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Ab initio grid chemical software ports –transferring knowledge from EGEE to Polish NGI

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Chemical software, especially with ab initio methods, have been developed over several years of research in the field of numerical methods in chemistry. As the research was performed by many groups of scientists this resulted in a variety of software suites. From this set the commercial packages are of particular interest among the community due to the availability of many computational methods, the fast development of new ones and better user support. To attractthe chemical community to grid computing a set of frequently used software suites have been ported to the grid.

Conclusions and Future Work

The present solution has been applied only to serial versions of chemical codes . Future work will mainly focus on the parallel execution of program suites on the PL-Grid infrastructure, as the scientific problems chemists are dealing with are involving larger and larger molecules. Taking into consideration EGEE achievements in that field we expect this task to be done with similar ease. Further plans beyond this include the integration of all grid software ports within the Virtual Laboratory, to allow the execution of complicated chemical experiments by non-specialists.

Detailed analysis

The majority of most commonly used chemical software has been ported to the EGEE Grid during the second and third phases of EGEE projects. The most spectacular achievements include the grid ports of commercial packages like Gaussian, Turbomole and Wien2k (both serial and parallel versions), the most popular among chemical community. The major difficulty with grid ports of commercial packages is related to their strict license requirements. Those include not only a code protection against unauthorized use but, more importantly, the check of usage patterns compliance. Unfortunately the solutions worked out do not allow simultaneous use of several commercial packages during one job run, as in most cases commercial packages belong to different VOs. The model applied in PL-Grid is different. In contrast to the EGEE solution all the packages have been ported to a single VO. Such a model allows not only the simultaneous execution of several instances of chemical packages at the same time, but it also eases the execution of complicated experiments where the next step of an experiment depends on the result(s) obtained previously.

Impact

The EGEE infrastructure together with the grid ports of chemical software has proven its usefulness in research in the field of computational chemistry. Direct availability of easy to use chemical packages increased Grid attractiveness, ad resulted in better grid utilization by the community and enhanced user satisfaction, making the chemical communitythe second largest Grid user. The same results are expected for Pl-Grid and others National Grid Initiatives (NGI). It is important to point out that only a very little additional effort related to porting procedures was required, as the main obstacles for porting have been solved by the members of Computational Chemistry Scientific Discipline Cluster. On the same basis other NGI's can take advantage of EGEE acquired knowledge and expertise in several scientific areas.

Keywords

ab initio, chemical software, porting, NGI, PL-Grid

URL for further information

www.plgrid.pl (NGI www page)

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