Installed software

Consult the available software installed and ready to use in our HPC machines, including available versions.

If you would like us to install a program which is not currently available, please contact us using our ***support portal*** (registration required).

ADF

Purpose: Density Functional Theory
Latest version: 2021.104
License: ⚠ Must be provided by the user.
Proprietary License _ext-link
Website: *https://www.scm.com/ _ext-link*

Amsterdam Density Functional (ADF) is a proprietary software suite for density functional theory (DFT) calculation of molecular systems, especially inorganic systems.

ADF implements Kohn-Sham-type DFT calculations to finite molecular systems, in gas phase or in solution. It applies LDA, GGA, and in some cases hybrid and meta-GGA functionals, including relativistic effects, to Slater-type orbitals.

Amber

Purpose: Molecular Dynamics
Latest version: 20
Licence: ⚠ Must be provided by the user.
Proprietary licence ext-link
Website: *http://ambermd.org/_ext-link*

Amber is a collection of programs for setting-up, running and analysing molecular dynamics simulations.

Amber refers both to a collection of about 50 programs for building, configuring and minimising molecular structures, setting up force fields, running simulations, analysing trajectories, and computing system properties, and to a force field for biomolecules implemented by the Amber programs.

ASE

Purpose: Photo processing
Latest version: 3.16.2
Licence: Free of use
GNU LGPL
Website: *https://wiki.fysik.dtu.dk /ase/_ext-link*

The **A**tomic **S**imulation **E**nvironment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. The code is freely available under the GNU LGPL license.

ClustalW

Purpose: Bioinformatics
Latest version: 2.1
Licence: Free of use for academics users
Mixed
Website: *http://www.clustal.org /omega/ _ext-link*

Clustal is a series of widely used computer programs used in Bioinformatics for multiple sequence alignment.

ClustalW is the third generation, released in 1994, greatly improved upon the previous versions. It improved upon the progressive alignment algorithm in various ways, including allowing individual sequences to be weighted down or up according to similarity or divergence respectively in a partial alignment. It also included the ability to run the program in batch mode from the command line.

Code_Aster

Purpose: Finite Element Analysis
Latest version: 14.4
Licence: Free of use
GNU GPL _ext-link
Website: *https://code-aster.org/ _ ext-link*

Code_Aster is a computer-assisted engineering suite, with a focus on finite element methods.

The core of Code_Aster is a finite element solver for structural analysis, with additional programs for thermal flows, linear and non-linear static and dynamic analysis, fatigue, damage and fracture tools and multi-physics coupling. A companion open source pre- and post-processor, Salome, is also available.

Conda

Purpose: Statistics and Plotting
Latest version: 23.3.0
Licence: Free of use
Open Source - BSD ext-link
Website: *https://conda.io/en /latest/ ext-link*

Conda is an open source package management system and environment management system that quickly installs, runs and updates packages and their dependencies. It, also, easily creates, saves, loads and switches between environments. It was created for Python programs, but it can package and distribute software for any language (Python, R, Ruby, Lua, Scala, Java, JavaScript, C/ C++, FORTRAN...).

The 3.x version of Python should be your default choice, as the 2.7 version is ***deprecated as of 2020ext-link***.

CP2K

Purpose: Ab initio
Latest version: 9.1.0
License: Free of use
GNU GPL _ext-link
Website: *https://www.cp2k.org/_e xt-link*

CP2K is a program for ab initio electronic structure calculations and molecular dynamics.

CP2K is geared towards, but not restricted to, massive parallel computations using mixed plane-wave/Gaussian bases and pseudopotentials. It can implement a variety of methods, including semiempirical, HF, DFT (LDA, GGA, meta-GGA, hybrid), MP2 and TD-DFT, for molecular and periodic systems.

It can also perform both classical and ab initio molecular dynamics, Monte Carlo, and minimum energy path calculations.

CPMD

Purpose: Molecular Dynamics
Latest version: 4.1
Licence: ✅ Free of use for academics users
Mixed
Website: *http://www.cpmd.org/ _ext-link*

The **CPMD** code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.

CRYSTAL

Purpose: Electronic Structure Calculations
Latest version: 17
Licence: ⚠ Must be provided by the user.
Proprietary _ext-link
Website: *http://www.crystal.unito.it/ _ext-link*

CRYSTAL performs ab initio calculations of the ground state energy, energy gradient, electronic wave function and properties of periodic systems. Hartree-Fock or KohnSham Hamiltonians can be used.

Environment Modules

Purpose: Libraries & Environment Modules
Latest version: 3.2.10
Licence: Free of use
GNU GPL _ext-link
Website: *https://modules.sourceforge.net/ _ext-link*

Environment Modules is a software package released under GNU-GPL license and available at SourceForge website. It consists of an amount of instructions and information files (modulefiles), which provides an easy interface for the dynamic modification of a user's environment.

Each module contains the information needed to initialize the shell for an application. That is why it is useful when working with different versions from a same program. Modules can be loaded and unloaded dynamically and atomically in a clean fashion. Users can easily control their environment through these simple processes of loading and unloading modules.

FDS

Purpose: Fire Simulator
Latest version: 6.7.1
Licence: Free of use
Open Source
Website: *https://pages.nist.gov/fds-smv/_ext-link*

FDS is a program for fire simulations.

FDS is a computational fluid dynamics (CFD) program which implements large eddy simulations (LES) for the analysis of fire evolution and fire-driven fluid flows, including smoke and heat transfer. Its companion program Smokeview allows for the visualisation and analysis of fire dynamics.

FHI-aims

Purpose: Electronic Structure Calculations
Latest version: 220117
Licence: ⚠ Must be provided by the user.
Proprietary _ext-link
Website: *http://aimsclub.fhi-berlin.mpg.de/ _ext-link*

The **F**ritz **H**aber **I**nstitute ***ab-initio*** **m**olecular **s**imulations (FHI-aims) is a computer program package for computational materials science based on quantum-mechanical first principles. By using DFT or HF, it allows the resolution of molecular problems or periodical systems, the optimization of structures and the resolution of transport problems.

GAMESS

Purpose: Electronic Structure Calculations
Latest version: 2018
Licence: ✓ Free of use
Free of charge research licence _ext-link
Website: *http://www.msg.ameslab.gov/_ext-link*

GAMESS is a program for ab initio molecular electronic structure calculations.

Functionality includes HF, GVB, MCSCF, CI, MP2, CC and DFT methods, excited states, geometry optimisation, vibrational frequencies, solvation effects, relativistic corrections, pseudopotentials and nuclear wavefunctions.

Gaussian

Purpose: Electronic Structure Calculations
Latest version: Gaussian16 C.02
License: ✓ Provided by CSUC
Closed-source
Website: *http://gaussian.com/_ext-link*

Gaussian is a program implementing a variety of computational chemistry methods.

The range of computational methods includes molecular mechanics, semi-empirical methods, Hartree-Fock SCF, Møller-Plesset perturbation theory, DFT methods, QM/MM calculations, CI methods and CC calculations. Calculations employing these methods can be carried out in order to optimise molecular geometry, electronic structure and derived chemical properties.

Gromacs

Purpose: Molecular Dynamics
Latest version: 2021.3
License: Free of use
GNU LGPL _ext-link
Website: *http://www.gromacs.org/ _ext-link*

Gromacs is a program for general molecular dynamics, notable for its fast computation of 1-4 interactions.

It can implement regular molecular dynamics simulations using a variety of integrators, Langevin dynamics, energy minimisation, test-particle insertion, etc. It implements a variety of methods to calculate electrostatics and Van der Waals interactions, thermostats and barostats, 2- and 3-dimensional periodic boundary conditions, etc.

LAMMPS

Purpose: Molecular Dynamics
Latest version: 23Jun2022
License: Free of use
GNU GPL _ext-link
Website: *http://lammps.sandia.gov/ _ext-link*

LAMMPS is a classical molecular dynamics application.

It performs atomistic or coarse-grained simulations of molecular, macromolecular and mesoscale systems with a variety of force fields.

MOLCAS

Purpose: Electronic Structure Calculations
Latest version: 8.2
License: ⚠ Must be provided by the user.
Proprietary
Website: *http://www.molcas.org/_ext-link*

MOLCAS is an electronic structure calculations package.

It provides a particular emphasis on multi-configurational methods for highly degenerated ground states. MOLCAS can implement methods for single determinant ground states (SCF, MP2, CC, DFT), but focuses on treating accurately highly degenerate states (excited states, heavy metals, transition states, etc.) through methods such as multi-configurational self-consistent field (MCSCF), complete active space (CASSCF), and including correlation effects via second-order perturbation theory (CASPT2).

Molden

Purpose: Visualization
Latest version: 5.8
Licence: ✓ Free of use for non-commercial users
Proprietary _ext-link
Website: *http://cheminf.cmbi.ru.nl/molden/ _ext-link*

Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK , GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac, it also supports a number of other programs via the Molden Format.

NAMD

Purpose: Molecular Dynamics
Latest version: 2.13
License: ✓ Free of use for non-commercial users
Mixed license _ext-link
Website: *http://www.ks.uiuc.edu/ _ext-link*

NAMD is a molecular dynamics package.

NAMD implements standard MD capabilities (variety of integrators, thermostats, barostats, force field compatibility, PME electrostatics, time-step integration, replica exchange, free energy calculations, etc.).

NAMD is also available to run on GPU NODES showing up to 8X performance (at same number of cores as std nodes). To perform GPU computations, please ***contact us***.

NewtonX

Purpose: Excited-state molecular dynamics
Latest version: 2b18
Licence: ✔ Free of use for non-commercial users
Proprietary _ext-link
Website: *http://newtonx.org/ _ext-link*

NewtonX is a general-purpose program package for excited-state molecular dynamics, including nonadiabatic methods (Trajectory Surface Hopping), and can be used to simulate absorption and emission spectra with the nuclear ensemble approach.

NewtonX modular development allows it to be easily linked to any quantum chemistry package that can provide energy gradients and nonadiabatic couplings

NWChem

Purpose: Electronic Structure Calculations
Latest version: 6.8
License: ✔ Free of use
EDL _ext-link
Website: *http://www.nwchem-sw.org/ _ext-link*

NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.

OpenFOAM

Purpose: Computational Fluid Dynamics
Latest version: v2112
Licence: Free of use
GNU GPL _ext-link
Website: *http://www.openfoam.com/ _ext-link*

OpenFOAM is a software environment for computational fluid dynamics (CFD) and related computations.

OpenFOAM provides a C++ library and tools for setting up, meshing, solving, computing properties, and post-processing continuum mechanics, especially computational fluid dynamics. OpenFOAM includes solvers for a number of applications and provides an environment in which users can build their own.

OpenMOLCAS

Purpose: Electronic Structure Calculations
Latest version: v21.02
License: Open/Free
Website: *https://gitlab.com/Molcas/OpenMolcas*

OpenMOLCAS (The open version of MOLCAS) is an electronic structure calculations package.

It provides a particular emphasis on multi-configurational methods for highly degenerated ground states. OpenMOLCAS can implement methods for single determinant ground states (SCF, MP2, CC, DFT), but focuses on treating accurately highly degenerate states (excited states, heavy metals, transition states, etc.) through methods such as multi-configurational self-consistent field (MCSCF), complete active space (CASSCF), and including correlation effects via second-order perturbation theory (CASPT2).

ORCA

Purpose: electronic Structure Calculations
Latest version: 5.0.4
License: ✅ Free of use for academics
Mixed
Website: *https://orcaforum.kofo.mpg.de/_ext-link*

ORCA is a program that implements HF, DFT, semi-empirical, and high level ab initio (CI and CC) methods with gaussian basis sets for electronic structure calculations.

ORCA implements a variety of standard quantum chemistry methods, but is especially tailored at geometry optimisation and prediction of spectroscopic parameters in open-shell molecular systems. It can be coupled to ***Gromacs*** for QM/MM calculations.

ParaView

Purpose: Excited-state molecular dynamics
Latest version: 5.8
Licence: ✅ Free of use
BSD _ext-link
Website: *http://www.paraview.org/ _ext-link*

ParaView is an open-source, multi-platform data analysis and visualization application. ParaView users can quickly build visualizations to analyze their data using qualitative and quantitative techniques. The data exploration can be done interactively in 3D or programmatically using ParaView's batch processing capabilities.

PhotoScan

Purpose: Photo processing
Latest version: 1.4.5
Licence: ⚠️ Must be provided by the user.
Proprietary License
Website: *https://www.agisoft.es/_ext-link*

Agisoft PhotoScan is a desktop software to process digital images and, by combining digital photogrammetry and computer vision techniques, generate a 3D reconstruction of the environment.

Quantum ESPRESSO

Purpose: Electronic structure, materials modelling
Latest version: 7.1
License: Free of use
GNU GPL_ext-link
Website: *https://www.quantum-espresso.org/_ext-link*

Quantum ESPRESSO is a suite for electronic structure calculations and simulation of nano-structured materials.

The core of Quantum ESPRESSO are density functional theory (DFT) electronic calculations using plane-wave basis sets and pseudo-potential.

R

Purpose: Statistics and plotting
Latest version: 4.0.2
License: Free of use
Open Source - *GNU GPL _ext-link*
Website: *https://www.r-project.org/ _ext-link*

R is a language and environment for statistical computing and plotting.

R implements tools for data analysis, array operators (especially matrices), I/O features, graphical output features, and a high-level language (S) for integrating all of them, including user-defined variables, loops, etc.

RDKit

Purpose: Cheminformatics and ML
Latest version: 1.4.5
Licence: Free of use
BSD _ext-link
Website: *https://www.rdkit.org/_ext-link*

RDKit is a collection of cheminformatics and machine-learning software written in C++ and Python.

SALOME

Purpose: CFD & Engineering
Latest version: 9.3
Licence: Free of use
GNU LGPL _ext-link
Website: *https://www.salome-platform.org/ _ext-link*

SALOME is an open-source software that provides a generic Pre- and Post-Processing platform for numerical simulation. It is based on an open and flexible architecture made of reusable components.

SALOME-Meca

Purpose: CFD & Engineering
Latest version: 2016
Licence: Free of use
GNU LGPL _ext-link
Website: *https://www.code-aster.org/ _ext-link*

SALOME-Meca is a standalone application which represents integration of the ***Code_Aster*** solver in the ***SALOME*** platform.

Schrödinger

Purpose: Drug design, Molecular Dynamics
Latest version: 2022-2
Licence: ⚠ Must be provided by the user.
Proprietary License
Website: *https://www.schrodinger.com/_ext-link*

Schrödinger is a suite of programs for drug design, bioinformatics and molecular dynamics.

Schrödinger is a highly modular suite of programs for a variety of simulation, design, visualisation, docking, modelling and bio /chemoinformatics purposes. Several distributions focus on drug design, materials science, biological systems and data treatment and visualisation, providing tools for pre- and post-processing, interfaces, analysis and optimisation for custom workflows between the programs and integrated environments. Schrödinger suites contain programs also available as stand-alone releases, such as *Desmond* or *Jaguar*.

SIESTA

Purpose: Ab initio electronic structure, Molecular Dynamics
Latest version: 4.1
License: ✓ Free of use for academics users
Mixed
Website: *https://departments.icmab.es/_ext-link*

SIESTA is a program for ab initio electronic structure and molecular dynamics of solids and molecules.

SIESTA applies DFT hamiltonians (LDA, GGA) to strictly localized numerical basis sets and non-local pseudopotentials to obtain electronic structures. From these it can compute solid properties (band structure, DOS, k-space sampling, dielectric polarisation, phonons), perform Born-Oppenheimer molecular dynamics (NVT and NPT), and, in recent versions, Van der Waals potentials and ballistic electron transport properties (TranSIESTA).

STAR-CCM+

Purpose: Fluid Dynamics & Engineering
Latest version: 12.06.011
License: ⚠ Must be provided by the user
Propietary License _ext -link
Website: *https://www.plm. automation.siemens.com/ ext-link*

STAR-CCM+ is a multi-physics simulation package.

Built around a core for simultaneous resolution of computational fluid dynamics and heat transfer, STAR-CCM+ includes multiphase simulation, polyhedral meshing of solids and fluids, a fuel cells package, phase changes, chemical reactions, electromagnetic, etc.

STATA

Purpose: Mathematics & Statistics
Latest version: 15
Licence: ⚠ Must be provided by the user.
Propietary _ext-link
Website: *https://www.stata.com/ _ ext-link*

STATA is a statistical software that integrates and provides plenty of tools for statistical analysis and graphics.

VASP

Purpose: ab initio Molecular Dynamics
Latest version: 6.1.2
License: ⚠ Must be provided by the user
Proprietary
Website: *https://www.vasp.at/_ext -link*

Vienna Ab-Initio Simulation Package (VASP) is a program for plane-wave ab initio molecular dynamics.

VASP is a package to perform Born-Oppenheimer ab initio molecular dynamics (MD) simulations, employing a plane-wave DFT approach (LDA, GGA, meta-GGA, hybrids) to electronic structure. It implements either Vanderbilt pseudopotentials or the projector-augmented wave (PAW) method and Pulay-Broyden convergence to compute the ground electronic state at each step, as opposed to Car-Parrinello molecular dynamics.

VMD

Purpose: Molecular Dynamics
Latest version: 1.9.4
Licence: Free of use
GNU GPL
Website: *https://www.ks.uiuc.edu/_ext-link*

Visual Molecular Dynamics (VMD) is a visualisation program to visualise, model and analyse bio-molecular systems. Can generate PSF (Protein Structure File) files, perform live simulations using NAMD and modelling and analyse systems through its plugins. Is also fully compatible with the most part of Molecular file formats (PDB, PSF, CHARM, AMBER...).

The GPU compatibility makes VMD able to manage large atom number bio-molecules in various representations.

WESTPA

Purpose: Molecular Dynamics
Latest version: 1.0 beta
License: Free of use
GNU GPL _ext-link
Website: *https://westpa.github.io/_ext-link*

The **Weighted Ensemble Simulation Toolkit with Parallelization and Analysis (WESTPA)** is a high-performance framework for carrying out extended-timescale simulations of rare events with rigorous kinetics using the weighted ensemble algorithm of ***Huber and Kim (1996)***.

The software works with any dynamics engine and has already been used with a variety of molecular dynamics (e.g. GROMACS, NAMD, AMBER) and cell-modeling packages (e.g. BioNetGen, MCell).

WRF

Purpose: Climate Sciences
Latest version: 4.0.3
Licence: Free of use
Public domain _ext-link
Website: *https://www2.mmm.ucar.edu/wrf/ _ext-link*

The **Weather Research & Forecasting Model** (WRF) is a next-generation numerical mesoscale weather prediction system designed for atmospheric operational research and prediction needs. It has two dynamic cores, a data assimilation system, and a software architecture that facilitates parallel calculation and system extensibility. The model serves a wide range of meteorological applications through scales of tens of meters to thousands of kilometers.

WRF can generate atmospheric simulations using real data (observations, analysis) or idealized conditions.