MPI jobs with gLite

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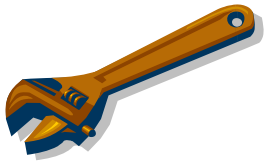
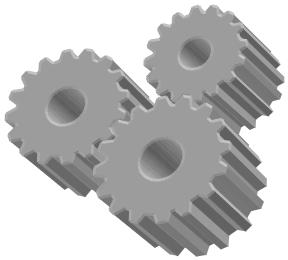
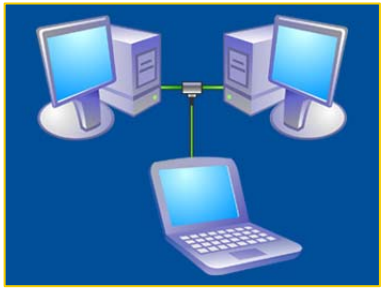
Outline

- Overview
  - Requirements & Settings 
  - Options 
- How to create a MPI job.
- MPI job in LCG middleware.
- MPI job in gLite (Lightweight Middleware for Grid Computing) middleware.

Overview

- Execution of parallel jobs is an essential issue for modern conceptions of informatics and application.



- Most used library for parallel jobs support is (Message Passing Interface) MPI

- At the state of the art, parallel jobs can run inside single Computing Elements (CE) only;

  - several projects are involved into studies concerning the possibility of executing parallel jos on Worker Nodes (WNs) belonging to differents CEs.

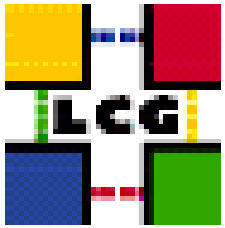
Requirements & Settings

- In order to garantee that MPI job can run, the following requirements MUST BE satisfied:
  - the MPICH software must be installed and placed in the PATH environment variable, on all the WNs of the CE.
  - Some MPI's applications required a shared filesystem among the WNs to run.
    - The variable VO_<name_of_VO>_SW_DIR will contain the name of a *directory* in case of SHARED filesystem.
    - The variable VO_<name_of_VO>_SW_DIR will contain "." if there is NO SHARED filesystem.

Requirements & Settings

- The *Executable* that is specified in the JDL must not be the MPI application directly, but a *wrapper* script that invokes the MPI applications by calling `mpirun` command.

How to create a MPI Job



- For the user's point of view, jobs to be run as MPI are specified setting the JDL `JobType` attribute to **MPICH** and specifying the `NodeNumber` attribute as well.

E.g.:

```
JobType = "MPICH";
NodeNumber = 4;
```

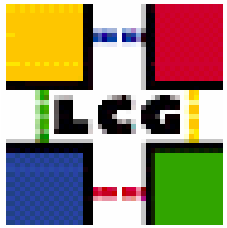
This attribute define the required number of CPUs needed for the application.

- When these two attributes are included in a JDL the User Interface (UI) *automatically* add the following expression

```
(other.GlueCEInfoTotalCPUs >= NodeNumber) &&
Member ("MPICH",other.GlueHostApplicationSoftwareRunTimeEnvironment)
```

to the JDL requirements expression in order to find out the best resource where the job can be executed.

MPI jobs with LCG middleware



the problem ...

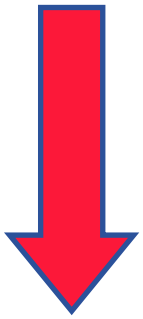
- Unfortunately LCG project was not synchronized with the latter requirement *avoiding to share disk space* with nodes inside the same CE.

- This drove us to spend our time in providing a *ad-hoc* solution in order to find an efficent workaround to this problem.

- The solution adopted bypasses the problem by putting some intelligence inside the script passed in Inputsandbox.

… the solution

- In detail each job has to *mirror*, via scp, its files on all nodes dedicated to it.



ssh hostbased authentication MUST BE well configured between all the WNs.

mpi.jdl

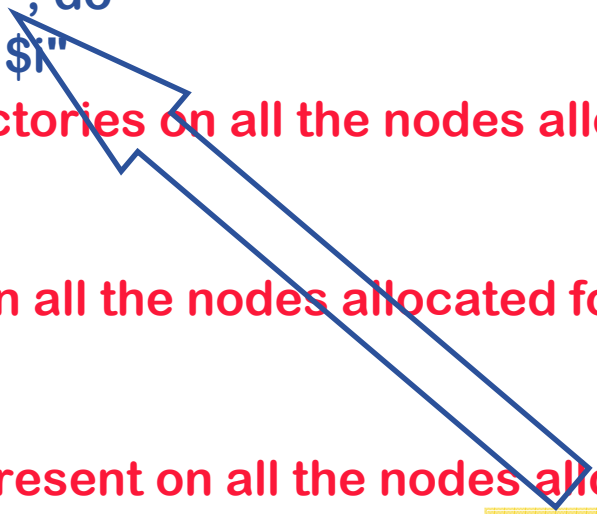
```
[
    Type = "Job";
    JobType = "MPICH";
    Executable = "MPItest.sh";
    NodeNumber = 5;
    Arguments = "cpi 5";
    StdOutput = "test.out"; StdError = "test.err";
    InputSandbox = {"MPItest.sh","cpi"};
    OutputSandbox =
    {"test.err","test.out","executable.out"};
    Requirements   = other.GlueCEInfoLRMSType == "PBS" ||
    other.GlueCEInfoLRMSType == "LSF";
]
```

The number of threads specified with NodeNumber attribute agrees with the second Argument. It will be used during the invoking of mpirun command.

MPItest.sh

```
for i in `cat $HOST_NODEFILE` ; do
    echo "Mirroring via SSH to $i"
    # creates the working directories on all the nodes allocated for parallel
    execution.
    ssh $i mkdir -p `pwd`
    # copies the needed files on all the nodes allocated for parallel
    execution.
    /usr/bin/scp -rp ./* $i:`pwd`
    # checks that all files are present on all the nodes allocated for parallel
    execution.
    ssh $i ls `pwd`
done

# execute the parallel job with mpirun.
echo "Executing $EXE"
chmod 755 $EXE
mpirun -np $CPU_NEEDED -machinefile $HOST_NODEFILE
    `pwd`/$EXE > executable.out
```



The Environment variable $HOST_NODEFILE contains the list of WNs allocated for the parallel execution.

MPI jobs with gLite middleware

- Unlike the LCG middleware, gLite WMS is able to support both configurations (*shared* and *not shared*) automatically for both LSF and Torque.

- With gLite-1.4 job wrapper will take care to mirror the working directory in all nodes dedicated to the mpi job if the home are not shared.

mpi-glite.jdl

```
[
   JobType = "MPICH";
   NodeNumber = 6;
   StdOutput = "cpi.out";
   StdError = "cpi.err";
   InputSandbox = {"cpi"};
   OutputSandbox = {"cpi.err","cpi.out"};

   Requirements =
   (Member("GLITE-1.4",
   other.GlueHostApplicationSoftwareRunTimeEnvironment) && (other.GlueCEInfoTotalCPUs >= 10));
]
```

- **The command sequence to submit this example is this one:**

```
voms-proxy-init --voms gilda

edg-job-submit mpi.jdl
edg-job-status <JobID>
```


```
glite-job-submit mpi-glite.jdl
glite-job-status <JobID>
```

mpi job @ work !

pi is approximately 3.1415926544231239, Error is 0.0000000008333307

wall clock time = 10.008261

Process 0 of 6 on grid036.ct.infn.it

Process 1 of 6 on grid036.ct.infn.it

Process 2 of 6 on grid033.ct.infn.it

Process 3 of 6 on grid033.ct.infn.it

Process 5 of 6 on grid034.ct.infn.it

Process 4 of 6 on grid034.ct.infn.it

Conclusion

The limitation of the actual middleware, according to the RB schedule the MPI jobs only on a single CE reducing dramatically the number of WNs available for the parallel computation, can be overcome using the CrossGrid testbed based on LCG middleware.

To get more information you can contact Jesus Marco (marco@ifca.unican.es) or Harald Kornmayer (harald.kornmayer@iwr.fzk.de).

MPI on the web..

- **LCG-2 User Guide Manuals Series**
  - https://edms.cern.ch/file/454439/LCG-2-UserGuide.pdf
- **http://oscinfo.osc.edu/training/**
- **http://www.netlib.org/mpi/index.html**
- **http://www-unix.mcs.anl.gov/mpi/learning.html**
- **http://www.ncsa.uiuc.edu/UserInfo/Training**

Questions…