Scientific Application Packages

- **Astrophysics on HPC Systems**
- **Bioinformatics Tools for HPC Systems**
  - Cell Ranger
  - Hail
  - PICRUSt2
- **Computational Chemistry and Material Science Software**
  - ABINIT
  - CP2K
  - CPMD
  - GAMESS
  - Gaussian
  - MOLPRO
  - ORCA - An ab initio, DFT and semiempirical SCF-MO package
  - Quantum ESPRESSO
  - Schrödinger-Suite
  - SIESTA
  - TURBOMOLE
  - VASP
  - Wannier90
  - WIEN2k
- **Computer Algebra for HPC**
  - Mathematica on HPC
  - MATLAB on HPC Systems
  - Octave on HPC
- **Data Analysis and Statistics Software for HPC Systems**
  - Gurobi Optimization on HPC Systems
  - 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
- **Machine Learning on HPC Systems**
  - Tensorflow on CoolMUC-3
- **Molecular Modelling Software for HPC Systems**
  - AMBER
  - GROMACS
  - lammps
  - NAMD
  - NWChem
  - Schrödinger
- **Visualisation Software on HPC Systems**
  - ParaView
  - Tecplot 360
  - VMD