GAMESS application in BG– an example of scientific research task

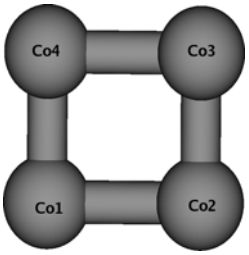
Description of the task

The application task is to establish the geometrical structure of the small Co nanoparticles. The investigation starts from small size Co-cluster modeling, due to several reasons:

1) the large cluster could be formed from small particles;
2) computing of clusters of very small size, consisting of only a few atoms or even single isolated atom, is now possible.

On the other hand, the magnetic properties of nanoparticles depend of crystal symmetry and atomic composition. These processes affect even the structural parameters od cluster, such as shape of particles or interatomic distances. Thus, the study of electronic structure of the Co nanoparticles helps us to understand the reason of dependence above.

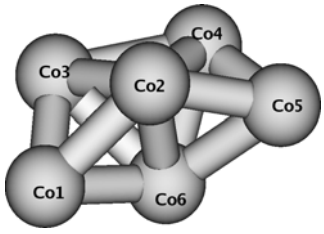
B3LYP/6-31G					
Bond	Bond length	Angle		Dihedral angle	
1 – 2	2.16	1 – 2 – 3	90.0	1 – 2 – 3 – 4	0.0
2 – 3	1.94	2 – 3 – 4	90.0		
3 – 4	2.16	3 – 4 – 1	90.0		
4 – 1	1.94				



Description of requirements for the application

The application is very time consuming, because of the number of different structures and shapes increase rapidly while increasing number of Co atoms. As an example, the Co_4 have three different structures, while more than six different structures could form six Co atoms. All proposed structures are investigated in order to find the most stable compounds. In addition, the increasing of atom number in nanoparticles leads to larger computing resource needs.

B3LYP/6-31G					
Bond	Bond length	Angle		Dihedral angle	
1 – 2	2.24	3 – 2 – 1	59.41	1 – 2 – 3 - 4	-80.63
1 – 3	2.24	4 – 3 – 2	61.02	2 – 3 – 4 – 5	42.41
1 – 6	2.16	5 – 4 – 3	109.61	3 – 4 – 5 – 6	-21.18
2 – 3	2.16	6 – 5 – 4	110.84		
2 – 4	2.33				
2 – 5	2.15				
2 – 6	2.11				
3 – 4	2.33				
3 – 6	2.31				
4 – 5	2.04				
4 – 6	2.18				
5 – 6	2.23				



Why the application is important for scientists of the Baltic States

As mentioned above the aim of our investigation is to establish the geometrical structure of Co nanoparticle and to understand why and how magnetic properties of the nanoparticle are structurally depended. The obtained knowledge would create opportunities for new nano material discoveries. It would be possible to create large capability storage devices. The

nanoparticle may be used as nanophotonic devices, or in similar way. Hence, such calculations would help Lithuania to join the international efforts to create new promising nano devices and materials.

Description of computing procedure

The structural origin of clusters has been studied by the Hartree-Fock method with 6-31G basis set within geometry optimization. The method describes structural parameters of clusters and allows us to select the most stable isomers of the nanoparticles without using huge computing time resources rather well. The stabilities and electronic structure of the selected small cluster Co_n (n=4, 6, 8) were re-investigated by using generalized gradient approximation for exchange-correlation potential in the density functional theory (DFT) as described by Becke's three-parameter hybrid functional using the non-local correlation and provided by Lee, Yang, and Parr. The DFT methods are commonly referred to as B3LYP. The 6-31G basis set for Co has been used as well. The structures of the investigated nanoparticles have been optimized globally without any symmetry constraint and by starting from various initial geometries.

Description of software

The research is performed by using ab initio quantum chemistry package such as GAMESS. Additionally we are interested to have possibility to use Gaussian or Dalton program packages to evaluate g-tenzor and the direction of its component.

Description of the prerequisites for grid, needed to run the application

To run the application one must have the possibility to apply GAMESS or the other quantum chemistry package that is installed on different clusters. Preferably, that one may use the same version of the programs. Today it is possible to foresee that the computer resource amount (particularly memory) will increase, because the result precision depends on the basis set and method and the investigated compounds are grown also. On the other hand, it will be very useful to receive the output file of the aborted problem especially the long running one.

Brief instructions, demonstrations, suitable snapshots

To run GAMESS one has to provide it with input file called gamess.inp where gamess is an arbitrarily chosen strings. You will find the input description within every possible input keywords on web page: http://www.msg.ameslab.gov/GAMESS/.

To executing GAMESS one must additionally have gamess.jdl and gamess.csh files.

The example of the gamess.jdl file is the following:

```
JobType        = "MPICH";
NodeNumber     = 2;
MyProxyServer = "grid3.mif.vu.lt";
LRMS_Type      = "pbs";
Executable     = "gamess.csh";
StdOutput      = "gamess.out";
```

```
StdError       = "gamess.err";
InputSandbox   = {"gamess.csh", "gamess.inp"};
OutputSandbox  = {"gamess.out", "gamess.err", "gamess.log", "gamess.dat"};
Requirements                    =                    Member("VO-gamess-GAMESS",
other.GlueHostApplicationSoftwareRunTimeEnvironment);
```

The example of the gamess.csh file is:

```
#!/bin/csh
#set echo

$VO_GAMESS_SW_DIR/GAMESS-sockets-Jun272005R5/rungms gamess.inp >& gamess.log
exit 0
```

When executing GAMESS on the cluster Atom one type:

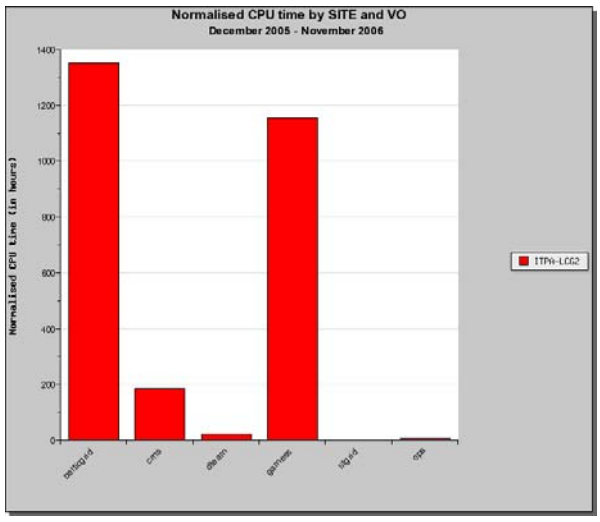
```
glite-job-submit -r atomas.itpa.lt:2119/jobmanager-lcgpbs-gamess -lrms pbs -o jobs gamess.jdl
```

The all files gamess.inp, gamess.jdl, gamess.csh are assumed to be located in the submit directory. As results, a file called gamess.log, gamess.dat, gamess.err, and gamess.out will be produced in the separate directory.

Statistics of runs, results achieved, hours used, jobs successful, jobs failed, other comments.

At present, we are running 8 problems (on an average) per day on three clusters: Atom, KTU and VU. The result achieving is problem dependent. Some results were achieved after 2-6 hours of the calculations on the average, while the results of other ones were waited for one month. Usually, 4 to 8 problems are successfully finished, 1 problem is failed per day. One problem current status is “waiting” from 26th October.

The problems are returned with message: ”Please rename/errase/home/gmo13/.mpi/.... “ 2-3 times per week. Hours used on the cluster Atomas are presented in the figure below.



Normalized CPU time by used for GAMESS application on cluster Atomas