

Application of Gaussian package on the EGEE Grid to chemical reaction study

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Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

A vast number of methods available for computational chemistry caused that community is accustomed to software packages rather than single programs. To attract the community a port of many freely available chemical packages is now available on the Grid. In order to make the Grid even more attractive for the community we present solution which enables use of commercial chemical software on the Grid which makes it a perfect platform for chemistry application.

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

The Grid advantages in chemical applications were demonstrated by us several times. This mainly includes the numerical frequency calculations, molecular dynamics simulations and vibrational averaging study with help of freely available chemical software. In this report we apply commercial software installed on the Grid to chemical reaction study. Chemical reactions are the most interesting and the most demanding computational chemistry challenges. In general such a study requires detailed insight not only in to the structure and properties of products and substrates but also into so called reaction path which describe how changes in substrates structure lead to the product. We shortly characterize a whole procedure and demonstrate how researchers can benefit from the Grid at each computation step.

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possible, point out the experience limitations (both in terms of existing services or missing functionality)

Presented solution is currently being applied to other commercial chemical packages and we recommend similar procedure to be employed to other commercial. With a little of negotiation with commercial companies all the license issues may be solved making the desired product available on the Grid. There are however, still unsolved issues which will need to be addressed in the future like 'floating' type licenses for which the Grid solution is highly needed.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

Among existing chemical applications commercial ones are the most needed. This is due to availability of many computational methods, fast development of new ones and better user support. However, the main reasons blocking wide use of commercial

packages on the Grid are their strict license requirements. These include not only a code protection against unauthorized use but what is equally important check of usage patterns compliance. Confirmation of fulfilling the license requirements is the key step in porting software to the Grid and then using it. In case of Gaussian program our solution was based on the negotiations with Gaussian Inc,. As a result a new virtual organization Gaussian was created. Due to availability of Gaussian for all EGEE users other disciplines such as medicine, biochemistry or physics may benefit from it. This is also a sign for business companies to attempt porting of their software to the Grid.

Author: Dr STERZEL, Mariusz (ACC Cyfronet AGH)

Co-authors: Mr SZEPIENIEC, Tomasz (ACC Cyfronet AGH); Dr PISKORZ, Witold (Dep. of Chemistry, Jagiellonian University)

Presenter: Dr STERZEL, Mariusz (ACC Cyfronet AGH)

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