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
- lrztools 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
  - 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
- lrztools 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)
  - 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
    • ORCA
    • PLUMED
    • Quantum ESPRESSO
    • SCHRODINGER
    • 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
    • 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
    • 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