COMPUTATIONAL CHEMISTRY APPLICATIONS

The Computational Chemistry Virtual Organisation has been established to run the Grid Enabled Molecular Simulator (GEMS). Several applications have been ported to the Grid and have been run in production. Efforts are also underway to port additional applications to the EGEE infrastructure and to promote wider collaboration between the computational chemistry research groups.

The **GEMS** application is used to implement a simulation environment to study reaction dynamics of complex chemical systems.

ABCtraj calculates the observables of the atom-diatom reactions in gas phase. The events are generated using Monte Carlo techniques. The program is linked to a molecular virtual reality environment that shows the outcomes of the simulation in virtual monitors.

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 **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.

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

GAMESS is a program for *ab initio* molecular quantum chemistry that can compute SCF wavefunctions. Correlation corrections to these SCF wavefunctions 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 programs widely used by scientists for research in established and emerging areas of chemical interest. Starting from the basic laws of quantum mechanics, Gaussian is used to predict 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 web page.

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In the near future other applications will be deployed in the CompChem VO, such as:

- **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.
- **Dalton** represents a powerful quantum chemistry program for the calculation of molecular properties with SCF, MP2 or MCSCF wave functions. The strengths of the program 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.
- **CPMD** - The Car-Parrinello Molecular Dynamics code is a parallelized plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for *ab-initio* molecular dynamics.
- **ACES II** - Advanced Concepts in Electronic Structure is a series of programs for performing high-level quantum chemical *ab-initio* calculations. Its major strength is the accurate calculation of atomic and molecular energies as well as properties using “many-body” techniques such as many-body perturbation theory (MBPT) and, in particular coupled-cluster techniques to treat electron correlation.
- **Turbomole** is a program 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 will be available via a separate VO.
- **NAMD** is a parallel, object-oriented molecular dynamics code designed for high-performance simulations of large biomolecular systems.

In addition the CompChem VO will experiment with the **CHARON** system to interface the Grid with a custom user interface suitable to fulfil specific requirements of the Computational Chemistry community.

EGEE is keen to consider other applications. For further information on how to participate, as well as more information about the applications running on EGEE, visit the User and Application Portal at http://egeena4.lal.in2p3.fr/.

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