Software

OpenFOAM
Nov 03, 2021 • updated by Jack Ogaja • view change

R
Sep 10, 2021 • updated by Christian Tuma • view change

ParaView
Sep 10, 2021 • updated by Christian Tuma • view change

Charm++
Sep 10, 2021 • updated by Christian Tuma • view change

Python
Sep 09, 2021 • updated by Marcus Boden • view change

Chemistry

Add new Chemistry Software

- GPAW — a density functional theory Python code based on the projector-augmented wave method.
- GROMACS — A versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.
- NAMD — a parallel, object-oriented molecular dynamics code designed for high-performance simulations of large biomolecular systems using force fields.
- RELION — REgularised LIkelihood OptimisatioN is a stand-alone computer program that employs an empirical Bayesian approach to refinement of (multiple) 3D reconstructions or 2D class averages in electron cryo-microscopy(cryo-EM)
- VASP — A complex package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations using pseu-do-po-ten-tials or the projector-augmented wave method and a plane wave basis set.

- ASE – The Atomic Simulation Environment – a set of tools and Python modules for setting up, manipulating, running, visualizing, and analyzing atomistic simulations.
- GPAW – A density functional theory Python code based on the projector-augmented wave method. It uses real-space uniform grids and multi-grid methods, atom-centered basis functions, or plane waves.
- CP2K – A package for atomistic simulations of solid state, liquid, molecular, and biological systems offering a wide range of computational methods; see "module avail cp2k"
- LAMMPS – A parallel, classical potential molecular dynamics code for solid-state materials, soft matter and coarse-grained or mesoscopic systems.
- TURBOMOLE – A program package for *ab initio* electronic structure calculations. (see "module avail turbomole" on the SMP cluster)
- NWChem – A general computational chemistry code with capabilities from classical molecular dynamics to highly correlated electronic structure methods, designed to run on massively parallel machines.
- MOLPRO – A comprehensive system of ab initio programs for advanced molecular electronic structure calculations.
- PLUMED – A tool for trajectory analysis and plugin for molecular dynamics codes for free energy calculations in molecular systems
- CPMD – A plane wave / pseudopotential implementation of DFT, designed for massively parallel ab-initio molecular dynamics.
- Quantum ESPRESSO – An integrated suite of codes for electronic structure calculations and materials modeling at the nanoscale, based on DFT, plane waves, and pseudopotentials.
- BandUP – Band unfolding for plane wave based electronic structure calculations.

Data manipulation, tools and libraries

Add new Data Manipulation Software

- CDO — The Climate Data Operators
- ECCODES — ECMWF application programming interface
- HDF5 Libraries and Binaries — HDF5 - hierarchical data format
- libtiff — A software package containing a library for reading and writing _Tag Image File Format_(TIFF), and a small collection of tools for simple manipulations of TIFF images
- NCO — The NetCdf Operators
- netCDF — Network Common Data Form

- Octave — Add short Excerpt. This will be included in the Software list
- pigz — A parallel implementation of gzip for modern multi-processor, multi-core machine
- PROJ — Cartographic Projections Library
- R — R - statistical computing and graphics
- Szip — Szip, fast and lossless compression of scientific data
- The Unidata UDUNITS2 Package — Conversion and manipulation of units

- Boost – Boost C++ libraries
- CGAL – The Computational Geometry Algorithms Library

Development tools, compilers, translators, languages, performance analysis

Add new Development/Debugging Tool or Compiler

- antlr — Another Tool for Language Recognition
- Arm DDT — Parallel debugger, including MPI/OpenMP programs.
- Charm++ — Parallel Programming Framework
- Patchelf — a simple utility for modifying existing ELF executables and libraries.
- Python — An Overview over the different Python Versions available on our System
- Valgrind instrumentation framework — an instrumentation framework for building dynamic analysis tools

- CMake – CMake build environment
- GCC – GNU Compiler Collection for C, C++, Fortran, Go, Objc, Objc++ and Lto
- OpenMPI – High Performance Message Passing Library

Engineering

Add Engineering Software

- ABAQUS — A Finite Element Analysis Package for Engineering Application
- ANSYS CFX — Computational fluid dynamics solver focused on turbo-machinery (vertex-centered FVM)
- ANSYS Fluent — General computational fluid dynamics solver (cell-centered FVM)
- ANSYS Mechanical — A Package for Coupled Physics Simulations
- Foam-extend — The Open Source CFD Toolbox
- How to bring your own license
- OpenFOAM — An object-oriented Computational Fluid Dynamics(CFD) toolkit
- STAR-CCM+ — A Package for Computational Fluid Dynamics Simulations

- ParaView — An interactive data analysis and visualisation tool with 3D rendering capability

Miscellaneous

Add new Miscellaneous Software

- nocache — nocache - minimize caching effects in lustre filesystems
- Singularity — enables users to have full control of their environment

- texlive – LaTeX distribution, typesetting system
- git – A fast, scalable, distributed revision control system

Numerics

Add new Numerics Software

- BLAS — BLAS (Basic Linear Algebra Subprograms)
- FFTW3 — A C-subroutine library for computing discrete Fourier transforms
- GSL — The GNU Scientific Library (GSL)- a numerical library for C and C++ programmers
- MUMPS — MUltifrontal Massively Parallel sparse direct Solver.
- NFFT — Discrete Fourier transform (DFT) in one or more dimensions
- ScaLAPACK — Scalable LAPACK
- Scotch — Software package and libraries for sequential and parallel graph partitioning, static mapping, sparse matrix block ordering, and sequential mesh and hypergraph partitioning.

- METIS – A set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices.

- ParMETIS – An MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices.

Visualisation

Add new Visualisation Software

- Ferret - Data Visualization and Analysis — your ferret in large and complex gridded data sets.
- GraDS — An interactive desktop tool for easy access, manipulation, and visualization of earth science data
- NCL
- NcView — Ncview - a visual browser for netCDF formated files.
- ParaView — An interactive data analysis and visualisation tool with 3D rendering capability
- pyfesom2 — Python library and tools for handling of FESOM2 ocean model output