HPC Software and Programming

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>`.

- Code and Performance Analysis Tools for HPC Systems
  - 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

- Compilers and Languages for HPC
  - GNU Compiler Collection
  - Intel Compilers
  - NAG Fortran Compiler
  - Overview: Compilers, Languages, Programming Tools
  - Portland Group Compiler
  - The Fortran Programming Language

- Environment Modules
  - HPC Environment: Spack Generated Modules

- I/O Libraries and Tools for HPC Systems
  - Adaptable IO System (ADIOS)
  - CFD General Notation System (CGNS)
  - Darshan Tool
  - HDF5 (Hierarchical Data Format Version 5)
  - MPI-IO (Message-Passing Interface IO)
  - NCAR Command Language (NCL)
  - Network Common Data Form (NetCDF)
  - PnetCDF (Parallel I/O Library for NetCDF Files)
  - Scalable I/O library (SIONlib)

- 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

- Scientific Application Packages
  - Bioinformatics Tools for HPC Systems
  - Computational Chemistry Software for HPC Systems
  - 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
  - Scientific Application Packages: Astrophysics
  - Visualisation Software for HPC Systems

- Secure Shell on LRZ HPC Systems

- Workflow Tools for HPC Applications
  - Documentation Generators - Doxygen
  - IDEs - Eclipse CDT
  - Interpreters - Java programming language