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
    - Intel OneAPI
    - NAG Fortran Compiler
    - Portland Group Compiler
    - Python for HPC
    - The Fortran Programming Language
- Environment Modules
  - Building software in user space with spack
  - Spack Modules Release 18.2
  - Spack Modules Release 19.1
  - Spack Modules Release 20.1
- IO Libraries and Tools for HPC Systems
  - ADIOS
  - CGNS
  - Darshan
  - HDF5
  - MPI-IO
  - 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
  - CERN Root - A modular scientific software toolkit.
  - 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)
- SLES15: Intel Performance Libraries (MKL, TBB, IPP, DAAL)
- ScalAPACK - scalable parallel LAPACK

- **Parallel Execution Environments for HPC Systems**
  - HPX - A Parallel Standard Conformal C++ Library
  - 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
    - PICRUSt2
  - Computational Chemistry, Molecular Modelling and Materials Science Software for HPC Systems
    - ABINIT
    - AMBER
    - CP2K
    - CPMD
    - Dalton
    - GAMESS
    - Gaussian
    - GROMACS
    - lammps
    - MOLPRO
    - NAMD
    - NWChem
    - OpenMM
    - ORCA
    - PLUMED
    - Quantum ESPRESSO
    - Schrodinger
    - SIEESTA
    - 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
  - Dassault Systems Software on HPC Systems
  - Gmsh
  - 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**
  - Gnuplot
  - Jmol
  - 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