HPC Software and Programming Support

Module system

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, tools and packages, and optionally their versions. Specific information about the application, links to the documentation and – if applicable – licensing restrictions are provided via the command

```
module help <appl>
```

or to view the specific settings done by the module:

```
module show <appl>
```

Categories

- Access and Data Transfer on LRZ HPC systems
- Compilers and Languages for HPC
- Environment Modules
- IO Libraries and Tools for HPC Systems
- Irztools and lrzlib on SuperMUC-NG
- Numerical Libraries for HPC Applications
- Parallel Execution Environments for HPC Systems
- Performance and Code Analysis Tools for HPC
- Scientific Application Packages
- Virtualization and Containers
- Workflow Tools for HPC Applications

- Submit a Ticket for Support

Full list

- Access and Data Transfer on LRZ HPC systems
  - GSISSH on LRZ HPC Systems
  - ssh - Secure Shell on LRZ HPC Systems
- Compilers and Languages for HPC
  - Comparison of Compiler Options (intel vs. pgi vs. gcc)
  - GNU Compiler Collection
  - Intel Compilers
    - Most important Intel Compiler Options and Directives
  - NAG Fortran Compiler
  - Portland Group Compiler
  - Python for HPC
  - The Fortran Programming Language
- Environment Modules
  - Spack Modules Release 18.2
  - Spack Modules Release 19.1
- IO Libraries and Tools for HPC Systems
  - ADIOS
  - CGNS
  - Darshan
  - HDF5
  - MPI-I0
  - NCL
  - NetCDF
  - PnetCDF
  - SIONlib
- Irztools and lrzlib on SuperMUC-NG
- 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
    - FGSL - A Fortran interface to the GNU Scientific Library
  - Intel Performance Libraries (MKL, TBB, IPP, DAAL)
  - ScALAPACK - scalable parallel LAPACK
- Parallel Execution Environments for HPC Systems
  - MPI - Message Passing Interface
    - Intel MPI
- OpenMPI
- OpenMP - shared memory and device parallelism
- PGAS parallel languages
  - Coarray Fortran on LRZ's HPC systems
  - Cray Chapel on LRZ's HPC systems
  - Unified Parallel C on LRZ's HPC systems
- Performance and Code Analysis Tools for HPC
  - Energy Aware Runtime
  - 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
    - Cell Ranger
    - Hail
    - PICRUS2
  - Computational Chemistry, Materials Science and Molecular Modelling Software for HPC Systems
    - ABINIT
    - AMBER
    - CP2K
    - CPMD
    - Dalton
    - GAMESS
    - Gaussian
    - GROMACS
    - lammps
    - MOLPRO
    - NAMD
    - NWChem
    - ORCA
    - Quantum ESPRESSO
    - SCHRÖDINGER
    - SIESTA
    - TURBOMOLE
    - VASP
    - Wannier90
    - WIEN2k
  - Computer Algebra for HPC
    - Maple
    - Mathematica on HPC
    - MATLAB on HPC Systems
    - Octave on HPC
  - Data Analysis and Statistics Software for HPC Systems
    - Gurobi Optimization on HPC Systems
    - How to setup a Jupyter Server in the Cloud for Courses
    - Jupyter Notebook on the Linux Cluster
    - R on HPC Systems
    - Spark on the Linux Cluster
  - Engineering and Finite Elements on HPC Systems
    - ANSA Pre-processor
    - ANSYS on HPC Systems
    - Comsol on HPC Systems
    - MSC Nastran on HPC Systems
    - OpenFOAM on HPC Systems
    - Patran
    - Siemens PLM on HPC Systems
  - Machine Learning on HPC Systems
    - Tensorflow on CoolMUC-3
  - Visualisation Software on HPC Systems
    - ParaView
    - PyMOL
    - Tecplot 360
    - Visit
    - VMD
- Virtualization and Containers
  - Charliecloud at LRZ
- Workflow Tools for HPC Applications
  - Doxygen Documentation Generator
  - Eclipse CDT
  - Java
- Submit a Ticket for Support