Software

Here you can find a list of the installed software. It is possible that in the meantime new software packages are installed, that have not yet been added to this list. To get an exact overview of all available modules and their versions, you can query a list via the command:

```
module avail
```

For software requests please contact us: phoenix-support@tu-bs.de.

Chemistry

- Gromacs - A versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.
- NAMD - A parallel, object-oriented molecular dynamics code designed for high-performance simulations of large biomolecular systems using force fields.
- LAMMPS - A parallel, classical potential molecular dynamics code for solid-state materials, soft matter and coarse-grained or mesoscopic systems.
- LIGGGHTS - An Open Source Discrete Element Method Particle Simulation Software.
- DL_POLY Classic - A general purpose classical molecular dynamics (MD) simulation software.
- Gaussian - A general purpose computational chemistry software package.
- GOMC - A software for simulating molecular systems using the Metropolis Monte Carlo algorithm.
- Towhee - A Monte Carlo molecular simulation code originally designed for the prediction of fluid phase equilibria using atom-based force fields.

Biology

- Bowtie - A fast and memory-efficient short read aligner that aligns short DNA sequences to the human genome.
- BLAST - A basic local alignment search tool that finds regions of local similarity between protein or nucleotide sequences.
- Exonerate - A generic tool for pairwise sequence comparison with many alignment models, either exhaustive dynamic programming or a variety of heuristics.
- ANTs - A tool for high-dimensional mappings to capture the statistics of brain structure and function.

- SAMtools - A Sequence Alignment/Map format for storing large nucleotide sequence alignments.
- trimAl - A tool for the automated removal of spurious sequences or poorly aligned regions from a multiple sequence alignment.

Engineering

- ABAQUS - A Finite Element Analysis Package for Engineering Application.
- ANSYS CFX - A computational fluid dynamics solver focused on turbo-machinery (vertex-centered FVM).
- ANSYS Fluent - A general computational fluid dynamics solver (cell-centered FVM).
- ANSYS Mechanical - A Package for Coupled Physics Simulations.
- LS-DYNA - One of the most advanced simulation tools for nonlinear structural analysis, its core-competency lies in highly nonlinear transient dynamic finite element analysis (FEA).
- OpenFOAM - An object-oriented Computational Fluid Dynamics (CFD) toolkit.
- ParaView - An interactive data analysis and visualisation tool with 3D rendering capability.
- FDS - A large-eddy simulation code for low-speed flows, with an emphasis on smoke and heat transport from fires.
- HyperWorks - A CAE program that enables finite element analysis, modeling, and simulation.
- LS-DYNA - An advanced general-purpose multiphysics simulation software package, corecompetency is highly nonlinear transient dynamic finite element analysis (FEA) using explicit time integration.
- PAM-CRASH - A software package used for crash simulation and the design of occupant safety systems, primarily in the automotive industry.
- SU2 - An open-source suite for multiphysics simulation and design.

Numerics

- OpenBLAS - BLAS (Basic Linear Algebra Subprograms).
- FFTW3 - A C-subroutine library for computing discrete Fourier transforms.
- GSL - The GNU Scientific Library (GSL)- a numerical library for C and C++ programmers.
- Scotch - Software package and libraries for sequential and parallel graph partitioning, static mapping, sparse matrix block ordering, and sequential mesh and hypergraph partitioning.
- METIS - A set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices.
- Octave - A software featuring a high-level programming language, primarily intended for numerical computations, data analysis and visualisation.

- Eigen - A C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
- Matlab - A proprietary multi-paradigm programming language and numeric computing environment that allows matrix manipulations, plotting of functions and data, among other things.
- PETSc - A suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations.

Data manipulation, tools and libraries

- HDF5 - A hierarchical data format.
- NCO - A toolkit to manipulate and analyze data stored in NetCDF-accessible formats.
- NetCDF - Network Common Data Format, a set of software libraries and machine-independent data formats.
- boost - Boost C++ libraries that provides support for tasks and structures such as linear algebra, pseudorandom number generation, multithreading, image processing, regular expressions, and unit testing.
- CGAL - A computational geometry algorithms library.
- CGNS - A general, portable, and extensible standard for the storage and retrieval of computational fluid dynamics (CFD) analysis data.
- curl - A command line tool and library for transerring data with URLs.
- OpenSSL - A software library for applications that secure communications over computer networks against eavesdropping or need to identify the party at the other end.

Development tools, compilers, translators, languages, performance analysis

- Charm++ - A parallel object-oriented programming framework.
- Patchelf - A simple utility for modifying existing ELF executables and libraries.
- Python - A high-level, general-purpose programming language.
- CMake - A cross-platform family of tools designed to build, test and package software.
- GCC - A GNU Compiler Collection for C, C++, Fortran, Go, Objc, Objc++ and Lto.
- Make - A GNU tool which controls the generation of executables and other non-source files of a program from the program's source files.
- OpenMPI - An open source Message Passing Interface (MPI) implementation.
- MPICH - A high performance and widely portable implementation of MPI.
- Intel MPI - A MPI implementation of Intel with two compiler wrappers (for GCC and for Intel compilers).

- MVAPICH - A MPI implementation, that particularly performs good on computing systems using InfiniBand and Omni-Path.
- Threading Building Blocks (TBB) - A C++ template library developed by Intel for parallel programming on multi-core processors.
- Binutils - A collection of binary tools, e.g. GNU linker, GNU assembler.
- MPC - A GNU C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result.
- MPFR - A GNU C library for multiple-precision floating-point computations with correct rounding.
- GMP - A GNU library for arbitrary precision arithmetic.
- LLVM - A set of compiler and toolchain technologies, which can be used to develop a front end for any programming language and a back end for any instruction set architecture.
- Ccache - A compiler cache that speeds up recompilation.
- Clang - A compiler front end for languages in the C language family, as well as the OpenMP, OpenCL, RenderScript, CUDA, and HIP frameworks.
- Intel System Studio - An all-in-one, cross-platform tool suite, purpose-built to simplify system bring-up and improve system performance on Intel platforms.
- Intel Advisor - A design and analysis tool for SIMD vectorization, threading, memory use and GPU offload optimization.
- Julia - A general-purpose, high-level, high-performance, dynamic programming language. Many features are well suited for numerical analysis and computational science.
- Lua - A powerful, efficient, lightweight, embeddable scripting language. It supports procedural programming, object-oriented programming, functional programming, data-driven programming, and data description.
- DejaGnu - A framework for testing other programs. Its purpose is to provide a single front end for all tests.
- GNU Debugger (GDB) - A portable debugger that works for many programming languages.
- Bison - 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.
- Flex - A fast lexical analyzer generator to recognize lexical patterns in text.
- GNU C Library (glibc) - A library that provides the core libraries for the GNU system.
- CUDA - A parallel computing platform and programming model developed by NVIDIA for general computing on graphical processing units (GPUs).

Computer Graphics

- NVIDIA OptiX - An application framework for achieving optimal ray tracing performance on the GPU.

- OpenCV - A library of programming functions for image processing and computer vision.
- Embree - A collection of high-performance ray tracing kernels, developed at Intel.

Visualisation

- ParaView - An interactive data analysis and visualisation tool with 3D rendering capability.
- VisIt - An interactive parallel visualization and graphical analysis tool for viewing scientific data.
- VTK - A visualization toolkit for manipulating and displaying scientific data.

Miscellaneous

- Singularity - Enables users to have full control of their environment.
- Texinfo - A typesetting syntax used for generating documentation in both on-line and printed form (creating filetypes as dvi, html, pdf, etc., and its own hypertext format, info) with a single source file.
- Git - A fast, scalable, distributed revision control system.

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