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Porting of basic linear algebra algorithms on the EGI parallel platform

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Overview

The increasing availability of computer power on distributed platforms makes it easier to implement basic linear algebra algorithms that are low level complexity codes taken from typical library routines or algorithms popular among the Molecular and Material Science (MMS) community members.
In this report we outline the work carried out in our laboratory by porting on the EGI Infrastructure a set of these algorithms and performing MPI calculations to test the parallel performance of the used platform.

Impact

The availability of MPI on the virtually unlimited set of CPUs grafted on Grid platforms has shown to be a strong incentive to implement different scientific applications (from simple basic linear algebra algorithms to complex suites of codes) on distributed systems and to develop appropriate distribution models. On this ground the virtual organization (VO) COMPCHEM assembled out of a group of molecular and material sciences laboratories, committed itself to implement their computer codes on the section of the production European Grid Infrastructure available to the VO using MPI. From the tests performed by running the parallel MPI version of a set of common matrix multiplication algorithms in the EGI environment has emerged that the number of jobs requiring up to 8 CPUs and terminated successfully has increased of about 20% and the number of jobs requiring from 16 up to 32 CPUs has increased of about 30% if compared with 2009 results. The obtained results indicate an increase of reliability on the use of MPI on the present Grid environment.

Description of the work

All the Grid nodes that support COMPCHEM VO have been tested using three different matrix multiplication algorithms (Cannon algorithm, Fox algorithm and Strassen algorithm) as benchmark. Each executable has been compiled statically in the UI machine used by COMPCHEM VO (SLC4.8 Berillium, gLite 3.1) in order to assure binary compatibility. The compiler used was ifort (academic license) linked with MPICH1 libraries. From a preliminary analysis performed by running the glite-wms-job-listmatch and the related JDL file in which the requirements MPI-START & MPICH have been specified, it was found that 16 over a total of 25 sites supporting COMPCHEM VO support also MPI applications. The reduction in sites that support MPI registered in the last year (in 2009 were 22/25) is basically due to the introduction of the MPI-SAM tests (now NAGIOS tests). The tests now assure the basic requirements for a job submitted with MPI tags.
The performance of each site has been obtained running the codes sequentially in one node and in parallel in 2 ,4 ,8, 16, 32 nodes on the same cluster, evaluating statistics and performances. The global performances and the statistical analysis carried out by submitting MPI jobs have been compared with those obtained in 2009.

Conclusions

The porting of basic linear algebra algorithms onto the Grid infrastructures can be seen as part of a more general effort to build a solid platform to implement the parallel versions of complex suites of codes. The presented case study demonstrates the possibility of using the parallel capabilities of the European Grid and can be used as an example for those Communities which are interested in the porting of their parallel applications into the Grid environment.

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