EGEE User Forum

Contribution ID: **82** Type: **Oral contribution**

An Attempt at Applying EGEE Grid to Quantum Chemistry

Wednesday 1 March 2006 16:30 (15 minutes)

The EGEE Grid Project enables access to huge computing and storage resources. Taking this oportunity we have tried to identyfie chemical problems that could be computed in this environment. Some of the results considered within this work are presented with description focused on requirements for the computational enviroment as well as techniques of Grid-enabling computations based on packages like GAMESS and GAUSIAN.
Recently lots of work has been done in the area of parallelizing the existing codes and discovering new ones used in quantum chemistry. That allows calculations to run much faster now than even ten years ago. However, there still exist tasks where without a large number of processors it is not possible to obtain satisfactory results. The two main challenges are harmonic frequency calculations and ab-initio (AI) molecular dynamics (MD) simulations. The former ones are mainly used to analyze molecular vibrations. Despite the fact that the algorithm for analytic harmonic frequency calculations has been known for over 20 years, only few quantum chemical codes have it implemented. The other still use numerical scheme where for a given number of atoms (N) in a molecule, , and for more accurate calculations independent steps (energy + gradients) have to be done to get harmonic frequencies. To achieve this as many processors as possible is needed to fit that huge number of calculations. This makes grids technology an ideal solution for that kind of application. The second challenge, MD simulations are mainly used in a case where 'static'calculation like for example determination of Nuclear Magnetic Resonance (NMR) chemical shifts gives wrong results. MD consists usually of two steps. In the first one the nuclear gradients are calculated, in the second one, based on obtained gradients, the actual classical forces acting on an atom are calculated. Knowing these forces one can estimate accelerations, velocities and guess new position of the atom after a given short period of time (so called time step). Finally the whole process is repeated for every new position of each atom. In case of mentioned NMR experiment we are interested in the average value of chemical shift over simulation. Of course NMR calculations are also very time consuming themselves and have to be done for many different geometries which again makes grid technology an ideal solution to final NMR chemical shift calculations.
We present here two kinds of calculations. First we show results for geometry optimization and frequency calculations for a few carotenoids. These molecules are of almost constant interest since they cooperate with chlorophyll in photosynthesis process. All the calculations have been done within EGEE Grid (VOCE VO). We also present an example of MD calculations and share our knowledge about what kind of problems can be found during such studies.

Primary authors: Dr STERZEL, Mariusz (Academic Computer Centre "Cyfronet"); Mrs SZEPIENIEC, Tomasz

(Academic Computer Centre ”Cyfronet”)

Co-authors: Dr FIEDOR, Leszek (Faculty of Biotechnology, Jagiellonian University); Dr PILCH, Mariusz (Faculty of Chemistry, Jagiellonian University)

Presenter: Dr STERZEL, Mariusz (Academic Computer Centre ”Cyfronet”)

Session Classification: 1d: Computational Chemistry - Lattice QCD - Finance

Track Classification: Computational Chemistry - Lattice QCD - Finance