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The Molecular Science challenges in EGEE

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The understanding of the behavior of molecular systems is important for the progress of life sciences and industrial applications. In both cases is increasingly necessary to perform a study of the relevant molecular systems by using simulations and computational procedures which heavily demand computational resources. In some of these studies it is mandatory to put together the resource and complementary competencies of various laboratories. The Grid is indeed the infrastructure that allows such a cooperative modality of work. In particular for scientific purposes
the EGEE Grid is the proper environment. For this reason a Virtual Organization (VO) called CompChem has been created within EGEE. Its goal is to support the computational needs of the Chemistry and Molecular Science community and pivot the user access to the EGEE Grid facilities.
Using the simulator being implemented in CompChem the study of molecular systems is carried out by adopting various computational approaches bearing approximations of different levels.
These computational approaches can be grouped into three categories:
1. Classical and Quasiclassical: these are the less rigorous approaches. They are, however, the most popular. The main characteristic of these computational procedures is that the related computer codes are naturally parallel. They consist in fact of a set of independent tasks, with few communications at the beginning and at the end of each task.
Related computational codes are suitable to exploit the power of the Grid in terms of the high number of computing elements (CEs) available.
2. Semi-classical: these approaches introduce appropriate corrections the deviations of quasiclassical estimates from quantum ones. The Grid infrastructure is exploited for massive calculations by varying the initial conditions of the simulation and performing the statistical analysis of the results.
3. Quantum: this is the most accurate computational approach heavily demanding in terms of computational and storage resources. Grid facilities and services will be only seldomly able to support them in a proper way using present
hardware and middleware utilities. Therefore they will represent a real challenge for Grid service development.

The computational codes presently used are mainly produced by the laboratories member of the VO. However some popular commercial programs (DL POLY, Venus, MolPro, GAMESS, Columbus, etc) are also being implemented. These packages are at present executed only on the computing element (CE) owning the license. We are planning to implement in the Resource Broker (RB) the mapping of the licensed sites via the Job Description Language (JDL). In this way the RB will be able to schedule properly the jobs requiring licensed software. The VO is implementing[1] an algorithm to reward each participating laboratory for contributions given to the VO providing hardware resources, licensed software and specific competences.
One of the most advanced activities we are carrying out in EGEE is the simulation

on the Grid of the ionic permeability of some cellular micropores. To this end we use molecular dynamics simulations to mimic the behavior of a solvated ion when driven by an electronic field through a simple model of the channel. As a model channel a carbon nanotube (CNT) was used as done in a recent molecular dynamics simulation of water filling and emptying of the interior of an open-end carbon nanotube[3-6]. In this way we have been able to calculate the ionic permeability
of several solvated ions (Na+, Mg++, K+, Ca++, Cs+) by counting the ions forced to flow into the nanotube by the applied potential diffence along z-axis.

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