Software for HPC

Software is generally made available via the Environment Modules. The output of the command `module avail` provides an up-to-date list of available libraries and versions.

Specific information about the application, links to the documentation and – if applicable – licensing restrictions are provided via the command `module help <appl>`.

Categories

- Compilers and Languages for HPC
- Environment Modules
- I/O Libraries and Tools for HPC Systems
- Numerical Libraries for HPC Applications
- Parallel Execution Environments for HPC Systems
- Performance and Code Analysis Tools for HPC
- Scientific Application Packages
- Tools for Access and Data Transfer on LRZ HPC systems
- Workflow Tools for HPC Applications

Full list

- Compilers and Languages for HPC
  - GNU Compiler Collection
  - Intel Compilers
  - NAG Fortran Compiler
  - Portland Group Compiler
  - Python for HPC
  - The Fortran Programming Language
- Environment Modules
  - Spack Modules Release 18.2
- I/O Libraries and Tools for HPC Systems
  - ADIOS (Adaptable IO System)
  - CGNS (CFD General Notation System)
  - Darshan
  - HDF5 (Hierarchical Data Format Version 5)
  - MPI-IO (Message-Passing Interface IO)
  - NCL (NCAR Command Language)
  - NetCDF (Network Common Data Form)
  - PnetCDF (Parallel I/O Library for NetCDF Files)
  - SIONlib (Scalable I/O library)
- Numerical Libraries for HPC Applications
  - ARPACK - Arnoldi Package for sparse Eigenvalue Problems
  - BLAS and LAPACK: Numerical Linear Algebra
  - FFTW - Fastest Fourier Transform in the West
  - GSL: GNU Scientific Library
  - Intel Performance Libraries (MKL, TBB, IPP, DAAL)
  - ScaLAPACK - scalable parallel LAPACK
- Parallel Execution Environments for HPC Systems
  - MPI - Message Passing Interface
  - OpenMP - shared memory and device parallelism
  - PGAS parallel languages
- Performance and Code Analysis Tools for HPC
  - Intel Advisor: A tool to guide parallelization
  - Intel Inspector: Assuring Correctness of scientific codes
  - Intel Tracing Tools: Profiling and Correctness checking of MPI programs
  - Intel VTune Amplifier and Performance Snapshots
- Scientific Application Packages
  - Astrophysics on HPC Systems
  - Bioinformatics Tools for HPC Systems
  - Computational Chemistry and Material Science Software
  - Computer Algebra for HPC
  - Data Analysis and Statistics Software for HPC Systems
  - Engineering and Finite Elements on HPC Systems
  - Machine Learning on HPC Systems
  - Molecular Modelling Software for HPC Systems
  - Visualisation Software on HPC Systems
- Tools for Access and Data Transfer on LRZ HPC systems
  - GSISSH on LRZ HPC Systems
  - Secure Shell on LRZ HPC Systems
- Workflow Tools for HPC Applications
  - Doxygen Documentation Generator
  - Eclipse CDT
  - Java