19, hg38, as well as mouse, worm, fly, yeast and many others).

More Information

<http://annovar.openbioinformatics.org/en/latest/>

Available Versions:

20191024-GCCcore-8.3.0-Perl-5.28.1

1.511 ant

Description

Apache Ant is a Java library and command-line tool whose mission is to drive processes described in build files as targets and extension points dependent upon each other. The main known usage of Ant is the build of Java applications.

More Information

<https://ant.apache.org/>

Available Versions:

```
1.10.12-Java-11
1.10.9-Java-11
1.10.7-Java-11
1.10.11-Java-11
1.10.8-Java-11
```

1.512 any2fasta

Description

Convert various sequence formats to FASTA

More Information

<https://github.com/tseemann/any2fasta>

Available Versions:

```
0.4.2-GCCcore-11.2.0
```

1.513 archspec

Description

A library for detecting, labeling, and reasoning about microarchitectures

More Information

<https://github.com/archspec/archspec>

Available Versions:

```
0.1.0-GCCcore-9.3.0-Python-3.8.2
0.1.3-GCCcore-11.2.0
0.1.2-GCCcore-10.3.0
```

1.514 aria2

Description

aria2 is a lightweight multi-protocol & multi-source command-line download utility.

More Information

<https://aria2.github.io>

Available Versions:

1.35.0-GCCcore-10.3.0

1.515 arpack-ng

Description

ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.

More Information

<https://github.com/opencollab/arpack-ng>

Available Versions:

3.7.0-foss-2019b
3.7.0-intel-2020a
3.7.0-foss-2020a
3.8.0-foss-2021b

1.516 arrow-R

Description

R interface to the Apache Arrow C++ library

More Information

<https://cran.r-project.org/web/packages/arrow>

Available Versions:

6.0.0.2-foss-2021b-R-4.1.2
8.0.0-foss-2022a-R-4.2.1

1.517 at-spi2-atk

Description

AT-SPI 2 toolkit bridge

More Information

<https://wiki.gnome.org/Accessibility>

Available Versions:

```
2.32.0-GCCcore-8.2.0
2.34.1-GCCcore-8.3.0
2.38.0-GCCcore-10.2.0
2.38.0-GCCcore-11.2.0
2.38.0-GCCcore-11.3.0
```

1.518 at-spi2-core

Description

Assistive Technology Service Provider Interface.

More Information

<https://wiki.gnome.org/Accessibility>

Available Versions:

```
2.32.0-GCCcore-8.2.0
2.40.3-GCCcore-11.2.0
2.44.1-GCCcore-11.3.0
2.34.0-GCCcore-8.3.0
2.38.0-GCCcore-10.2.0
```

1.519 attrdict3

Description

AttrDict is a Python library that provides mapping objects that allow their elements to be accessed both as keys and as attributes.

More Information

<https://github.com/pirofti/AttrDict3>

Available Versions:

```
2.0.2-GCCcore-11.2.0
```

1.520 autode

Description

autodE is a Python module initially designed for the automated calculation of reaction profiles from SMILES strings of reactant(s) and product(s). Current features include: transition state location, conformer searching, atom mapping, Python wrappers for a range of electronic structure theory codes, SMILES parsing, association complex generation, and reaction profile generation.

More Information

<https://github.com/duartegroup/autodE>

Available Versions:

1.3.3

1.521 bcl2fastq2

Description

bcl2fastq Conversion Software both demultiplexes data and converts BCL files generated by Illumina sequencing systems to standard FASTQ file formats for downstream analysis.

More Information

https://support.illumina.com/sequencing/sequencing_software/bcl2fastq-conversion-software.html

Available Versions:

2.20.0-GCC-10.2.0
2.20.0-foss-2018b

1.522 beagle-lib

Description

beagle-lib is a high-performance library that can perform the core calculations at the heart of most Bayesian and Maximum Likelihood phylogenetics packages.

More Information

<https://github.com/beagle-dev/beagle-lib>

Available Versions:

3.1.2-GCC-10.2.0
3.1.2-GCC-8.2.0-2.31.1
3.1.2-GCC-7.3.0-2.30

1.523 binutils

Description

binutils: GNU binary utilities

More Information

<https://directory.fsf.org/project/binutils/>

Available Versions:

```
2.31.1
2.39-GCCcore-12.2.0
2.32
2.27
2.39
2.38
2.31.1-GCCcore-8.2.0
2.38-GCCcore-11.3.0
2.35
2.36.1-GCCcore-10.3.0
2.36.1
2.35-GCCcore-10.2.0
2.34
2.34-GCCcore-9.3.0
2.31.1-GCCcore-8.3.0
2.25
2.26
2.30-GCCcore-7.3.0
2.30-GCCcore-8.1.0
2.32-GCCcore-8.3.0
2.30
2.37
2.37-GCCcore-11.2.0
2.28
2.32-GCCcore-9.3.0
```

1.524 bokeh

Description

Statistical and novel interactive HTML plots for Python

More Information

<https://github.com/bokeh/bokeh>

Available Versions:

```
2.4.3-foss-2022a
2.2.3-foss-2020b
2.2.3-fosscuda-2020b
1.4.0-foss-2019b-Python-3.7.4
```

1.525 breseq

Description

breseq is a computational pipeline for the analysis of short-read re-sequencing data

More Information

<https://barricklab.org/breseq>

Available Versions:

0.36.1-foss-2021b

1.526 bwidget

Description

The BWidget Toolkit is a high-level Widget Set for Tcl/Tk built using native Tcl/Tk 8.x namespaces.

More Information

<https://core.tcl-lang.org/bwidget/home>

Available Versions:

1.9.13-GCCcore-8.2.0
1.9.14-GCCcore-8.3.0

1.527 bzip2

Description

bzip2 is a freely available, patent free, high-quality data compressor. It typically compresses files to within 10% to 15% of the best available techniques (the PPM family of statistical compressors), whilst being around twice as fast at compression and six times faster at decompression.

More Information

<https://sourceware.org/bzip2>

Available Versions:

1.0.6-GCCcore-8.3.0
1.0.8-GCCcore-11.2.0
1.0.6-GCCcore-8.2.0
1.0.8-GCCcore-8.3.0
1.0.8-GCCcore-7.3.0
1.0.8-GCCcore-9.3.0
1.0.6-GCCcore-7.3.0
1.0.6-GCCcore-10.2.0
1.0.8-GCCcore-11.3.0
1.0.8-GCCcore-10.2.0
1.0.8-GCCcore-12.2.0
1.0.8-GCCcore-10.3.0

1.528 c-ares

Description

c-ares is a C library for asynchronous DNS requests (including name resolves)

More Information

<https://c-ares.haxx.se>

Available Versions:

```
1.17.2-GCCcore-10.3.0
1.18.1-GCCcore-11.2.0
```

1.529 c2x

Available Versions:

```
2.40
```

1.530 cURL

Description

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.

More Information

<https://curl.haxx.se>

Available Versions:

```
7.72.0-GCCcore-10.2.0
7.63.0-GCCcore-8.2.0
7.60.0-GCCcore-7.3.0
7.86.0-GCCcore-12.2.0
7.78.0-GCCcore-11.2.0
7.60.0-GCCcore-10.2.0
7.66.0-GCCcore-7.3.0
7.76.0-GCCcore-10.3.0
7.83.0-GCCcore-11.3.0
7.66.0-GCCcore-8.3.0
7.69.1-GCCcore-9.3.0
```

1.531 cairo

Description

Cairo is a 2D graphics library with support for multiple output devices. Currently supported output targets include the X Window System (via both Xlib and XCB), Quartz, Win32, image buffers, PostScript, PDF, and SVG file output. Experimental backends include OpenGL, BeOS, OS/2, and DirectFB

More Information

<https://cairographics.org>

Available Versions:

```
1.16.0-GCCcore-9.3.0
1.17.4-GCCcore-12.2.0
1.16.0-GCCcore-8.2.0
1.16.0-GCCcore-10.3.0
1.16.0-GCCcore-8.3.0
1.16.0-GCCcore-11.2.0
1.17.4-GCCcore-11.3.0
1.14.12-GCCcore-7.3.0
1.16.0-GCCcore-10.2.0
```

1.532 ccache

Description

Ccache (or “ccache”) is a compiler cache. It speeds up recompilation by caching previous compilations and detecting when the same compilation is being done again

More Information

<https://ccache.dev/>

Available Versions:

```
4.6.1-GCCcore-11.2.0
```

1.533 cfx

Available Versions:

```
2021R2
```

1.534 chewBBACA

Description

chewBBACA stands for “BSR-Based Allele Calling Algorithm”.chewBBACA is a comprehensive pipeline including a set of functions for thecreation and validation of whole genome and core genome MultiLocus SequenceTyping (wg/cgMLST) schemas, providing an allele calling algorithm based on BlastScore Ratio that can be run in multiprocessor settings and a set of functions tovisualize and validate allele variation in the loci.

More Information

<https://github.com/B-UMMI/chewBBACA>

Available Versions:

2.5.5-intel-2020a-Python-3.8.2

1.535 colossalai

Description

Colossal-AI: A Unified Deep Learning System for Big Model Era

More Information

<https://colossalai.org/>

Available Versions:

0.1.8-foss-2021a-CUDA-11.3.1

1.536 configurable-http-proxy

Description

HTTP proxy for node.js including a REST API for updating the routing table. Developed as a part of the Jupyter Hub multi-user server.

More Information

<https://github.com/jupyterhub/configurable-http-proxy>

Available Versions:

4.2.1-GCCcore-10.2.0

1.537 constraint

Description

The Python constraint module offers solvers for Constraint Satisfaction Problems (CSPs) over finite domains in simple and pure Python. CSP is class of problems which may be represented in terms of variables (a, b, ...), domains (a in [1, 2, 3], ...), and constraints (a < b, ...).

More Information

<https://github.com/python-constraint/python-constraint>

Available Versions:

1.4.0-foss-2020a-Python-3.8.2

1.538 cppy

Description

A small C++ header library which makes it easier to write Python extension modules. The primary feature is a PyObject smart pointer which automatically handles reference counting and provides convenience methods for performing common object operations.

More Information

<https://github.com/nucleic/cppy>

Available Versions:

1.2.1-GCCcore-11.3.0
1.1.0-GCCcore-11.2.0

1.539 crest

Description

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 analysis of structure ensembles.

More Information

<https://xtb-docs.readthedocs.io/en/latest/crest.html>

Available Versions:

2.10.2

1.540 cuDNN

Description

The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.

More Information

<https://developer.nvidia.com/cudnn>

Available Versions:

```
8.1.1.33-CUDA-11.2.2
7.6.4.38-gccuda-2019b
8.0.4.30-CUDA-11.1.1
8.2.1.32-CUDA-11.3.1
8.0.4.30-CUDA-11.0.2
8.4.1.50-CUDA-11.7.0
8.2.2.26-CUDA-11.4.1
```

1.541 cutadapt

Description

Cutadapt finds and removes adapter sequences, primers, poly-A tails and other types of unwanted sequence from your high-throughput sequencing reads.

More Information

<https://opensource.scilifelab.se/projects/cutadapt/>

Available Versions:

```
4.2-GCCcore-11.3.0
1.18-foss-2018b-Python-3.6.6
3.5-GCCcore-11.2.0
4.3-GCCcore-11.3.0
2.7-GCCcore-8.3.0-Python-3.7.4
```

1.542 cylv

Available Versions:

```
7.8.7
```

1.543 dask

Description

Dask natively scales Python. Dask provides advanced parallelism for analytics, enabling performance at scale for the tools you love.

More Information

<https://dask.org/>

Available Versions:

```
2022.10.0-foss-2022a
2021.2.0-fosscuda-2020b
2.8.0-foss-2019b-Python-3.7.4
2021.2.0-foss-2020b
```

1.544 datamash

Description

GNU datamash performs basic numeric, textual and statistical operations on input data files

More Information

<https://www.gnu.org/software/datamash/>

Available Versions:

```
1.5-GCCcore-10.2.0
```

1.545 dbus-glib

Description

D-Bus is a message bus system, a simple way for applications to talk to one another.

More Information

<https://dbus.freedesktop.org/doc/dbus-glib>

Available Versions:

```
0.110-GCCcore-8.3.0
0.112-GCCcore-11.2.0
```

1.546 deepdiff

Description

DeepDiff: Deep Difference of dictionaries, iterables and almost any other object recursively.

More Information

<https://deepdiff.readthedocs.io/en/latest/>

Available Versions:

4.0.6-GCCcore-8.2.0-Python-3.7.2

1.547 dftd4

Available Versions:

3.4.0
3.4.0-keep

1.548 dijitso

Description

dijitso is a Python module for distributed just-in-time shared library building.

More Information

<https://bitbucket.org/fenics-project/dijitso>

Available Versions:

2019.1.0-foss-2019b-Python-3.7.4

1.549 dill

Description

dill extends python's pickle module for serializing and de-serializing python objects to the majority of the built-in python types. Serialization is the process of converting an object to a byte stream, and the inverse of which is converting a byte stream back to on python object hierarchy.

More Information

<https://pypi.org/project/dill/>

Available Versions:

0.3.4-GCCcore-11.2.0
0.3.4-GCCcore-10.3.0
0.3.3-foss-2020a-Python-3.8.2

1.550 dm-tree

Description

dm-tree provides tree, a library for working with nested data structures. In a way, tree generalizes the builtin map function which only supports flat sequences, and allows to apply a function to each “leaf” preserving the overall structure.

More Information

<https://github.com/deepmind/tree>

Available Versions:

```
0.1.6-GCCcore-10.3.0
0.1.6-GCCcore-11.2.0
0.1.5-GCCcore-10.2.0
```

1.551 dmd

Available Versions:

```
2
```

1.552 dot

Available Versions:

1.553 double-conversion

Description

Efficient binary-decimal and decimal-binary conversion routines for IEEE doubles.

More Information

<https://github.com/google/double-conversion>

Available Versions:

```
3.1.4-GCCcore-8.3.0
3.2.0-GCCcore-11.3.0
3.1.5-GCCcore-11.2.0
3.1.5-GCCcore-10.3.0
3.1.5-GCCcore-9.3.0
3.1.5-GCCcore-10.2.0
```


1.554 ecCodes

Description

ecCodes is a package developed by ECMWF which provides an application programming interface and a set of tools for decoding and encoding messages in the following formats: WMO FM-92 GRIB edition 1 and edition 2, WMO FM-94 BUFR edition 3 and edition 4, WMO GTS abbreviated header (only decoding).

More Information

<https://software.ecmwf.int/wiki/display/ECC/ecCodes+Home>

Available Versions:

2.20.0-gompi-2020b

1.555 eilmer

Available Versions:

4.0-9c87a327

1.556 einops

Description

Flexible and powerful tensor operations for readable and reliable code. Supports numpy, pytorch, tensorflow, jax, and others.

More Information

<https://einops.rocks/>

Available Versions:

0.4.1-GCCcore-10.3.0

1.557 elfutils

Description

The elfutils project provides libraries and tools for ELF files and DWARF data.

More Information

<https://elfutils.org/>

Available Versions:

0.185-GCCcore-8.3.0

0.183-GCCcore-10.2.0

0.187-GCCcore-11.3.0

1.558 enaBrowserTools

Description

enaBrowserTools is a set of scripts that interface with the ENA web services to download data from ENA easily, without any knowledge of scripting required.

More Information

<https://github.com/enasequence/enaBrowserTools/>

Available Versions:

1.6-GCCcore-8.2.0-Python-3.7.2

1.559 enchant-2

Description

Enchant aims to provide a simple but comprehensive abstraction for dealing with different spell checking libraries in a consistent way. A client, such as a text editor or word processor, need not know anything about a specific spell-checker, and since all back-ends are plugins, new spell-checkers can be added without needing any change to the program using Enchant.

More Information

<https://github.com/AbiWord/enchant>

Available Versions:

2.3.3-GCCcore-11.2.0

1.560 exiv2

Description

Exiv2 is a Cross-platform C++ library and a command line utility to manage image metadata.

More Information

<https://exiv2.org>

Available Versions:

0.27.5-GCCcore-11.2.0

1.561 expat

Description

Expat is an XML parser library written in C. It is a stream-oriented parser in which an application registers handlers for things the parser might find in the XML document (like start tags)

More Information

<https://libexpat.github.io>

Available Versions:

```
2.4.8-GCCcore-11.3.0
2.2.9-GCCcore-9.3.0
2.2.5-GCCcore-7.3.0
2.2.7-GCCcore-7.3.0
2.2.5-GCCcore-10.2.0
2.2.5-GCCcore-8.1.0
2.2.6-GCCcore-8.2.0
2.4.1-GCCcore-11.2.0
2.2.7-GCCcore-9.3.0
2.2.9-GCCcore-10.2.0
2.2.7-GCCcore-8.3.0
2.2.6-GCCcore-8.3.0
2.4.9-GCCcore-12.2.0
2.2.9-GCCcore-10.3.0
```

1.562 expecttest

Description

This library implements expect tests (also known as “golden” tests). Expect tests are a method of writing tests where instead of hard-coding the expected output of a test, you run the test to get the output, and the test framework automatically populates the expected output. If the output of the test changes, you can rerun the test with the environment variable EXPECTTEST_ACCEPT=1 to automatically update the expected output.

More Information

<https://github.com/ezyang/expecttest>

Available Versions:

```
0.1.3-GCCcore-11.3.0
0.1.3-GCCcore-10.3.0
```

1.563 fast-gbs

Available Versions:

v2

1.564 fastahack

Description

Utilities for indexing and sequence extraction from FASTA files.

More Information

<https://github.com/ekg/fastahack>

Available Versions:

1.0.0-GCCcore-11.2.0

1.565 fdmnes

Available Versions:

2021-08-10

1.566 fdmnes-parallel

Available Versions:

2021-08-10

1.567 fermi-lite

Description

Standalone C library for assembling Illumina short reads in small regions.

More Information

<https://github.com/lh3/fermi-lite>

Available Versions:

20190320-GCCcore-11.2.0

1.568 file

Description

The file command is ‘a file type guesser’, that is, a command-line tool that tells you in words what kind of data a file contains.

More Information

<https://www.darwinsys.com/file/>

Available Versions:

```
5.39-GCCcore-10.2.0
5.35-GCCcore-7.3.0
5.43-GCCcore-11.3.0
```

1.569 filevercmp

Description

filevercmp function as in sort –version-sort.

More Information

<https://github.com/ekg/filevercmp>

Available Versions:

```
20191210-GCCcore-11.2.0
```

1.570 fineRADstructure

Description

A package for population structure inference from RAD-seq data

More Information

<http://cichlid.gurdon.cam.ac.uk/fineRADstructure.html>

Available Versions:

```
20180709-intel-2020a
```

1.571 fineSTRUCTURE

Description

fineSTRUCTURE is a fast and powerful algorithm for identifying population structure using dense sequencing data.

More Information

https://people.maths.bris.ac.uk/~madjl/finestructure/finestructure_info.html

Available Versions:

2.1.3-intel-2020a

1.572 flappie

Available Versions:

2.1.3

1.573 flatbuffers

Description

FlatBuffers: Memory Efficient Serialization Library

More Information

<https://github.com/google/flatbuffers/>

Available Versions:

2.0.0-GCCcore-10.3.0
1.12.0-GCCcore-9.3.0
1.12.0-GCCcore-8.3.0
2.0.0-GCCcore-11.2.0
1.12.0-GCCcore-10.2.0

1.574 flatbuffers-python

Description

Python Flatbuffers runtime library.

More Information

<https://github.com/google/flatbuffers/>

Available Versions:

1.12-GCCcore-10.2.0
2.0-GCCcore-11.2.0
2.0-GCCcore-10.3.0

1.575 flex

Description

Flex (Fast Lexical Analyzer) is a tool for generating scanners. A scanner, sometimes called a tokenizer, is a program which recognizes lexical patterns in text.

More Information

<http://flex.sourceforge.net/>

Available Versions:

```
2.6.4
2.6.4-GCCcore-8.3.0
2.6.3
2.6.4-GCCcore-12.2.0
2.6.4-GCCcore-7.3.0
2.6.0
2.6.4-GCCcore-10.2.0
2.6.4-GCCcore-11.2.0
2.5.39-GCCcore-8.3.0
2.6.4-GCCcore-10.3.0
2.5.39
2.6.4-GCCcore-8.2.0
2.6.4-GCCcore-8.1.0
2.6.4-GCCcore-9.3.0
2.6.4-GCCcore-11.3.0
```

1.576 fluent

Available Versions:

```
2021R2
```

1.577 fontconfig

Description

Fontconfig is a library designed to provide system-wide font configuration, customization and application access.

More Information

<https://www.freedesktop.org/wiki/Software/fontconfig/>

Available Versions:

```
2.13.92-GCCcore-9.3.0
2.13.1-GCCcore-8.2.0
2.13.93-GCCcore-10.3.0
2.14.1-GCCcore-12.2.0
2.13.1-GCCcore-9.3.0
2.13.94-GCCcore-11.2.0
```

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```
2.14.0-GCCcore-11.3.0
2.13.0-GCCcore-7.3.0
2.13.92-GCCcore-10.2.0
2.13.1-GCCcore-8.3.0
```

1.578 foss

Description

GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support, OpenBLAS (BLAS and LAPACK support), FFTW and ScaLAPACK.

More Information

<https://easybuild.readthedocs.io/en/master/Common-toolchains.html#foss-toolchain>

Available Versions:

```
2019a
2022a
2018b
2020b
2019b
2021b
2021a
2020a
2022b
```

1.579 fosscuda

Description

GCC based compiler toolchain __with CUDA **support**__, and including OpenMPI for MPI support

More Information

(none)

Available Versions:

```
2020g
2020b
2020a
2019b
2018b
```


1.580 freebayes

Description

Bayesian haplotype-based genetic polymorphism discovery and genotyping.

More Information

<https://github.com/freebayes/freebayes>

Available Versions:

1.3.6-foss-2021b-R-4.1.2

1.581 freeglut

Description

freeglut is a completely OpenSourced alternative to the OpenGL Utility Toolkit (GLUT) library.

More Information

<http://freeglut.sourceforge.net/>

Available Versions:

3.2.1-GCCcore-10.3.0
3.2.1-GCCcore-9.3.0
3.2.1-GCCcore-11.2.0
3.2.1-GCCcore-8.3.0

1.582 freetype

Description

FreeType 2 is a software font engine that is designed to be small, efficient, highly customizable, and portable while capable of producing high-quality output (glyph images). It can be used in graphics libraries, display servers, font conversion tools, text image generation tools, and many other products as well.

More Information

<http://freetype.org>

Available Versions:

2.9.1-GCCcore-8.2.0
2.11.0-GCCcore-11.2.0
2.12.1-GCCcore-12.2.0
2.10.1-GCCcore-9.3.0
2.10.4-GCCcore-10.3.0
2.12.1-GCCcore-11.3.0
2.10.1-GCCcore-8.3.0
2.9.1-GCCcore-7.3.0
2.10.3-GCCcore-10.2.0

1.583 fsom

Description

A tiny C library for managing SOM (Self-Organizing Maps) neural networks.

More Information

<https://github.com/ekg/fsom>

Available Versions:

20141119-GCCcore-11.2.0

1.584 garlic

Available Versions:

22

1.585 gawk

Description

The awk utility interprets a special-purpose programming language that makes it possible to handlesimple data-reformatting jobs with just a few lines of code.

More Information

<https://www.gnu.org/software/gawk>

Available Versions:

5.1.1-GCC-11.2.0

1.586 gc

Description

The Boehm-Demers-Weiser conservative garbage collector can be used as a garbage collecting replacement for C malloc or C++ new.

More Information

<https://hboehm.info/gc/>

Available Versions:

7.6.10-GCCcore-8.2.0
8.2.2-GCCcore-11.3.0
8.2.0-GCCcore-11.2.0
7.6.12-GCCcore-9.3.0
7.6.12-GCCcore-8.3.0

1.587 gccuda

Description

GNU Compiler Collection (GCC) based compiler toolchain, along with CUDA toolkit.

More Information

(none)

Available Versions:

2019b
2020b
2020a
2018b

1.588 gdc-client

Description

The gdc-client provides several convenience functions over the GDC API which provides general download/upload via HTTPS.

More Information

<https://gdc.nci.nih.gov/access-data/gdc-data-transfer-tool>

Available Versions:

1.6.0-GCCcore-10.2.0

1.589 geopandas

Description

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.

More Information

<https://github.com/geopandas/geopandas>

Available Versions:

0.8.1-foss-2020a-Python-3.8.2

1.590 geth

Available Versions:

2022

1.591 gettext

Description

GNU ‘gettext’ is an important step for the GNU Translation Project, as it is an asset on which we may build many other steps. This package offers to programmers, translators, and even users, a well integrated set of tools and documentation

More Information

<https://www.gnu.org/software/gettext/>

Available Versions:

0.21.1
0.19.8.1-GCCcore-8.2.0
0.21-GCCcore-10.3.0
0.20.1-GCCcore-9.3.0
0.21-GCCcore-11.2.0
0.19.8.1-GCCcore-7.3.0
0.21-GCCcore-11.3.0
0.21-GCCcore-10.2.0
0.19.8.1
0.21
0.21.1-GCCcore-12.2.0
0.20.1
0.20.1-GCCcore-8.3.0

1.592 gflags

Description

The gflags package contains a C++ library that implements commandline flags processing. It includes built-in support for standard types such as string and the ability to define flags in the source file in which they are used.

More Information

<https://github.com/gflags/gflags>

Available Versions:

2.2.2-GCCcore-8.2.0

1.593 giflib

Description

giflib is a library for reading and writing gif images. It is API and ABI compatible with libungif which was in wide use while the LZW compression algorithm was patented.

More Information

<http://giflib.sourceforge.net/>

Available Versions:

```
5.2.1-GCCcore-10.3.0
5.2.1-GCCcore-9.3.0
5.2.1-GCCcore-11.2.0
5.2.1-GCCcore-8.3.0
5.2.1-GCCcore-11.3.0
5.1.4-GCCcore-8.2.0
5.2.1-GCCcore-10.2.0
```

1.594 git

Description

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.

More Information

<https://git-scm.com/>

Available Versions:

```
2.33.1-GCCcore-11.2.0-nodocs
2.38.1-GCCcore-12.2.0-nodocs
2.32.0-GCCcore-10.3.0-nodocs
2.23.0-GCCcore-8.3.0-nodocs
2.23.0-GCCcore-8.3.0
2.36.0-GCCcore-11.3.0-nodocs
2.23.0-GCCcore-9.3.0-nodocs
2.28.0-GCCcore-10.2.0-nodocs
```

1.595 git-lfs

Description

Git Large File Storage (LFS) replaces large files such as audio samples, videos, datasets, and graphics with text pointers inside Git, while storing the file contents on a remote server like GitHub.com

More Information

<https://git-lfs.github.com>

Available Versions:

2.11.0

1.596 glew

Description

The OpenGL Extension Wrangler LibraryThe OpenGL Extension Wrangler Library (GLEW) is a cross-platform open-source C/C++ extension loading library. GLEW provides efficient run-time mechanisms for determining which OpenGL extensions are supported on the target platform. OpenGL core and extension functionality is exposed in a single header file. GLEW has been tested on a variety of operating systems, including Windows, Linux, Mac OS X, FreeBSD, Irix, and Solaris.

More Information

<http://glew.sourceforge.net/>

Available Versions:

2.1.0-GCCcore-8.3.0
2.1.0-GCCcore-9.3.0
2.2.0-GCCcore-11.2.0-egl

1.597 glib-networking

Description

Network extensions for GLib

More Information

<https://gitlab.gnome.org/GNOME/glib-networking>

Available Versions:

2.72.1-GCCcore-11.2.0

1.598 glog

Description

A C++ implementation of the Google logging module.

More Information

<https://github.com/google/glog>

Available Versions:

0.4.0-GCCcore-8.2.0

1.599 gmpy2

Description

GMP/MPFR, MPFR, and MPC interface to Python 2.6+ and 3.x

More Information

<https://github.com/aleaxit/gmpy>

Available Versions:

```
2.1.0b5-GCC-10.3.0
2.1.0b5-GCC-9.3.0
2.1.0b4-GCC-8.3.0
```

1.600 gmsh

Description

Gmsh is a 3D finite element grid generator with a build-in CAD engine and post-processor.

More Information

<https://gmsh.info/>

Available Versions:

```
4.7.1-intel-2020a-Python-3.8.2
```

1.601 gnuplot

Description

Portable interactive, function plotting utility

More Information

<http://gnuplot.sourceforge.net>

Available Versions:

```
5.4.4-GCCcore-11.3.0
5.4.1-GCCcore-10.2.0
5.4.2-GCCcore-10.3.0
5.2.8-GCCcore-8.3.0
5.4.2-GCCcore-11.2.0
5.2.8-GCCcore-9.3.0
```

1.602 gOMPI

Description

GNU Compiler Collection (GCC) based compiler toolchain, including OpenMPI for MPI support.

More Information

(none)

Available Versions:

2019b
2019b-dba
2019a
2020b
2020a
2021a
2018b
2022a
2021b
2022b

1.603 gOMPIC

Description

GNU Compiler Collection (GCC) based compiler toolchain along with CUDA toolkit, including OpenMPI for MPI support with CUDA features enabled.

More Information

(none)

Available Versions:

2018b
2020a
2019b
2020b

1.604 googletest

Description

Google's framework for writing C++ tests on a variety of platforms

More Information

<https://github.com/google/googletest>

Available Versions:


```
1.10.0-GCCcore-10.2.0
1.11.0-GCCcore-11.3.0
1.11.0-GCCcore-11.2.0
```

1.605 gperf

Description

GNU gperf is a perfect hash function generator. For a given list of strings, it produces a hash function and hash table, in form of C or C++ code, for looking up a value depending on the input string. The hash function is perfect, which means that the hash table has no collisions, and the hash table lookup needs a single string comparison only.

More Information

<https://www.gnu.org/software/gperf/>

Available Versions:

```
3.1-GCCcore-10.3.0
3.1-GCCcore-8.2.0
3.1-GCCcore-12.2.0
3.1-GCCcore-8.3.0
3.1-GCCcore-11.2.0
3.1-GCCcore-11.3.0
3.1-GCCcore-7.3.0
3.1-GCCcore-10.2.0
3.1-GCCcore-9.3.0
```

1.606 gperftools

Description

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.

More Information

<https://github.com/gperftools/gperftools>

Available Versions:

```
2.9.1-GCCcore-10.3.0
2.7.90-GCCcore-8.3.0
```

1.607 graphite2

Description

Graphite is a “smart font” system developed specifically to handle the complexities of lesser-known languages of the world.

More Information

https://scripts.sil.org/cms/scripts/page.php?site_id=projects&item_id=graphite_home

Available Versions:

<code>1.3.14-GCCcore-11.3.0</code> <code>1.3.14-GCCcore-11.2.0</code>
--

1.608 grib_api

Description

The ECMWF GRIB API is an application program interface accessible from C, FORTRAN and Python programs developed for encoding and decoding WMO FM-92 GRIB edition 1 and edition 2 messages. A useful set of command line tools is also provided to give quick access to GRIB messages.

More Information

<https://software.ecmwf.int/wiki/display/GRIB/Home>

Available Versions:

<code>1.24.0-intel-2020b</code>

1.609 groff

Description

Groff (GNU troff) is a typesetting system that reads plain text mixed with formatting commands and produces formatted output.

More Information

<https://www.gnu.org/software/groff>

Available Versions:

<code>1.22.4-GCCcore-9.3.0</code> <code>1.22.4-GCCcore-10.3.0</code> <code>1.22.4-GCCcore-11.2.0</code> <code>1.22.4-GCCcore-11.3.0</code> <code>1.22.4-GCCcore-12.2.0</code>

1.610 gromacs

Available Versions:

2018.4-fosscuda-2019b

1.611 gromacs-cp2k

Available Versions:

2021.1-foss-2020a

1.612 gromos

Available Versions:

1.5.0

1.613 gubbins

Description

Gubbins (Genealogies Unbiased By recomBinations In Nucleotide Sequences) is an algorithm that iteratively identifies loci containing elevated densities of base substitutions while concurrently constructing a phylogeny based on the putative point mutations outside of these regions. Simulations demonstrate the algorithm generates highly accurate reconstructions under realistic models of short-term bacterial evolution, and can be run in only a few hours on alignments of hundreds of bacterial genome sequences.

More Information

<https://sanger-pathogens.github.io/gubbins>

Available Versions:

2.4.0

1.614 gzip

Description

gzip (GNU zip) is a popular data compression program as a replacement for compress

More Information

<https://www.gnu.org/software/gzip/>

Available Versions:

```
1.10-GCCcore-10.2.0
1.10-GCCcore-11.2.0
1.10-GCCcore-10.3.0
1.10-GCCcore-9.3.0
1.12-GCCcore-12.2.0
1.10-GCCcore-8.3.0
1.12-GCCcore-11.3.0
```

1.615 h5py

Description

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.

More Information

<https://www.h5py.org/>

Available Versions:

```
2.10.0-foss-2019b-Python-3.7.4
2.10.0-intel-2020a-Python-3.8.2
2.10.0-fosscuda-2019b-Python-3.7.4
2.9.0-foss-2019a
2.10.0-fosscuda-2020a-Python-3.8.2
3.6.0-foss-2021b
2.10.0-foss-2020a-Python-3.8.2
3.2.1-foss-2021a
3.1.0-fosscuda-2020b
2.8.0-foss-2018b-Python-2.7.15
3.1.0-foss-2020b
```

1.616 help2man

Description

help2man produces simple manual pages from the ‘-help’ and ‘-version’ output of other commands.

More Information

<https://www.gnu.org/software/help2man/>

Available Versions:

```
1.47.7-GCCcore-8.2.0
1.48.3-GCCcore-11.2.0
1.49.2-GCCcore-11.3.0
1.47.4
1.47.16-GCCcore-10.2.0
1.47.6-GCCcore-8.1.0
1.47.4-GCCcore-7.3.0
1.47.12-GCCcore-9.3.0
```

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```
1.49.2-GCCcore-12.2.0
1.47.8-GCCcore-8.3.0
1.48.3-GCCcore-10.3.0
```

1.617 hiredis

Description

Hiredis is a minimalistic C client library for the Redis database. It is minimalistic because it just adds minimal support for the protocol, but at the same time it uses a high level printf-like API in order to make it much higher level than otherwise suggested by its minimal code base and the lack of explicit bindings for every Redis command.

More Information

<https://github.com/redis/hiredis>

Available Versions:

```
1.0.2-GCCcore-11.2.0
```

1.618 hptt

Available Versions:

```
1.0.5
```

1.619 htop

Description

An interactive process viewer for Unix

More Information

<http://hisham.hm/htop/>

Available Versions:

```
2.0.1
```

1.620 hunspell

Description

Hunspell is a spell checker and morphological analyzer library and program designed for languages with rich morphology and complex word compounding or character encoding.

More Information

<http://hunspell.github.io/>

Available Versions:

1.7.1-GCCcore-11.2.0

1.621 hwloc

Description

The Portable Hardware Locality (hwloc) software package provides a portable abstraction (across OS, versions, architectures, ...) of the hierarchical topology of modern architectures, including NUMA memory nodes, sockets, shared caches, cores and simultaneous multithreading. It also gathers various system attributes such as cache and memory information as well as the locality of I/O devices such as network interfaces, InfiniBand HCAs or GPUs. It primarily aims at helping applications with gathering information about modern computing hardware so as to exploit it accordingly and efficiently.

More Information

<https://www.open-mpi.org/projects/hwloc/>

Available Versions:

2.4.1-GCCcore-10.3.0
1.11.12-GCCcore-8.3.0
2.2.0-GCCcore-10.2.0
1.11.10-GCCcore-7.3.0
2.5.0-GCCcore-11.2.0
2.8.0-GCCcore-12.2.0
1.11.12-GCCcore-9.3.0
2.2.0-GCCcore-9.3.0
1.11.11-GCCcore-8.2.0
2.7.1-GCCcore-11.3.0

1.622 hypothesis

Description

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.

More Information

<https://github.com/HypothesisWorks/hypothesis>

Available Versions:

6.46.7-GCCcore-11.3.0
6.13.1-GCCcore-10.3.0
5.41.2-GCCcore-10.2.0
5.41.5-GCCcore-10.2.0
4.44.2-GCCcore-8.3.0-Python-3.7.4
6.14.6-GCCcore-11.2.0
4.23.4-GCCcore-8.2.0

1.623 icc

Description

Intel C and C++ compilers

More Information

<https://software.intel.com/en-us/intel-compilers/>

Available Versions:

```
2019.1.144-GCC-8.2.0-2.31.1
2018.3.222-GCC-7.3.0-2.30
```

1.624 iccifort

Description

Intel C, C++ & Fortran compilers

More Information

<http://software.intel.com/en-us/intel-cluster-toolkit-compiler/>

Available Versions:

```
2019.1.144-GCC-8.2.0-2.31.1
2019.5.281
2018.3.222-GCC-7.3.0-2.30
2020.4.304
2020.1.217
```

1.625 iccifortcuda

Description

Intel C, C++ & Fortran compilers with CUDA toolkit

More Information

(none)

Available Versions:

```
2020b
```

1.626 ifort

Description

Intel Fortran compiler

More Information

<https://software.intel.com/en-us/intel-compilers/>

Available Versions:

2019.1.144-GCC-8.2.0-2.31.1
2018.3.222-GCC-7.3.0-2.30

1.627 iimpi

Description

Intel C/C++ and Fortran compilers, alongside Intel MPI.

More Information

<https://software.intel.com/parallel-studio-xe>

Available Versions:

2022b
2021a
2022.05
2021b
2022a
2020a
2020b

1.628 iimpic

Description

Intel C/C++ and Fortran compilers, alongside Intel MPI and CUDA.

More Information

(none)

Available Versions:

2020b

1.629 imkl

Description

Intel oneAPI Math Kernel Library

More Information

<https://software.intel.com/content/www/us/en/develop/tools/oneapi/components/onemkl.html>

Available Versions:

```
2021.4.0
2020.1.217-gompi-2020a
2022.1.0
2020.4.304-iimpic-2020b
2020.4.304-iimpi-2020b
2021.2.0-iimpi-2021a
2022.2.1
2021.2.0-iompi-2021a
2020.1.217-iimpi-2020a
```

1.630 imkl-FFTW

Description

FFTW interfaces using Intel oneAPI Math Kernel Library

More Information

<https://software.intel.com/content/www/us/en/develop/tools/oneapi/components/onemkl.html>

Available Versions:

```
2022.2.1-iimpi-2022b
2022.1.0-iimpi-2022.05
2021.4.0-iimpi-2021b
2022.1.0-iimpi-2022a
```

1.631 impi

Description

Intel MPI Library, compatible with MPICH ABI

More Information

<https://software.intel.com/en-us/intel-mpi-library/>

Available Versions:

```
2019.7.217-iccifort-2020.1.217
2019.9.304-iccifortcuda-2020b
2021.4.0-intel-compilers-2021.4.0
2019.9.304-iccifort-2020.4.304
```

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```
2021.2.0-intel-compilers-2021.2.0
2021.6.0-intel-compilers-2022.1.0
2021.7.1-intel-compilers-2022.2.1
```

1.632 intel

Description

Compiler toolchain including Intel compilers, Intel MPI and Intel Math Kernel Library (MKL).

More Information

<https://easybuild.readthedocs.io/en/master/Common-toolchains.html#intel-toolchain>

Available Versions:

```
2021b
2020a
2021a
2022b
2022a
2020b
2022.05
```

1.633 intel-compilers

Description

Intel C, C++ & Fortran compilers (classic and oneAPI)

More Information

<https://software.intel.com/content/www/us/en/develop/tools/oneapi/hpc-toolkit.html>

Available Versions:

```
2022.2.1
2022.1.0
2021.2.0
2021.4.0
```

1.634 intelcuda

Description

Intel Cluster Toolkit Compiler Edition provides Intel C/C++ and Fortran compilers, Intel MPI & Intel MKL, with CUDA toolkit

More Information

(none)

Available Versions:

2020b

1.635 intervaltree

Description

An interval tree can be used to efficiently find a set of numeric intervals overlapping or containing another interval. This library provides a basic implementation of an interval tree using C++ templates, allowing the insertion of arbitrary types into the tree.

More Information

<https://github.com/ekg/intervaltree>

Available Versions:

0.1-GCCcore-11.2.0

1.636 intltool

Description

intltool is a set of tools to centralize translation of many different file formats using GNU gettext-compatible PO files.

More Information

<http://freedesktop.org/wiki/Software/intltool/>

Available Versions:

0.51.0-GCCcore-8.2.0
0.51.0-GCCcore-12.2.0
0.51.0-GCCcore-8.3.0
0.51.0-GCCcore-11.3.0
0.51.0-GCCcore-10.2.0
0.51.0-GCCcore-7.3.0-Perl-5.28.0
0.51.0-GCCcore-10.3.0
0.51.0-GCCcore-11.2.0
0.51.0-GCCcore-9.3.0

1.637 iomkl

Description

Compiler toolchain including Intel compilers, Open MPI and Intel Math Kernel Library (MKL).

More Information

<https://software.intel.com/content/www/us/en/develop/tools/oneapi/hpc-toolkit.html>

Available Versions:

2021a

1.638 iompi

Description

Intel C/C++ and Fortran compilers, alongside Open MPI.

More Information

<https://software.intel.com/en-us/intel-cluster-toolkit-compiler/>

Available Versions:

2020b
2021a

1.639 itensor

Available Versions:

3.1.5
3.1.5-omp

1.640 jax

Description

Composable transformations of Python+NumPy programs: differentiate, vectorize, JIT to GPU/TPU, and more

More Information

<https://pypi.python.org/pypi/jax>

Available Versions:

0.3.9-foss-2021a-CUDA-11.3.1
0.3.23-foss-2021b-CUDA-11.4.1
0.2.19-foss-cuda-2020b

1.641 jbigkit

Description

JBIG-KIT is a software implementation of the JBIG1 data compression standard (ITU-T T.82), which was designed for bi-level image data, such as scanned documents.

More Information

<https://www.cl.cam.ac.uk/~mgk25/jbigkit/>

Available Versions:

```
2.1-GCCcore-11.2.0
2.1-GCCcore-11.3.0
2.1-GCCcore-12.2.0
```

1.642 jemalloc

Description

jemalloc is a general purpose malloc(3) implementation that emphasizes fragmentation avoidance and scalable concurrency support.

More Information

<http://jemalloc.net>

Available Versions:

```
5.2.1-GCCcore-10.3.0
5.2.1-GCCcore-8.3.0
5.2.1-GCCcore-11.2.0
5.2.1-GCCcore-10.2.0
```

1.643 jupyter-server

Description

The Jupyter Server provides the backend (i.e. the core services, APIs, and RESTendpoints) for Jupyter web applications like Jupyter notebook, JupyterLab, andVoila.

More Information

<https://jupyter.org/>

Available Versions:

```
1.21.0-GCCcore-11.3.0
```

1.644 kallisto

Description

kallisto is a program for quantifying abundances of transcripts from RNA-Seq data, or more generally of target sequences using high-throughput sequencing reads.

More Information

<https://pachterlab.github.io/kallisto/>

Available Versions:

```
0.46.1-foss-2019b
0.48.0-gompi-2021b
0.46.2-foss-2020b
```

1.645 kim-api

Description

Open Knowledgebase of Interatomic Models.KIM is an API and OpenKIM is a collection of interatomic models (potentials) for atomistic simulations. This is a library that can be used by simulation programs to get access to the models in the OpenKIM database. This EasyBuild only installs the API, the models can be installed with the package `openkim-models`, or the user can install them manually by running `kim-api-collections-management install user MODELNAME` or `kim-api-collections-management install user OpenKIM` to install them all.

More Information

<https://openkim.org/>

Available Versions:

```
2.1.3-foss-2020a
2.2.1-GCCcore-11.2.0
2.2.1-GCCcore-10.3.0
2.1.3-intel-2020a
2.3.0-GCCcore-11.2.0
```

1.646 kwant

Description

Kwant is a free (open source), powerful, and easy to use Python package for numerical calculations on tight-binding models with a strong focus on quantum transport.

More Information

<https://kwant-project.org/>

Available Versions:

```
1.4.1-foss-2019a-Python-3.7.2
```

1.647 libGLU

Description

The OpenGL Utility Library (GLU) is a computer graphics library for OpenGL.

More Information

<https://mesa.freedesktop.org/archive/glu/>

Available Versions:

```
9.0.1-GCCcore-9.3.0
9.0.1-GCCcore-8.3.0
9.0.2-GCCcore-12.2.0
9.0.1-GCCcore-10.3.0
9.0.2-GCCcore-11.2.0
9.0.0-foss-2018b
```

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```
9.0.2-GCCcore-11.3.0
9.0.1-GCCcore-10.2.0
```

1.648 libRmath

Description

The routines supporting the distribution and special functions in R and a few others are declared in C header file Rmath.h. These can be compiled into a standalone library for linking to other applications.

More Information

<https://cran.r-project.org/doc/manuals/r-release/R-admin.html#The-standalone-Rmath-library>

Available Versions:

```
4.1.2-GCCcore-11.2.0
```

1.649 libaio

Description

Asynchronous input/output library that uses the kernels native interface.

More Information

<https://pagure.io/libaio>

Available Versions:

```
0.3.112-GCCcore-10.2.0
0.3.111-GCCcore-8.3.0
0.3.112-GCCcore-10.3.0
```

1.650 libarchive

Description

Multi-format archive and compression library

More Information

<https://www.libarchive.org/>

Available Versions:

```
3.4.0-GCCcore-8.2.0
3.6.1-GCCcore-11.3.0
3.5.1-GCCcore-11.2.0
3.6.1-GCCcore-12.2.0
3.5.1-GCCcore-10.3.0
```

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3.5.1-GCCcore-8.3.0
3.4.3-GCCcore-10.2.0

1.651 libcerf

Description

libcerf is a self-contained numeric library that provides an efficient and accurate implementation of complex error functions, along with Dawson, Faddeeva, and Voigt functions.

More Information

<https://jugit.fz-juelich.de/mlz/libcerf>

Available Versions:

1.7-GCCcore-7.3.0
1.13-GCCcore-8.3.0
1.17-GCCcore-11.2.0
2.1-GCCcore-11.3.0
1.13-GCCcore-9.3.0
1.17-GCCcore-10.3.0
1.14-GCCcore-10.2.0

1.652 libcint

Description

libcint is an open source library for analytical Gaussian integrals.

More Information

<https://github.com/sunqm/libcint>

Available Versions:

4.4.0-foss-2021a
5.1.6-foss-2021a

1.653 libctl

Description

libctl is a free Guile-based library implementing flexible control files for scientific simulations.

More Information

<https://libctl.readthedocs.io/en/latest/>

Available Versions:

4.1.3-GCCcore-9.3.0

1.654 libdap

Description

A C++ SDK which contains an implementation of DAP 2.0 and DAP4.0. This includes both Client- and Server-side support classes.

More Information

<https://www.opendap.org/software/libdap>

Available Versions:

```
3.20.7-GCCcore-10.3.0
3.20.7-GCCcore-10.2.0
```

1.655 libdeflate

Description

Heavily optimized library for DEFLATE/zlib/gzip compression and decompression.

More Information

<https://github.com/ebiggers/libdeflate>

Available Versions:

```
1.8-GCCcore-11.2.0
1.10-GCCcore-11.3.0
1.15-GCCcore-12.2.0
```

1.656 libdrm

Description

Direct Rendering Manager runtime library.

More Information

<https://dri.freedesktop.org>

Available Versions:

```
2.4.102-GCCcore-10.2.0
2.4.99-GCCcore-8.3.0
2.4.92-GCCcore-7.3.0
2.4.99-GCCcore-9.3.0
2.4.107-GCCcore-11.2.0
2.4.97-GCCcore-8.2.0
2.4.114-GCCcore-12.2.0
2.4.100-GCCcore-9.3.0
2.4.110-GCCcore-11.3.0
2.4.106-GCCcore-10.3.0
```

1.657 libdwarf

Description

The DWARF Debugging Information Format is of interest to programmers working on compilers and debuggers (and anyone interested in reading or writing DWARF information))

More Information

<https://www.prevanders.net/dwarf.html>

Available Versions:

20201201-GCCcore-10.2.0

1.658 libedit

Description

This BSD-style licensed command line editor library provides generic line editing, history, and tokenization functions, similar to those found in GNU Readline.

More Information

<https://thrysoee.dk/editline/>

Available Versions:

20191231-GCCcore-9.3.0

1.659 libelf

Description

libelf is a free ELF object file access library

More Information

<https://sourceware.org/elfutils>

Available Versions:

0.8.13-GCCcore-10.2.0

1.660 libepoxy

Description

Epoxy is a library for handling OpenGL function pointer management for you

More Information

<https://github.com/anholt/libepoxy>

Available Versions:

```

1.5.4-GCCcore-8.3.0
1.5.8-GCCcore-11.2.0
1.5.10-GCCcore-11.3.0
1.5.3-GCCcore-8.2.0
1.5.4-GCCcore-10.2.0

```

1.661 libev

Description

A full-featured and high-performance (see benchmark) event loop that is loosely modelled after libevent, but without its limitations and bugs. It is used in GNU Virtual Private Ethernet, rxvt-unicode, auditd, the Deliantra MORPG Server and Client, and many other programs.

More Information

<http://software.schmorp.de/pkg/libev.html>

Available Versions:

```
4.33-GCC-11.2.0
```

1.662 libevent

Description

The libevent API provides a mechanism to execute a callback function when a specific event occurs on a file descriptor or after a timeout has been reached. Furthermore, libevent also support callbacks due to signals or regular timeouts.

More Information

<http://libevent.org/>

Available Versions:

```

2.1.8
2.1.12-GCCcore-11.3.0
2.1.11-GCCcore-9.3.0
2.1.12-GCCcore-10.2.0
2.1.11-GCCcore-8.3.0
2.1.12-GCCcore-10.3.0
2.1.12-GCCcore-12.2.0
2.1.12-GCCcore-11.2.0

```

1.663 libexif

Description

A library for parsing, editing, and saving EXIF data.

More Information

<https://libexif.github.io/>

Available Versions:

0.6.24-GCCcore-11.2.0

1.664 libfabric

Description

Libfabric is a core component of OFI. It is the library that defines and exports the user-space API of OFI, and is typically the only software that applications deal with directly. It works in conjunction with provider libraries, which are often integrated directly into libfabric.

More Information

<https://ofiwg.github.io/libfabric/>

Available Versions:

1.11.0-GCCcore-10.2.0
1.16.1-GCCcore-12.2.0
1.11.0-GCCcore-9.3.0
1.13.2-GCCcore-11.2.0
1.12.1-GCCcore-10.3.0
1.15.1-GCCcore-11.3.0

1.665 libffi

Description

The libffi library provides a portable, high level programming interface to various calling conventions. This allows a programmer to call any function specified by a call interface description at run-time.

More Information

<https://sourceware.org/libffi/>

Available Versions:

3.3-GCCcore-9.3.0
3.2.1-GCCcore-7.3.0
3.2.1-GCCcore-9.3.0
3.4.4-GCCcore-12.2.0
3.3-GCCcore-10.3.0
3.2.1-GCCcore-8.3.0
3.4.2-GCCcore-11.3.0

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```
3.4.2-GCCcore-11.2.0
3.2.1-GCCcore-10.2.0
3.3-GCCcore-10.2.0
3.2.1-GCCcore-8.2.0
```

1.666 libgcrypt

Description

Libgcrypt is a general purpose cryptographic library originally based on code from GnuPG

More Information

https://gnupg.org/related_software/libgcrypt/index.html

Available Versions:

```
1.9.3-GCCcore-11.2.0
```

1.667 libgd

Description

GD is an open source code library for the dynamic creation of images by programmers.

More Information

<https://libgd.github.io>

Available Versions:

```
2.3.3-GCCcore-11.2.0
2.3.1-GCCcore-10.3.0
2.2.5-GCCcore-8.3.0
2.3.0-GCCcore-9.3.0
2.2.5-GCCcore-7.3.0
2.3.3-GCCcore-11.3.0
2.3.0-GCCcore-10.2.0
```

1.668 libgdiplus

Description

Libgdiplus is the Mono library that provides a GDI+-compatible API on non-Windows operating systems.

More Information

<https://www.mono-project.com/docs/gui/libgdiplus>

Available Versions:

```
6.1-GCCcore-11.2.0
```

1.669 libgeotiff

Description

Library for reading and writing coordinate system information from/to GeoTIFF files

More Information

<https://directory.fsf.org/wiki/Libgeotiff>

Available Versions:

```
1.5.1-GCCcore-8.3.0
1.6.0-GCCcore-10.3.0
1.7.0-GCCcore-11.2.0
1.4.2-foss-2018b
1.5.1-GCCcore-9.3.0
1.7.1-GCCcore-11.3.0
1.6.0-GCCcore-10.2.0
1.5.1-GCCcore-8.2.0
```

1.670 libgit2

Description

libgit2 is a portable, pure C implementation of the Git core methods provided as a re-entrantlinkable library with a solid API, allowing you to write native speed custom Git applications in any language which supports C bindings.

More Information

<https://libgit2.org/>

Available Versions:

```
1.1.1-GCCcore-11.2.0
1.4.3-GCCcore-11.3.0
1.1.0-GCCcore-10.3.0
```

1.671 libglade

Description

Libglade is a library for constructing user interfaces dynamically from XML descriptions.

More Information

<https://developer.gnome.org/libglade/>

Available Versions:

```
2.6.4-foss-2018b
```

1.672 libglvnd

Description

libglvnd is a vendor-neutral dispatch layer for arbitrating OpenGL API calls between multiple vendors.

More Information

<https://gitlab.freedesktop.org/glvnd/libglvnd>

Available Versions:

```
1.3.3-GCCcore-11.2.0
1.3.3-GCCcore-10.3.0
1.2.0-GCCcore-9.3.0
1.6.0-GCCcore-12.2.0
1.3.2-GCCcore-10.2.0
1.4.0-GCCcore-11.3.0
```

1.673 libgpg-error

Description

Libgpg-error is a small library that defines common error values for all GnuPG components.

More Information

https://gnupg.org/related_software/libgpg-error/index.html

Available Versions:

```
1.42-GCCcore-11.2.0
```

1.674 libgpuarray

Description

Library to manipulate tensors on the GPU.

More Information

<http://deeplearning.net/software/libgpuarray/>

Available Versions:

```
0.7.6-fosscuda-2019b-Python-3.7.4
0.7.6-fosscuda-2020b
```

1.675 libiconv

Description

Libiconv converts from one character encoding to another through Unicode conversion

More Information

<https://www.gnu.org/software/libiconv>

Available Versions:

```
1.17-GCCcore-11.3.0
1.16-GCCcore-9.3.0
1.16-GCCcore-8.3.0
1.15-GCCcore-7.3.0
1.16-GCCcore-10.2.0
1.16-GCCcore-11.2.0
1.16-GCCcore-8.2.0
1.16-GCCcore-10.3.0
```

1.676 libidn

Description

GNU Libidn is a fully documented implementation of the Stringprep, Punycode and IDNA specifications. Libidn's purpose is to encode and decode internationalized domain names.

More Information

<http://www.gnu.org/software/libidn>

Available Versions:

```
1.41-GCCcore-11.3.0
1.38-GCCcore-11.2.0
```

1.677 libidn2

Description

Libidn2 implements the revised algorithm for internationalized domain names called IDNA2008/TR46.

More Information

<http://www.gnu.org/software/libidn2>

Available Versions:

```
2.3.2-GCCcore-11.3.0
2.3.2-GCCcore-11.2.0
2.3.0-GCCcore-10.2.0
```


1.678 libjpeg-turbo

Description

libjpeg-turbo is a fork of the original IJG libjpeg which uses SIMD to accelerate baseline JPEG compression and decompression. libjpeg is a library that implements JPEG image encoding, decoding and transcoding.

More Information

<https://sourceforge.net/projects/libjpeg-turbo/>

Available Versions:

```
2.0.3-GCCcore-8.3.0
2.0.6-GCCcore-10.3.0
2.0.5-GCCcore-10.2.0
2.0.0-GCCcore-7.3.0
2.0.2-GCCcore-8.2.0
2.1.4-GCCcore-12.2.0
2.1.3-GCCcore-11.3.0
2.0.4-GCCcore-9.3.0
2.0.6-GCCcore-11.2.0
```

1.679 libmatheval

Description

GNU libmatheval is a library (callable from C and Fortran) to parse and evaluate symbolic expressions input as text.

More Information

<http://www.gnu.org/software/libmatheval/>

Available Versions:

```
1.1.11-GCCcore-8.2.0
1.1.11-GCCcore-9.3.0
1.1.11-GCCcore-8.3.0
```

1.680 libogg

Description

Ogg is a multimedia container format, and the native file and stream format for the Xiph.org multimedia codecs.

More Information

<https://xiph.org/ogg/>

Available Versions:

```
1.3.4-GCCcore-10.3.0
1.3.5-GCCcore-12.2.0
1.3.4-GCCcore-10.2.0
```

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1.3.5-GCCcore-11.3.0
1.3.5-GCCcore-11.2.0

1.681 libopus

Description

Opus is a totally open, royalty-free, highly versatile audio codec. Opus is unmatched for interactive speech and music transmission over the Internet, but is also intended for storage and streaming applications. It is standardized by the Internet Engineering Task Force (IETF) as RFC 6716 which incorporated technology from Skype's SILK codec and Xiph.Org's CELT codec.

More Information

<https://www.opus-codec.org/>

Available Versions:

1.3.1-GCCcore-12.2.0
1.3.1-GCCcore-11.3.0

1.682 libpciaccess

Description

Generic PCI access library.

More Information

<http://cgit.freedesktop.org/xorg/lib/libpciaccess/>

Available Versions:

0.14-GCCcore-8.2.0
0.16-GCCcore-10.3.0
0.14-GCCcore-8.3.0
0.16-GCCcore-9.3.0
0.16-GCCcore-10.2.0
0.14-GCCcore-7.3.0
0.16-GCCcore-11.3.0
0.16-GCCcore-11.2.0
0.17-GCCcore-12.2.0

1.683 libpng

Description

libpng is the official PNG reference library

More Information

<http://www.libpng.org/pub/png/libpng.html>

Available Versions:

```
1.6.34-GCCcore-7.3.0
1.6.37-GCCcore-9.3.0
1.6.37-GCCcore-11.2.0
1.6.36-GCCcore-8.2.0
1.6.37-GCCcore-11.3.0
1.6.38-GCCcore-12.2.0
1.6.37-GCCcore-10.2.0
1.6.37-GCCcore-8.3.0
1.6.37-GCCcore-10.3.0
```

1.684 libpsl

Description

C library for the Public Suffix List

More Information

<https://rockdaboot.github.io/libpsl>

Available Versions:

```
0.21.1-GCCcore-11.2.0
0.21.1-GCCcore-11.3.0
```

1.685 libpsortb

Description

PSORT family of programs for subcellular localization prediction as well as other datasets and resources relevant to localization prediction.

More Information

<http://psort.org/>

Available Versions:

```
1.0-foss-2021b
```

1.686 libreadline

Description

The GNU Readline library provides a set of functions for use by applications that allow users to edit command lines as they are typed in. Both Emacs and vi editing modes are available. The Readline library includes additional functions to maintain a list of previously-entered command lines, to recall and perhaps reedit those lines, and perform csh-like history expansion on previous commands.

More Information

<https://tiswww.case.edu/php/chet/readline/rltop.html>

Available Versions:

```
8.1-GCCcore-10.3.0
8.0-GCCcore-10.2.0
8.2-GCCcore-12.2.0
8.0-GCCcore-8.3.0
8.0-GCCcore-8.2.0
8.1.2-GCCcore-11.3.0
7.0-GCCcore-7.3.0
8.1-GCCcore-11.2.0
8.0-GCCcore-7.3.0
7.0-GCCcore-10.2.0
8.0-GCCcore-9.3.0
```

1.687 librtdtopo

Description

The RT Topology Library exposes an API to create and manage standard (ISO 13249 aka SQL/MM) topologies using user-provided data stores.

More Information

<https://git.osgeo.org/gitea/rttopo/librtdtopo>

Available Versions:

```
1.1.0-GCC-11.2.0
```

1.688 libsigc++

Description

The libsigc++ package implements a typesafe callback system for standard C++.

More Information

<https://libsigcplusplus.github.io/libsigcplusplus/>

Available Versions:

```
2.10.2-GCCcore-8.3.0
2.10.8-GCCcore-10.3.0
```

1.689 libsndfile

Description

Libsndfile is a C library for reading and writing files containing sampled sound (such as MS Windows WAV and the Apple/SGI AIFF format) through one standard library interface.

More Information

<http://www.mega-nerd.com/libsndfile>

Available Versions:

```
1.0.31-GCCcore-10.3.0
1.0.28-GCCcore-9.3.0
1.0.28-GCCcore-8.3.0
1.0.28-GCCcore-7.3.0
1.0.28-GCCcore-10.2.0
1.1.0-GCCcore-11.3.0
1.2.0-GCCcore-12.2.0
1.0.31-GCCcore-11.2.0
```

1.690 libsodium

Description

Sodium is a modern, easy-to-use software library for encryption, decryption, signatures, password hashing and more.

More Information

<https://doc.libsodium.org/>

Available Versions:

```
1.0.18-GCCcore-11.2.0
1.0.18-GCCcore-10.3.0
1.0.18-GCCcore-11.3.0
1.0.18-GCCcore-10.2.0
1.0.18-GCCcore-9.3.0
1.0.18-GCCcore-8.3.0
```

1.691 libspatialindex

Description

C++ implementation of R*-tree, an MVR-tree and a TPR-tree with C API

More Information

<https://libspatialindex.org>

Available Versions:

1.9.3-GCCcore-11.2.0

1.692 libspatialite

Description

Spatialite is an open source library intended to extend the SQLite core to support fully fledged Spatial SQL capabilities.

More Information

<https://www.gaia-gis.it/fossil/libspatialite/home>

Available Versions:

5.0.1-GCC-11.2.0

4.3.0a-GCC-8.3.0-Python-3.7.4

1.693 libtasn1

Description

Libtasn1 is the ASN.1 library used by GnuTLS, GNU Shishi and some other packages. It was written by Fabio Fiorina, and has been shipped as part of GnuTLS for some time but is now a proper GNU package.

More Information

<https://www.gnu.org/software/libtasn1/>

Available Versions:

4.19.0-GCCcore-11.3.0

4.18.0-GCCcore-11.2.0

1.694 libtirpc

Description

Libtirpc is a port of Suns Transport-Independent RPC library to Linux.

More Information

<https://sourceforge.net/projects/libtirpc/>

Available Versions:

```
1.3.2-GCCcore-11.3.0
1.3.2-GCCcore-10.3.0
1.2.6-GCCcore-8.3.0
1.3.1-GCCcore-10.2.0
1.3.2-GCCcore-11.2.0
```

1.695 libtool

Description

GNU libtool is a generic library support script. Libtool hides the complexity of using shared libraries behind a consistent, portable interface.

More Information

<http://www.gnu.org/software/libtool>

Available Versions:

```
2.4.6-GCCcore-8.3.0
2.4.6-GCCcore-8.1.0
2.4.6-GCCcore-10.2.0
2.4.6-GCCcore-9.3.0
2.4.7-GCCcore-11.3.0
2.4.6-GCCcore-7.3.0
2.4.7-GCCcore-12.2.0
2.4.6-GCCcore-10.3.0
2.4.6-GCCcore-8.2.0
2.4.6-GCCcore-11.2.0
```

1.696 libunistring

Description

This library provides functions for manipulating Unicode strings and for manipulating C strings according to the Unicode standard.

More Information

<https://www.gnu.org/software/libunistring/>

Available Versions:

```
0.9.10-GCCcore-9.3.0
0.9.10-GCCcore-8.2.0
1.0-GCCcore-11.3.0
1.0-GCCcore-11.2.0
0.9.10-GCCcore-8.3.0
```

1.697 libunwind

Description

The primary goal of libunwind is to define a portable and efficient C programming interface (API) to determine the call-chain of a program. The API additionally provides the means to manipulate the preserved (callee-saved) state of each call-frame and to resume execution at any point in the call-chain (non-local goto). The API supports both local (same-process) and remote (across-process) operation. As such, the API is useful in a number of applications

More Information

<https://www.nongnu.org/libunwind/>

Available Versions:

```
1.6.2-GCCcore-11.3.0
1.3.1-GCCcore-8.3.0
1.4.0-GCCcore-10.3.0
1.5.0-GCCcore-11.2.0
1.6.2-GCCcore-12.2.0
1.3.1-GCCcore-8.2.0
1.3.1-GCCcore-9.3.0
1.2.1-GCCcore-7.3.0
1.4.0-GCCcore-10.2.0
```

1.698 libvdwxc

Description

libvdwxc is a general library for evaluating energy and potential forexchange-correlation (XC) functionals from the vdW-DF family that can be used with variousof density functional theory (DFT) codes.

More Information

<https://libvdwxc.org>

Available Versions:

```
0.4.0-foss-2020b
0.4.0-foss-2022a
0.4.0-foss-2021a
```


1.699 libvorbis

Description

Ogg Vorbis is a fully open, non-proprietary, patent-and-royalty-free, general-purpose compressed audio format

More Information

<https://xiph.org/vorbis/>

Available Versions:

```
1.3.7-GCCcore-12.2.0
1.3.7-GCCcore-11.3.0
1.3.7-GCCcore-10.3.0
1.3.7-GCCcore-11.2.0
1.3.7-GCCcore-10.2.0
```

1.700 libwebp

Description

WebP is a modern image format that provides superior lossless and lossy compression for images on the web. Using WebP, webmasters and web developers can create smaller, richer images that make the web faster.

More Information

<https://developers.google.com/speed/webp/>

Available Versions:

```
1.0.2-GCCcore-8.2.0
1.2.4-GCCcore-11.3.0
1.2.0-GCCcore-11.2.0
1.1.0-GCCcore-10.2.0
```

1.701 libwpe

Description

WPE is the reference WebKit port for embedded and low-consumption computer devices. It has been designed from the ground-up with performance, small footprint, accelerated content rendering, and simplicity of deployment in mind, bringing the excellence of the WebKit engine to countless platforms and target devices.

More Information

<https://webkit.org/wpe>

Available Versions:

```
1.13.3-GCCcore-11.2.0
```

1.702 libxc

Description

Libxc is a library of exchange-correlation functionals for density-functional theory. The aim is to provide a portable, well tested and reliable set of exchange and correlation functionals.

More Information

<https://www.tddft.org/programs/libxc>

Available Versions:

```
4.3.4-intel-2020a
5.1.5-intel-compilers-2021.2.0
5.1.6-GCC-11.2.0
4.3.4-GCC-10.2.0
4.3.4-GCC-8.3.0
5.1.5-GCC-10.3.0
5.1.6-intel-compilers-2021.4.0
4.3.4-iccifort-2020.1.217
5.2.3-GCC-11.3.0
3.0.1-GCC-8.2.0-2.31.1
4.3.4-iccifort-2019.5.281
4.3.4-iccifort-2020.4.304
4.3.4-GCC-9.3.0
4.3.4-GCC-8.2.0-2.31.1
4.3.4-GCC-7.3.0-2.30
5.2.3-GCC-10.3.0
3.0.1-foss-2020a
5.1.2-GCC-10.2.0
5.2.3-intel-compilers-2022.1.0
5.1.6-GCC-11.3.0
```

1.703 libxml++

Description

libxml++ is a C++ wrapper for the libxml XML parser library.

More Information

<http://libxmlplusplus.sourceforge.net>

Available Versions:

```
2.40.1-GCCcore-8.3.0
2.42.1-GCC-10.3.0
```

1.704 libxml2

Description

Libxml2 is the XML C parser and toolchain developed for the Gnome project (but usable outside of the Gnome platform).

More Information

<http://xmlsoft.org/>

Available Versions:

```
2.10.3-GCCcore-12.2.0
2.9.8-GCCcore-8.2.0
2.9.10-GCCcore-10.2.0
2.9.9-GCCcore-9.3.0
2.9.10-GCCcore-11.2.0
2.9.8-GCCcore-7.3.0
2.9.10-GCCcore-10.3.0
2.9.10-GCCcore-9.3.0
2.9.9-GCCcore-8.3.0
2.9.13-GCCcore-11.3.0
```

1.705 libxslt

Description

Libxslt is the XSLT C library developed for the GNOME project (but usable outside of the Gnome platform).

More Information

<http://xmlsoft.org/>

Available Versions:

```
1.1.34-GCCcore-9.3.0
1.1.32-GCCcore-7.3.0
1.1.34-GCCcore-10.2.0
1.1.34-GCCcore-10.3.0
1.1.34-GCCcore-11.2.0
1.1.37-GCCcore-12.2.0
1.1.34-GCCcore-11.3.0
```

1.706 libxsmm

Description

LIBXSMM is a library for small dense and small sparse matrix-matrix multiplication targeting Intel Architecture (x86).

More Information

<https://github.com/hfp/libxsmm>

Available Versions:

```
1.10-foss-2019b
1.16.2-GCC-10.3.0
1.16.1-iccifort-2020.1.217
1.10-GCC-8.2.0-2.31.1
1.16.1-iccifort-2020.4.304
1.16.1-GCC-10.2.0
1.16.1-GCC-9.3.0
```

1.707 libyaml

Description

LibYAML is a YAML parser and emitter written in C.

More Information

<https://pyyaml.org/wiki/LibYAML>

Available Versions:

```
0.2.5-GCCcore-10.3.0
0.2.2-GCCcore-8.2.0
0.2.5-GCCcore-10.2.0
0.2.2-GCCcore-8.3.0
0.2.5-GCCcore-11.3.0
0.2.2-GCCcore-9.3.0
0.2.5-GCCcore-11.2.0
```

1.708 libzip

Description

libzip is a C library for reading, creating, and modifying zip archives.

More Information

<https://libzip.org/>

Available Versions:

```
1.7.3-GCCcore-11.2.0
```

1.709 likwid

Description

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.

More Information

<https://github.com/RRZE-HPC/likwid>

Available Versions:

5.0.1-GCCcore-8.3.0

1.710 Ipsolve

Description

Mixed Integer Linear Programming (MILP) solver

More Information

<https://sourceforge.net/projects/ipsolve/>

Available Versions:

5.5.2.5-GCC-8.3.0
5.5.2.11-GCC-10.2.0

1.711 lxml

Description

The lxml XML toolkit is a Pythonic binding for the C libraries libxml2 and libxslt.

More Information

<http://lxml.de/>

Available Versions:

4.2.5-foss-2018b-Python-2.7.15
4.9.1-GCCcore-11.3.0
4.6.3-GCCcore-11.2.0
4.5.2-foss-2020a-Python-3.8.2
4.6.3-GCCcore-10.3.0

1.712 lz4

Description

LZ4 is lossless compression algorithm, providing compression speed at 400 MB/s per core. It features an extremely fast decoder, with speed in multiple GB/s per core.

More Information

<https://lz4.github.io/lz4/>

Available Versions:

1.9.2-GCCcore-10.2.0
1.9.3-GCCcore-11.3.0
1.9.3-GCCcore-10.3.0

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```
1.9.2-GCCcore-8.3.0
1.9.2-GCCcore-9.3.0
1.9.4-GCCcore-12.2.0
1.9.3-GCCcore-11.2.0
```

1.713 magma

Description

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.

More Information

<https://icl.cs.utk.edu/magma/>

Available Versions:

```
2.6.2-foss-2022a-CUDA-11.7.0
2.6.1-foss-2021a-CUDA-11.3.1
2.5.4-fosscuda-2019b
2.5.4-fosscuda-2020b
2.5.1-fosscuda-2019b
```

1.714 make

Description

GNU version of make utility

More Information

<https://www.gnu.org/software/make/make.html>

Available Versions:

```
4.3-GCCcore-10.2.0
4.3-GCCcore-9.3.0
4.3-GCCcore-11.2.0
```

1.715 makeinfo

Description

makeinfo is part of the Texinfo project, the official documentation format of the GNU project.

More Information

<https://www.gnu.org/software/texinfo/>

Available Versions:

```
6.8-GCCcore-11.2.0
6.7-GCCcore-10.3.0
6.7-GCCcore-9.3.0
6.7-GCCcore-10.3.0-minimal
```

1.716 matplotlib

Description

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.

More Information

<https://matplotlib.org>

Available Versions:

```
3.2.1-intel-2020a-Python-3.8.2
2.2.3-foss-2018b-Python-2.7.15
3.4.3-foss-2021b
2.2.4-fosscuda-2019b-Python-2.7.16
2.2.4-foss-2019b-Python-2.7.16
2.2.3-fosscuda-2018b-Python-2.7.15
3.1.1-foss-2019b-Python-3.7.4
3.2.1-foss-2020a-Python-3.8.2
3.0.3-foss-2019a-Python-3.7.2
3.5.2-foss-2022a
3.3.3-foss-2020b
3.4.2-foss-2021a
3.5.2-foss-2021b
3.3.3-fosscuda-2020b
3.5.2-intel-2022a
```

1.717 mdtep

Available Versions:

2022

1.718 minimap2

Description

Minimap2 is a fast sequence mapping and alignment program that can find overlaps between long noisy reads, or map long reads or their assemblies to a reference genome optionally with detailed alignment (i.e. CIGAR). At present, it works efficiently with query sequences from a few kilobases to ~100 megabases in length at an error rate ~15%. Minimap2 outputs in the PAF or the SAM format. On limited test data sets, minimap2 is over 20 times faster than most other long-read aligners. It will replace BWA-MEM for long reads and contig alignment.

More Information

<https://github.com/lh3/minimap2>

Available Versions:

2.22-GCCcore-11.2.0
2.17-GCC-8.3.0
2.24-GCCcore-11.3.0

1.719 minizip

Description

Mini zip and unzip based on zlib

More Information

<https://www.winimage.com/zLibDll/minizip.html>

Available Versions:

1.1-GCCcore-11.2.0

1.720 mm-common

Description

The mm-common module provides the build infrastructure and utilities shared among the GNOME C++ binding libraries.

More Information

<https://gitlab.gnome.org/GNOME/mm-common>

Available Versions:

1.0.4-GCCcore-10.3.0

1.721 module-git

Available Versions:

1.722 module-info

Available Versions:

1.723 modules

Available Versions:

1.724 molmod

Description

MolMod is a Python library with many components that are useful to write molecular modeling programs.

More Information

<https://molmod.github.io/molmod/>

Available Versions:

1.4.5-intel-2020a-Python-3.8.2
1.4.5-foss-2020a-Python-3.8.2

1.725 motif

Description

Motif refers to both a graphical user interface (GUI) specification and the widget toolkit for building applications that follow that specification under the X Window System on Unix and other POSIX-compliant systems. It was the standard toolkit for the Common Desktop Environment and thus for Unix.

More Information

<https://motif.ics.com/>

Available Versions:

2.3.8-GCCcore-8.3.0
2.3.8-GCCcore-11.2.0
2.3.8-foss-2019a

1.726 mpi

Available Versions:

openmpi-x86_64

1.727 mpitest

Available Versions:

1.0

1.728 mpmath

Description

mpmath can be used as an arbitrary-precision substitute for Python's float/complex types and math/cmath modules, but also does much more advanced mathematics. Almost any calculation can be performed just as well at 10-digit or 1000-digit precision, with either real or complex numbers, and in many cases mpmath implements efficient algorithms that scale well for extremely high precision work.

More Information

<https://mpmath.org/>

Available Versions:

1.1.0-GCCcore-9.3.0-Python-3.8.2
1.0.0-foss-2018b-Python-2.7.15

1.729 mule

Available Versions:

4.4.0

1.730 multichoose

Description

generate multiset combinations (n multichoose k).

More Information

<https://github.com/ekg/multichoose>

Available Versions:

`1.0.3-GCCcore-11.2.0`

1.731 muparserx

Description

A C++ Library for Parsing Expressions with Strings, Complex Numbers, Vectors, Matrices and more.

More Information

<https://beltoforion.de/en/muparserx/>

Available Versions:

`4.0.8-GCCcore-10.3.0`

1.732 ncbi-vdb

Description

The SRA Toolkit and SDK from NCBI is a collection of tools and libraries for using data in the INSDC Sequence Read Archives.

More Information

<https://github.com/ncbi/ncbi-vdb>

Available Versions:

`2.10.9-gompi-2020b`
`3.0.2-gompi-2022a`
`2.9.3-foss-2018b`

1.733 ncdf4

Description

ncdf4: Interface to Unidata netCDF (version 4 or earlier) format data files

More Information

<https://cran.r-project.org/web/packages/ncdf4>

Available Versions:

`1.17-foss-2021a-R-4.1.0`
`1.17-foss-2019b`

1.734 ncurses

Description

The Ncurses (new curses) library is a free software emulation of curses in System V Release 4.0, and more. It uses Terminfo format, supports pads and color and multiple highlights and forms characters and function-key mapping, and has all the other SYSV-curses enhancements over BSD Curses.

More Information

<http://www.gnu.org/software/ncurses/>

Available Versions:

6.1-GCCcore-8.3.0
6.1-GCCcore-8.2.0
6.1
6.1-GCCcore-10.2.0
6.3-GCCcore-11.3.0
6.1-GCCcore-7.3.0
6.1-GCCcore-9.3.0
6.3
6.2-GCCcore-9.3.0
6.0
6.2-GCCcore-10.3.0
6.3-GCCcore-12.2.0
6.2
6.2-GCCcore-10.2.0
6.2-GCCcore-11.2.0

1.735 ncview

Description

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.

More Information

https://meteora.ucsd.edu/~pierce/ncview_home_page.html

Available Versions:

2.1.7-foss-2019b

1.736 netCDF

Description

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.

More Information

<https://www.unidata.ucar.edu/software/netcdf/>

Available Versions:

```
4.9.0-gompi-2022a
4.7.4-gompi-2020a
4.6.1-fosscuda-2018b
4.8.0-gompi-2021a
4.7.1-gompi-2019b-dba
4.6.1-foss-2018b
4.7.4-iimpi-2020b
4.7.1-gompic-2019b
4.6.2-gompi-2019a
4.7.4-gompic-2020b
4.8.1-gompi-2021b
4.7.1-gompi-2019b
4.7.4-gompi-2020b
4.9.0-iimpi-2022a
4.7.4-iimpi-2020a
4.8.1-iimpi-2021b
```

1.737 netCDF-C++4

Description

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.

More Information

<https://www.unidata.ucar.edu/software/netcdf/>

Available Versions:

```
4.3.1-iimpi-2020a
4.3.1-gompi-2020b
4.3.1-gompi-2021a
```

1.738 netCDF-Fortran

Description

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.

More Information

<http://www.unidata.ucar.edu/software/netcdf/>

Available Versions:

```
4.4.4-foss-2018b
4.5.3-gompi-2021b
4.6.0-iimpi-2022a
4.5.2-iimpi-2020a
4.5.3-gompi-2021a
4.5.2-gompi-2019b
4.5.2-gompi-2020a
4.5.3-iimpi-2021b
4.5.2-gompic-2019b
4.5.3-gompic-2020b
4.5.3-iimpi-2020b
4.4.4-fosscuda-2018b
4.5.3-gompi-2020b
4.5.2-gompi-2019b-dba
```

1.739 netcdf4-python

Description

Python/numpy interface to netCDF.

More Information

<https://unidata.github.io/netcdf4-python/>

Available Versions:

```
1.5.3-foss-2020a-Python-3.8.2
1.6.1-foss-2022a
```

1.740 nettle

Description

Nettle is a cryptographic library that is designed to fit easily in more or less any context: In crypto toolkits for object-oriented languages (C++, Python, Pike, ...), in applications like LSH or GNUPG, or even in kernel space.

More Information

<http://www.lysator.liu.se/~nisse/nettle/>

Available Versions:

```

3.4-foss-2018b
3.7.2-GCCcore-10.3.0
3.8-GCCcore-11.3.0
3.7.3-GCCcore-11.2.0
3.5.1-GCCcore-8.3.0
3.8.1-GCCcore-12.2.0
3.6-GCCcore-10.2.0
3.4.1-GCCcore-8.2.0
3.5.1-GCCcore-9.3.0

```

1.741 networkx

Description

NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.

More Information

<https://pypi.python.org/pypi/networkx>

Available Versions:

```

2.4-foss-2019a-Python-3.7.2
2.6.3-foss-2021b
2.3-foss-2019a-Python-3.7.2
2.2-foss-2018b-Python-2.7.15
2.4-foss-2019b-Python-3.7.4
2.5.1-foss-2021a
2.4-foss-2020a-Python-3.8.2
2.5-foss-2020b

```

1.742 nghttp2

Description

This is an implementation of the Hypertext Transfer Protocol version 2 in C. The framing layer of HTTP/2 is implemented as a reusable C library. On top of that, we have implemented an HTTP/2 client, server and proxy. We have also developed load test and benchmarking tools for HTTP/2. An HPACK encoder and decoder are available as a public API.

More Information

<https://github.com/nghttp2/nghttp2>

Available Versions:

```

1.48.0-GCC-11.2.0

```

1.743 nghttp3

Description

nghttp3 is an implementation of RFC 9114 HTTP/3 mapping over QUIC and RFC 9204 QPACK in C. It does not depend on any particular QUIC transport implementation.

More Information

<https://github.com/ngtcp2/nghttp3>

Available Versions:

<code>0.6.0-GCCcore-11.2.0</code> <code>0.6.0-GCCcore-11.3.0</code>
--

1.744 ngsF

Available Versions:

<code>2022</code>

1.745 ngsLD

Available Versions:

<code>2020</code>

1.746 ngspice

Description

Ngspice is a mixed-level/mixed-signal circuit simulator. Its code is based on three open source software packages: Spice3f5, Cider1b1 and Xspice.

More Information

<https://ngspice.sourceforge.net>

Available Versions:

<code>31-foss-2019b</code>

1.747 ngtcp2

Description

‘Call it TCP/2. One More Time.’ngtcp2 project is an effort to implement RFC9000 QUIC protocol.

More Information

<https://github.com/ngtcp2/ngtcp2>

Available Versions:

0.7.0-GCC-11.2.0

1.748 nlohmann_json

Description

JSON for Modern C++

More Information

<https://github.com/nlohmann/json>

Available Versions:

3.10.5-GCCcore-11.3.0

3.10.0-GCCcore-10.3.0

1.749 nodejs

Description

Node.js is a platform built on Chrome’s JavaScript runtime for easily building fast, scalable network applications. Node.js uses an event-driven, non-blocking I/O model that makes it lightweight and efficient, perfect for data-intensive real-time applications that run across distributed devices.

More Information

<https://nodejs.org>

Available Versions:

14.17.0-GCCcore-10.3.0

14.17.6-GCCcore-11.2.0

10.15.1-foss-2020a

16.15.1-GCCcore-11.3.0

12.19.0-GCCcore-10.2.0

1.750 nsync

Description

nsync is a C library that exports various synchronization primitives, such as mutexes

More Information

<https://github.com/google/nsync>

Available Versions:

```
1.24.0-GCCcore-10.3.0
1.24.0-GCCcore-9.3.0
1.24.0-GCCcore-11.2.0
1.24.0-GCCcore-10.2.0
1.24.0-GCCcore-8.3.0
```

1.751 null

Available Versions:

1.752 numactl

Description

The numactl program allows you to run your application program on specific cpu's and memory nodes. It does this by supplying a NUMA memory policy to the operating system before running your program. The libnuma library provides convenient ways for you to add NUMA memory policies into your own program.

More Information

<http://oss.sgi.com/projects/libnuma/>

Available Versions:

```
2.0.11-GCCcore-8.1.0
2.0.16-GCCcore-12.2.0
2.0.12-GCCcore-8.2.0
2.0.14-GCCcore-11.3.0
2.0.13-GCCcore-9.3.0
2.0.14-GCCcore-11.2.0
2.0.12-GCCcore-8.3.0
2.0.14-GCCcore-10.3.0
2.0.11-GCCcore-7.3.0
2.0.13-GCCcore-10.2.0
```

1.753 numba

Description

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.

More Information

<https://numba.pydata.org/>

Available Versions:

```
0.53.1-foss-2021a
0.46.0-foss-2019a
```

1.754 nvidia

Description

htop-like GPU usage monitor

More Information

<https://github.com/Syllo/nvidia>

Available Versions:

```
1.2.1-GCCcore-10.3.0
```

1.755 orthomcl

Available Versions:

```
v2.0.9
```

1.756 p11-kit

Description

Provides a way to load and enumerate PKCS#11 modules. Provides a standard configuration setup for installing PKCS#11 modules in such a way that they're discoverable. Also solves problems with coordinating the use of PKCS#11 by different components or libraries living in the same process.

More Information

<https://p11-glue.freedesktop.org/p11-kit.html>

Available Versions:

```
0.24.1-GCCcore-11.2.0
0.24.1-GCCcore-11.3.0
```

1.757 parallel

Description

parallel: Build and execute shell commands in parallel

More Information

<https://savannah.gnu.org/projects/parallel/>

Available Versions:

```
20220722-GCCcore-11.3.0
20210322-GCCcore-10.2.0
20190922-GCCcore-8.3.0
20200522-GCCcore-9.3.0
20190622-GCCcore-8.2.0
20210622-GCCcore-10.3.0
20190222-GCCcore-7.3.0
20210722-GCCcore-11.2.0
```

1.758 patchelf

Description

PatchELF is a small utility to modify the dynamic linker and RPATH of ELF executables.

More Information

<https://github.com/NixOS/patchelf>

Available Versions:

```
0.12-GCCcore-10.3.0
0.10-GCCcore-8.3.0
```

1.759 petsc4py

Description

petsc4py are Python bindings for PETSc, the Portable, Extensible Toolchain for Scientific Computation.

More Information

<https://bitbucket.org/petsc/petsc4py>

Available Versions:

```
3.15.0-foss-2021a
3.12.0-foss-2019b-Python-3.7.4
```

1.760 picard

Description

A set of tools (in Java) for working with next generation sequencing data in the BAM format.

More Information

<https://sourceforge.net/projects/picard>

Available Versions:

2.6.0-Java-1.8.0_131

1.761 pigz

Description

pigz, which stands for parallel implementation of gzip, is a fully functional replacement for gzip that exploits multiple processors and multiple cores to the hilt when compressing data. pigz was written by Mark Adler, and uses the zlib and pthread libraries.

More Information

<https://zlib.net/pigz/>

Available Versions:

2.4-GCCcore-7.3.0
2.4-GCCcore-8.3.0
2.7-GCCcore-11.3.0

1.762 pixman

Description

Pixman is a low-level software library for pixel manipulation, providing features such as image compositing and trapezoid rasterization. Important users of pixman are the cairo graphics library and the X server.

More Information

<http://www.pixman.org/>

Available Versions:

0.40.0-GCCcore-10.3.0
0.38.0-GCCcore-8.2.0
0.34.0-GCCcore-7.3.0
0.42.2-GCCcore-12.2.0
0.40.0-GCCcore-10.2.0
0.38.4-GCCcore-9.3.0
0.40.0-GCCcore-11.2.0
0.38.4-GCCcore-8.3.0
0.40.0-GCCcore-11.3.0

1.763 pkg-config

Description

pkg-config is a helper tool used when compiling applications and libraries. It helps you insert the correct compiler options on the command line so an application can use `gcc -o test test.c pkg-config -libs -cflags glib-2.0` for instance, rather than hard-coding values on where to find glib (or other libraries).

More Information

<http://www.freedesktop.org/wiki/Software/pkg-config/>

Available Versions:

```
0.29.2
0.29.2-GCCcore-11.2.0
0.29.2-GCCcore-10.2.0
0.29.2-GCCcore-7.3.0
0.29.2-GCCcore-11.3.0
0.29.2-GCCcore-9.3.0
0.29.2-GCCcore-8.2.0
0.29.2-GCCcore-8.3.0
0.29.2-GCCcore-10.3.0
```

1.764 pkgconf

Description

pkgconf is a program which helps to configure compiler and linker flags for development libraries. It is similar to pkg-config from freedesktop.org.

More Information

<https://github.com/pkgconf/pkgconf>

Available Versions:

```
1.8.0-GCCcore-11.3.0
1.8.0-GCCcore-11.2.0
1.9.3-GCCcore-12.2.0
1.8.0
```

1.765 pkgconfig

Description

pkgconfig is a Python module to interface with the pkg-config command line tool

More Information

<https://github.com/matze/pkgconfig>

Available Versions:

```
1.5.1-GCCcore-9.3.0-Python-3.8.2
1.5.4-GCCcore-10.3.0-python
1.5.5-GCCcore-11.2.0-python
1.5.1-GCCcore-8.2.0-python
1.5.1-GCCcore-8.3.0-Python-3.7.4
1.5.1-GCCcore-10.2.0-python
1.3.1-foss-2018b-Python-2.7.15
```

1.766 plotly.py

Description

An open-source, interactive graphing library for Python

More Information

<https://plot.ly/python>

Available Versions:

```
4.8.1-GCCcore-9.3.0
```

1.767 pmi

Available Versions:

```
pmix-x86_64
```

1.768 pocl

Description

Pocl is a portable open source (MIT-licensed) implementation of the OpenCL standard

More Information

<https://portablecl.org>

Available Versions:

```
1.6-GCC-10.2.0
1.6-gccuda-2020b
```

1.769 preseq

Description

Software for predicting library complexity and genome coverage in high-throughput sequencing.

More Information

<http://smithlabresearch.org/software/preseq>

Available Versions:

3.1.2-foss-2020b
2.0.3-foss-2018b

1.770 prism

Available Versions:

4.4-beta

1.771 prodigal

Description

Prodigal (Prokaryotic Dynamic Programming Genefinding Algorithm) is a microbial (bacterial and archaeal) gene finding program developed at Oak Ridge National Laboratory and the University of Tennessee.

More Information

<https://github.com/hyattpd/Prodigal/>

Available Versions:

2.6.3-GCCcore-9.3.0
2.6.3-GCCcore-7.3.0

1.772 prokka

Description

Prokka is a software tool for the rapid annotation of prokaryotic genomes.

More Information

<https://www.vicbioinformatics.com/software/prokka.shtml>

Available Versions:

1.14.5-gompi-2021a

1.773 protobuf

Description

Google Protocol Buffers

More Information

<https://github.com/google/protobuf/>

Available Versions:

```
3.13.0-GCCcore-9.3.0
3.17.3-GCCcore-10.3.0
3.6.1-GCCcore-7.3.0
3.14.0-GCCcore-10.2.0
3.19.4-GCCcore-11.3.0
3.10.0-GCCcore-8.3.0
3.17.3-GCCcore-11.2.0
```

1.774 protobuf-python

Description

Python Protocol Buffers runtime library.

More Information

<https://github.com/google/protobuf/>

Available Versions:

```
3.13.0-fosscuda-2020a-Python-3.8.2
3.19.4-GCCcore-11.3.0
3.17.3-GCCcore-10.3.0
3.13.0-foss-2020a-Python-3.8.2
3.10.0-fosscuda-2019b-Python-3.7.4
3.14.0-GCCcore-10.2.0
3.10.0-foss-2019b-Python-3.7.4
3.17.3-GCCcore-11.2.0
```

1.775 psutil

Description

A cross-platform process and system utilities module for Python

More Information

<https://github.com/giampaolo/psutil>

Available Versions:

```
5.6.3-GCCcore-8.2.0
```

1.776 psycopg2

Description

Psycopg is the most popular PostgreSQL adapter for the Python programming language.

More Information

<https://psycopg.org/>

Available Versions:

2.9.5-GCCcore-11.2.0

1.777 pugixml

Description

pugixml is a light-weight C++ XML processing library

More Information

<https://pugixml.org/>

Available Versions:

1.12.1-GCCcore-11.2.0

1.778 pullseq

Description

Utility program for extracting sequences from a fasta/fastq file

More Information

<https://github.com/bcthomas/pullseq>

Available Versions:

1.0.2-GCCcore-7.3.0

1.779 pyABC

Description

Massively parallel, distributed and scalable ABC-SMC (Approximate BayesianComputation - Sequential Monte Carlo) for parameter estimation of complexstochastic models. Implemented in Python with support of the R language.

More Information

<https://github.com/icb-dcm/pyabc>

Available Versions:

0.10.4-foss-2019b-Python-3.7.4

1.780 pybedtools

Description

pybedtools wraps and extends BEDTools and offers feature-level manipulations from within Python.

More Information

<https://daler.github.io/pybedtools>

Available Versions:

0.8.1-foss-2019b

1.781 pybind11

Description

pybind11 is a lightweight header-only library that exposes C++ types in Python and vice versa, mainly to create Python bindings of existing C++ code.

More Information

<https://pybind11.readthedocs.io>

Available Versions:

2.9.2-GCCcore-11.3.0
2.6.0-GCCcore-10.2.0
2.7.1-GCCcore-11.2.0
2.6.2-GCCcore-10.3.0
2.4.3-GCCcore-8.3.0-Python-3.7.4
2.4.3-GCCcore-9.3.0-Python-3.8.2

1.782 pyproj

Description

Python interface to PROJ4 library for cartographic transformations

More Information

<https://pyproj4.github.io/pyproj>

Available Versions:

2.6.1.post1-GCCcore-9.3.0-Python-3.8.2

1.783 pytest-xdist

Description

xdist: pytest distributed testing pluginThe pytest-xdist plugin extends pytest with some unique test execution modes:

- * test run parallelization: if you have multiple CPUs or hosts you can use those for a combined test run. This allows to speed up development or to use special resources of remote machines.
- * `-looponfail`: run your tests repeatedly in a subprocess. After each run pytest waits until a file in your project changes and then re-runs the previously failing tests. This is repeated until all tests pass after which again a full run is performed.
- * Multi-Platform coverage: you can specify different Python interpreters or different platforms and run tests in parallel on all of them.

Before running tests remotely, pytest efficiently “rsyncs” your program source code to the remote place. All test results are reported back and displayed to your local terminal. You may specify different Python versions and interpreters.

More Information

<https://github.com/pytest-dev/pytest-xdist>

Available Versions:

```
2.3.0-GCCcore-10.3.0
2.5.0-GCCcore-11.2.0
2.3.0-GCCcore-10.2.0
```

1.784 python-isal

Description

Faster zlib and gzip compatible compression and decompression by providing python bindings for the isa-l library.

More Information

<https://github.com/pycompression/python-isal>

Available Versions:

```
0.11.1-GCCcore-11.2.0
1.1.0-GCCcore-11.3.0
```

1.785 qcint

Description

libcint is an open source library for analytical Gaussian integrals.qcint is an optimized libcint branch for the x86-64 platform.

More Information

<http://wiki.sunqm.net/libcint>

Available Versions:

```
3.0.18-foss-2019a
4.0.5-foss-2020a
3.1.1-foss-2020a
```

1.786 qupdate

Description

qupdate is a Fortran library for fast updates of QR and Cholesky decompositions.

More Information

<https://sourceforge.net/projects/qupdate/>

Available Versions:

```
1.1.2-GCCcore-11.2.0
1.1.2-GCCcore-8.3.0
```

1.787 rclone

Description

Rclone is a command line program to sync files and directories to and from a variety of online storage services

More Information

<https://rclone.org/>

Available Versions:

```
1.54.1-amd64
```

1.788 re2c

Description

re2c is a free and open-source lexer generator for C and C++. Its main goal is generating fast lexers: at least as fast as their reasonably optimized hand-coded counterparts. Instead of using traditional table-driven approach, re2c encodes the generated finite state automata directly in the form of conditional jumps and comparisons.

More Information

<https://re2c.org/>

Available Versions:

```
2.0.3-GCCcore-10.2.0
2.2-GCCcore-11.2.0
1.2.1-GCCcore-8.3.0
2.2-GCCcore-11.3.0
2.1.1-GCCcore-10.3.0
1.3-GCCcore-9.3.0
```

1.789 networkx

Description

networkx is a general purpose graph library for python3 written in Rust to take advantage of the performance and safety that Rust provides. It was built as a replacement for qiskit's previous (and current) networkx usage (hence the name) but is designed to provide a high performance general purpose graph library for any python application. The project was originally started to build a faster directed graph to use as the underlying data structure for the DAG at the center of qiskit-terra's transpiler, but it has since grown to cover all the graph usage in Qiskit and other applications.

More Information

<https://retworkx.readthedocs.io/en/latest/index.html>

Available Versions:

0.6.0-foss-2020a-Python-3.8.2
0.9.0-foss-2021a

1.790 rgdal

Description

Provides bindings to the 'Geospatial' Data Abstraction Library ('GDAL') ($\geq 1.11.4$ and $\leq 2.5.0$) and access to projection/transformation operations from the 'PROJ.4' library.

More Information

<http://rgdal.r-forge.r-project.org/>

Available Versions:

1.4-8-foss-2020a-R-4.0.2
1.5-23-foss-2021a-R-4.1.0

1.791 rose

Available Versions:

2019.01.4

1.792 rosetta

Available Versions:

3.10

1.793 rpy2

Description

rpy2 is an interface to R running embedded in a Python process.

More Information

<https://rpy2.bitbucket.io/>

Available Versions:

3.2.6-foss-2019b-Python-3.7.4

1.794 sabre

Available Versions:

2022

1.795 samclip

Description

Filter SAM file for soft and hard clipped alignments.

More Information

<https://github.com/tseemann/samclip>

Available Versions:

0.4.0-GCCcore-11.2.0
0.2-GCCcore-7.3.0-Perl-5.28.0

1.796 scVelo

Description

scVelo is a scalable toolkit for estimating and analyzing RNA velocities in single cells using dynamical modeling.

More Information

<https://scvelo.org>

Available Versions:

0.2.3-foss-2021a

1.797 scikit-build

Description

Scikit-Build, or skbuild, is an improved build system generator for CPython C/C++/Fortran/Cython extensions.

More Information

<https://scikit-build.readthedocs.io/en/latest>

Available Versions:

```
0.11.1-GCCcore-10.3.0
0.11.1-GCCcore-11.2.0
0.11.1-foss-2020b
```

1.798 scikit-learn

Description

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.

More Information

<https://scikit-learn.org/stable/index.html>

Available Versions:

```
0.24.2-foss-2021a
0.23.1-foss-2020a-Python-3.8.2
1.1.2-foss-2022a
0.21.3-foss-2019b-Python-3.7.4
0.20.3-foss-2019a
```

1.799 scipy

Description

SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension for Python.

More Information

<https://www.scipy.org>

Available Versions:

```
1.4.1-foss-2019b-Python-3.7.4
```


1.800 screen

Available Versions:

```
2023
11
```

1.801 semver

Description

A Python module for semantic versioning. Simplifies comparing versions.

More Information

<http://semver.org/>

Available Versions:

```
2.13.0-GCCcore-10.2.0
```

1.802 seqtk

Description

Seqtk is a fast and lightweight tool for processing sequences in the FASTA or FASTQ format. It seamlessly parses both FASTA and FASTQ files which can also be optionally compressed by gzip.

More Information

<https://github.com/lh3/seqtk/>

Available Versions:

```
1.3-foss-2018b
1.3-GCC-11.2.0
```

1.803 shovill

Description

Faster SPAdes assembly of Illumina reads

More Information

<https://github.com/tseemann/shovill>

Available Versions:

```
1.1.0-foss-2018b-Python-2.7.15
```

1.804 slepc4py

Description

Python bindings for SLEPc, the Scalable Library for Eigenvalue Problem Computations.

More Information

<https://bitbucket.org/slepc/slepc4py>

Available Versions:

3.12.0-foss-2019b-Python-3.7.4
3.15.1-foss-2021a

1.805 smilei

Available Versions:

4.6

1.806 smithwaterman

Description

smith-waterman-gotoh alignment algorithm.

More Information

<https://github.com/ekg/smithwaterman>

Available Versions:

20160702-GCCcore-11.2.0

1.807 snakemake

Description

The Snakemake workflow management system is a tool to create reproducible and scalable data analyses.

More Information

<https://snakemake.readthedocs.io>

Available Versions:

6.10.0-foss-2021b
6.1.0-foss-2020b

1.808 snappy

Description

Snappy is a compression/decompression library. It does not aim for maximum compression, or compatibility with any other compression library; instead, it aims for very high speeds and reasonable compression.

More Information

<https://github.com/google/snappy>

Available Versions:

```
1.1.8-GCCcore-9.3.0
1.1.8-GCCcore-10.3.0
1.1.9-GCCcore-11.3.0
1.1.8-GCCcore-10.2.0
1.1.9-GCCcore-11.2.0
1.1.7-GCCcore-8.3.0
```

1.809 snippy

Description

Rapid haploid variant calling and core genome alignment

More Information

<https://github.com/tseemann/snippy>

Available Versions:

```
4.6.0-foss-2021b-R-4.1.2
```

1.810 snp-sites

Description

Finds SNP sites from a multi-FASTA alignment file.

More Information

<https://sanger-pathogens.github.io/snp-sites/>

Available Versions:

```
2.5.1-GCCcore-11.2.0
```

1.811 snpEff

Description

SnpEff is a variant annotation and effect prediction tool. It annotates and predicts the effects of genetic variants (such as amino acid changes).

More Information

<https://pcingola.github.io/SnpEff/>

Available Versions:

5.0e-GCCcore-11.2.0-Java-11

1.812 spaln

Description

Spaln (space-efficient spliced alignment) is a stand-alone program that maps and aligns a set of cDNA or protein sequences onto a whole genomic sequence in a single job.

More Information

<https://github.com/ogotoh/spaln>

Available Versions:

2.4.03-foss-2019b

1.813 sparsehash

Description

An extremely memory-efficient hash_map implementation. 2 bits/entry overhead! The SparseHash library contains several hash-map implementations, including implementations that optimize for space or speed.

More Information

<https://github.com/sparsehash/sparsehash>

Available Versions:

2.0.3-GCCcore-8.3.0

1.814 spdlog

Description

Very fast, header-only/compiled, C++ logging library.

More Information

<https://github.com/gabime/spdlog>

Available Versions:

1.9.2-GCCcore-10.3.0

1.815 spglib

Description

Spglib is a library for finding and handling crystal symmetries written in C.

More Information

<https://atztogo.github.io/spglib/>

Available Versions:

1.9.9-intel-2020a

1.816 spglib-python

Description

Spglib for Python. Spglib is a library for finding and handling crystal symmetries written in C.

More Information

<https://pypi.python.org/pypi/spglib>

Available Versions:

2.0.0-foss-2022a
1.16.1-foss-2021a
1.16.0-foss-2020b
2.0.0-intel-2022a

1.817 spython

Description

Singularity Python is a Python API to work with the Singularity open source software.

More Information

<https://singularityhub.github.io/singularity-cli/>

Available Versions:

0.1.14-GCCcore-10.2.0

1.818 statsmodels

Description

Statsmodels is a Python module that allows users to explore data, estimate statistical models, and perform statistical tests.

More Information

<https://www.statsmodels.org/>

Available Versions:

0.12.2-foss-2021a

1.819 sympy

Description

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.

More Information

<http://sympy.org/>

Available Versions:

1.4-foss-2019a
1.8-foss-2021a
1.6.2-foss-2020a-Python-3.8.2
1.5.1-foss-2019b-Python-3.7.4

1.820 tabixpp

Description

C++ wrapper to tabix indexer

More Information

<https://github.com/ekg/tabixpp>

Available Versions:

1.1.0-GCC-11.2.0

1.821 tbb

Description

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.

More Information

<https://github.com/oneapi-src/oneTBB>

Available Versions:

2020.3-GCCcore-11.2.0
2018_U5-GCCcore-7.3.0
2020.1-GCCcore-9.3.0
2019_U9-GCCcore-8.3.0
2020.3-GCCcore-10.3.0
2020.3-GCCcore-10.2.0

1.822 tbl2asn

Description

Tbl2asn is a command-line program that automates the creation of sequence records for submission to GenBank

More Information

<https://www.ncbi.nlm.nih.gov/genbank/tbl2asn2/>

Available Versions:

20220427-linux64

1.823 tensorboard

Description

TensorBoard is a suite of web applications for inspecting and understanding your TensorFlow runs and graphs.

More Information

<https://github.com/tensorflow/tensorboard>

Available Versions:

```
2.10.0-foss-2022a
2.8.0-foss-2021a
```

1.824 tensorflow-probability

Description

TensorFlow Probability (TFP) is a library for probabilistic reasoning and statistical analysis.

More Information

<https://www.tensorflow.org/probability>

Available Versions:

```
0.12.1-foss-cuda-2020b
0.16.0-foss-2021b
```

1.825 tesseract

Description

Tesseract is an optical character recognition engine

More Information

<https://github.com/tesseract-ocr/tesseract>

Available Versions:

```
4.1.0-GCCcore-8.2.0
5.3.0-GCCcore-11.3.0
```


1.826 testapp

Available Versions:

1.0

1.827 texinfo

Description

Texinfo is the official documentation format of the GNU project.

More Information

<https://www.gnu.org/software/texinfo/>

Available Versions:

6.7-GCCcore-8.3.0

1.828 tmux

Description

tmux is a terminal multiplexer. It lets you switch easily between several programs in one terminal, detach them (they keep running in the background) and reattach them to a different terminal.

More Information

<http://tmux.sourceforge.net/>

Available Versions:

2.3

1.829 torchtext

Description

Data loaders and abstractions for text and NLP

More Information

<https://github.com/pytorch/text>

Available Versions:

0.7.0-foss-2019b-Python-3.7.4-PyTorch-1.6.0

1.830 torchvision

Description

Datasets, Transforms and Models specific to Computer Vision

More Information

<https://github.com/pytorch/vision>

Available Versions:

0.11.3-foss-2021a-CUDA-11.3.1

1.831 tqdm

Description

A fast, extensible progress bar for Python and CLI

More Information

<https://github.com/tqdm/tqdm>

Available Versions:

4.64.0-GCCcore-11.3.0

4.41.1-GCCcore-8.3.0

4.61.2-GCCcore-10.3.0

1.832 typing-extensions

Description

Typing Extensions – Backported and Experimental Type Hints for Python

More Information

https://github.com/python/typing/blob/master/typing_extensions/README.rst

Available Versions:

3.7.4.3-GCCcore-10.2.0

3.10.0.0-GCCcore-10.3.0

4.3.0-GCCcore-11.3.0

3.7.4.3-GCCcore-8.3.0-Python-3.7.4

1.833 use.own

Available Versions:

1.834 utf8proc

Description

utf8proc is a small, clean C library that provides Unicode normalization, case-folding, and other operations for data in the UTF-8 encoding.

More Information

<https://github.com/JuliaStrings/utf8proc>

Available Versions:

```
2.7.0-GCCcore-11.3.0
2.5.0-GCCcore-10.2.0
2.6.1-GCCcore-11.2.0
```

1.835 util-linux

Description

Set of Linux utilities

More Information

<https://www.kernel.org/pub/linux/utils/util-linux>

Available Versions:

```
2.34-GCCcore-9.3.0
2.32-GCCcore-7.3.0
2.36-GCCcore-10.2.0
2.33-GCCcore-8.2.0
2.38-GCCcore-11.3.0
2.36-GCCcore-10.3.0
2.35-GCCcore-9.3.0
2.34-GCCcore-8.3.0
2.38.1-GCCcore-12.2.0
2.37-GCCcore-11.2.0
```

1.836 vcflib

Description

vcflib provides methods to manipulate and interpret sequence variation as it can be described by VCF. The Variant Call Format (VCF) is a flat-file, tab-delimited textual format intended to concisely describe reference-indexed genetic variations between individuals.

More Information

<https://github.com/vcflib/vcflib>

Available Versions:

1.0.3-foss-2021b-R-4.1.2

1.837 vt

Description

A tool set for short variant discovery in genetic sequence data.

More Information

<https://genome.sph.umich.edu/wiki/Vt>

Available Versions:

0.57721-GCC-11.2.0

1.838 wget

Description

GNU Wget is a free software package for retrieving files using HTTP, HTTPS and FTP, the most widely-used Internet protocols. It is a non-interactive commandline tool, so it may easily be called from scripts, cron jobs, terminals without X-Windows support, etc.

More Information

<https://www.gnu.org/software/wget>

Available Versions:

1.21.2-GCCcore-11.2.0
1.20.3-GCCcore-10.2.0

1.839 wgsim

Description

Wgsim is a small tool for simulating sequence reads from a reference genome.

More Information

<https://github.com/lh3/wgsim/>

Available Versions:

20111017-GCC-11.2.0

1.840 wpebackend-fdo

Description

WPE WebKit allows embedders to create simple and performant systems based on Web platform technologies. It is a WebKit port designed with flexibility and hardware acceleration in mind, leveraging common 3D graphics APIs for best performance.

More Information

<https://wpewebkit.org/>

Available Versions:

1.13.1-GCCcore-11.2.0

1.841 wtdbg2

Description

Wtdbg2 is a de novo sequence assembler for long noisy reads produced by PacBio or Oxford Nanopore Technologies (ONT). It assembles raw reads without error correction and then builds the consensus from intermediate assembly output.

More Information

<https://github.com/ruanjue/wtdbg2>

Available Versions:

2.5-GCCcore-9.3.0

1.842 wxPython

Description

Wraps the wxWidgets C++ toolkit and provides access to the user interface portions of the wxWidgets API, enabling Python applications to have a native GUI on Windows, Macs or Unix systems, with a native look and feel and requiring very little (if any) platform specific code.

More Information

<https://www.wxpython.org/>

Available Versions:

4.2.0-foss-2021b

1.843 wxWidgets

Description

wxWidgets is a C++ library that lets developers create applications for Windows, Mac OS X, Linux and other platforms with a single code base. It has popular language bindings for Python, Perl, Ruby and many other languages, and unlike other cross-platform toolkits, wxWidgets gives applications a truly native look and feel because it uses the platform's native API rather than emulating the GUI.

More Information

<https://www.wxwidgets.org>

Available Versions:

3.2.0-GCC-11.2.0

1.844 x264

Description

x264 is a free software library and application for encoding video streams into the H.264/MPEG-4 AVC compression format, and is released under the terms of the GNU GPL.

More Information

<https://www.videolan.org/developers/x264.html>

Available Versions:

20190925-GCCcore-8.3.0
20220620-GCCcore-11.3.0
20190413-GCCcore-8.2.0
20210414-GCCcore-10.3.0
20191217-GCCcore-9.3.0
20201026-GCCcore-10.2.0
20210613-GCCcore-11.2.0

1.845 x265

Description

x265 is a free software library and application for encoding video streams into the H.265 AVC compression format, and is released under the terms of the GNU GPL.

More Information

<https://x265.org/>

Available Versions:

```
3.5-GCCcore-11.2.0
3.3-GCCcore-9.3.0
3.0-GCCcore-8.2.0
3.2-GCCcore-8.3.0
3.5-GCCcore-10.3.0
3.3-GCCcore-10.2.0
3.5-GCCcore-11.3.0
```

1.846 xorg-macros

Description

X.org macros utilities.

More Information

<https://cgit.freedesktop.org/xorg/util/macros>

Available Versions:

```
1.19.3-GCCcore-10.3.0
1.19.2-GCCcore-8.2.0
1.19.2-GCCcore-9.3.0
1.19.2-GCCcore-7.3.0
1.19.2-GCCcore-10.2.0
1.19.3-GCCcore-11.2.0
1.19.3-GCCcore-12.2.0
1.19.3-GCCcore-11.3.0
1.19.2-GCCcore-8.3.0
```

1.847 xprop

Description

The xprop utility is for displaying window and font properties in an X server. One window or font is selected using the command line arguments or possibly in the case of a window, by clicking on the desired window. A list of properties is then given, possibly with formatting information.

More Information

<https://www.x.org/wiki/>

Available Versions:

```
1.2.5-GCCcore-11.2.0
1.2.4-GCCcore-8.3.0
1.2.3-GCCcore-7.3.0
1.2.5-GCCcore-10.2.0
```

1.848 xtb

Description

xtb - An extended tight-binding semi-empirical program package.

More Information

<https://xtb-docs.readthedocs.io>

Available Versions:

```
6.3.3-GCCcore-9.3.0
6.4.1-intel-2021a
```

1.849 xxd

Description

xxd is part of the VIM package and this will only install xxd, not vim!xxd converts to/from hexdumps of binary files.

More Information

<https://www.vim.org>

Available Versions:

```
8.2.4220-GCCcore-11.2.0
8.2.4220-GCCcore-11.3.0
```

1.850 yaff

Description

Yaff stands for 'Yet another force field'. It is a pythonic force-field code.

More Information

<https://molmod.github.io/yaff/>

Available Versions:

```
1.6.0-intel-2020a-Python-3.8.2
1.6.0-foss-2020a-Python-3.8.2
```


1.851 yaml-cpp

Description

yaml-cpp is a YAML parser and emitter in C++ matching the YAML 1.2 spec

More Information

<https://github.com/jbeder/yaml-cpp>

Available Versions:

0.7.0-GCCcore-10.3.0

1.852 zlib

Description

zlib is designed to be a free, general-purpose, legally unencumbered – that is, not covered by any patents – lossless data-compression library for use on virtually any computer hardware and operating system.

More Information

<https://www.zlib.net/>

Available Versions:

1.2.11-GCCcore-10.3.0
 1.2.11-GCCcore-10.2.0
 1.2.8
 1.2.11-GCCcore-9.3.0
 1.2.11-GCCcore-8.3.0
 1.2.12
 1.2.11-GCCcore-8.1.0
 1.2.11-GCCcore-7.3.0
 1.2.12-GCCcore-11.3.0
 1.2.11
 1.2.11-intel-2020a
 1.2.12-GCCcore-12.2.0
 1.2.11-GCCcore-11.2.0
 1.2.11-GCCcore-8.2.0

1.853 zstd

Description

Zstandard is a real-time compression algorithm, providing high compression ratios. It offers a very wide range of compression/speed trade-off, while being backed by a very fast decoder. It also offers a special mode for small data, called dictionary compression, and can create dictionaries from any sample set.

More Information

<https://facebook.github.io/zstd>

Available Versions:

1.4.4-GCCcore-8.3.0
1.5.0-GCCcore-11.2.0
1.5.2-GCCcore-11.3.0
1.4.5-GCCcore-10.2.0
1.4.9-GCCcore-10.3.0
1.5.2-GCCcore-12.2.0
1.4.4-GCCcore-9.3.0