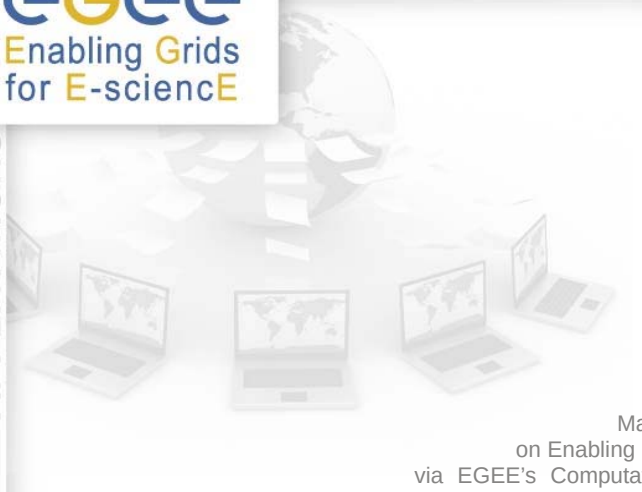
COMPUTATIONAL CHEMISTRY APPLICATIONS



While basic principles of experimental chemistry have remained unchanged for the last few decades, better access to computational power means that today's chemists can investigate and model larger, more complicated molecules at lower cost. After identifying a molecule of interest, the chemist tries to find its most likely structure by computing the lowest energy configuration of all possible shapes of the molecule. Upon finding the most stable structure, the chemist can calculate the molecule's properties. This information can be used by researchers from a suite of other disciplines: e.g. engineering, biology or astrophysics.

Many computational chemistry software applications are available for use on Enabling Grids for E-sciencE's (EGEE) grid. The majority of them can be accessed via EGEE's Computational Chemistry virtual organisation. Commercial packages are also available, requiring participation in the Gaussian or Turbomole Virtual Organisation (VO). All available packages are listed below.

ABCtraj calculates the properties of the atom-diatom reactions in gas phase. The events are generated using Monte Carlo techniques. The programme is linked to a molecular virtual reality environment that shows the outcomes of the simulation in virtual monitors. It can be also executed via P-Grade web interface.

COLUMBUS is a collection of programs for high-level *ab initio* molecular electronic structure calculations. The programs are designed primarily for extended multi-reference calculations on electronic ground, and excited states of atoms and molecules.

CPMD — Car-Parrinello Molecular Dynamics code — is a parallelised plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for *ab initio* molecular dynamics.

Dalton is a powerful quantum chemistry programme for the calculation of molecular properties with SCF, MP2 or MCSCF wave functions. The strengths of the programme are mainly in the areas of magnetic and (frequency-dependent) electric properties, and for studies of molecular potential energy surfaces, both for static and dynamical investigations.

The **DL-Poly** application performs the molecular dynamics simulation of complex systems. It is a de-facto standard in the computational chemistry and computational biology communities.

GAMESS is a programme for *ab initio* molecular quantum chemistry that can compute SCF wave functions. Correlation corrections to these SCF wave functions include Configuration Interaction, second order Perturbation Theory, and Coupled-Cluster approaches, as well as the Density Functional Theory approximation.

Gaussian is a set of electronic structure programmes widely used by scientists for research in established and emerging areas of chemical interest. Starting from the basic laws of quantum mechanics, Gaussian predicts properties of molecular systems under variety of conditions. Gaussian is a commercial product and, due to license restrictions, access to it is available only via the gaussian VO. Detailed information concerning participation can be found at the **http://egee.grid.cyfronet.pl/Gaussian** webpage. Numerical experiments using Gaussian can be performed via Chempo web portal.

MCTDH is a general algorithm to solve the time-dependent Schrödinger equation for multidimensional dynamical systems consisting of distinguishable particles. MCTDH can thus determine the quantum motion of the nuclei of a molecular system evolving on one or several coupled electronic potential energy surfaces. By its very nature, MCTDH is an approximate method. However, it can be made as accurate as any competing method, but its numerical efficiency deteriorates with growing accuracy.

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance simulations of large biomolecular systems.

NEWTON-X is a general-purpose programme package for excited-state molecular dynamics, including non-adiabatic methods (Tully's surface hopping). NX modular development allows it to be easily linked to any quantum chemistry package that can provide energy gradients and non-adiabatic coupling vectors. In the current version, NX can perform dynamics using COLUMBUS and TURBOMOLE programme packages.

The **RWAVEP** application computes chemical reactive quantum probabilities using the wave packet approach. Different events are generated for the various sets of initial conditions.

TURBOMOLE is a programme package for *ab initio* electronic structure calculations. Outstanding features of TURBOMOLE are: semi-direct algorithms with adjustable main memory and disk space requirements; full use of all point groups; efficient integral evaluation; stable and accurate grids for numerical integration. Turbomole is a commercial package and access to it is available via a separate VO.

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Venus calculates the cross-sections and rate coefficients for elementary chemical reactions by simulating the collisions between atoms and molecules whose initial conditions are sampled using a Monte Carlo scheme. In each collision the Hamilton equations governing the motion of the atoms are solved from reactants to products.

The programme package **WIEN2k** performs electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. In DFT the local (spin) density approximation (LDA) or the improved version of the generalized gradient approximation (GGA) can be used. WIEN2k is an all-electron scheme including relativistic effects and has many features. The Grid port includes a prototype of the grid workflow. Only users with valid Wien2k license are allowed to use it.

CHARON is a grid interface to fulfil the specific requirements of scientific communities.

Application webpages

EGEE is keen to consider other applications. For further information on how to participate see **http://technical.eu-egee.org/index.php?id=392**.
More information about the applications running on EGEE be found on the EGEE website at **http://technical.eu-egee.org/index.php?id=148**.

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