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Assessment of DEISA Grid Functionality

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Assessment of DEISA Grid Functionality

1 Introduction

This document describes effort produced according with work plan presented into “next 18 month” work program document [1], delivered at PM 24. In particular it is addressed to tasks T-JRA5-5.0.1 and T-JRA5-5.0.2, devoted to further investigation and activities that were necessary to solve problems encountered during DEISA grid assessment to perform computation with commercial CFD and CAA codes.

These activities, even if do not benefit of the full DEISA infrastructure yet, already show that an increase in the computational resources used, with respect to current level of industrial application, can lead to results with a significantly increased engineering relevance and potential for application.

In the phase described in this document we tested if in facts the infrastructure is able to support an application which needs to connect to a centralized license server. This issue is at the base of the main deal which is to verify as the infrastructure can distribute the workload between the internal sites. The model of workload distribution which we will refer is described on different deliverables of SA3 [especially 6].

With respect to time planning, activity was originally scheduled from PM 25 to PM 30, however solution of problems requested additional time, resulting in a delay of this deliverable. Finally a solution was reached and verified by submission of test jobs already available from light and medium application cases (D-JRA5-4 [2] and D-JRA5-5 [3]).

2 Exploitation of the DEISA infrastructure for commercial codes

During the deployment of DEISA infrastructure, we assessed two main issues that prevented an effective exploitation for applications that uses commercial licensing infrastructures, as the CFD++ one:

- licensing support on the whole DEISA infrastructure
- seamless application execution on the whole infrastructure.

These issues are interlaced because CFD++ simulation and JRA5 activities are constrained mainly by the network and system administration policies adopted by the partners that were preventing the simple deployment of centralized FLEXlm (tm) license servers and, as consequence, the seamless exploitation for the whole infrastructure.

Using the new “DEISA FLEXlm servers” the JRA5 (as well all the users) can in principle submit seamlessly a job on each DEISA site. In any case, a less critical but relevant issue still persists: license scheduling. In fact the users can submit their jobs to the DEISA machines only by means of a batch scheduler (LoadLeveler) that currently does not take in account external resources such as license tokens. This task is probably the most challenging, to submit to SA3.

3 Application deployment

With respect the status reported in the previous deliverable, the stuffs related to the application deployment are slightly changed in order to better accomplish the SA4 guidelines for *modulefiles* and the batch submission. The *modulefile* for the CFD++ application has been moved from the production “DEISA-Modules” to the special purpose user application module location *$DEISA_HOME/.modules*. This way enables the user to install its own applications leveraging the multi-cluster wide file system referenced by the shell environment variable *$DEISA_HOME*. The user now can install its own CFD++ under the shared file system and then use this *modulefile* to configure a CFD++ session.

The core application configuration in modulefile is based on the following tcl lines (excerpt from the file *.modules/sitelocal/applications/cfd++-5.1.1*):

```
set METACOMP_CFD_VERSION "5.1.1"
set METACOMP_CFD_INST_DIR \
“/deisa/cne/home/cne0crf0/cne0crf1/prod/CFDPP$METACOMP_CFD_VERSION"
set METACOMP_LICENSE_POINTER "7459@fe02-deisa.fec.cineca.it"
```

The latter line reflects the presence of the new “DEISA license server”, reachable from all the DEISA nodes.

The batch execution is now performed using a LoadLeveler script like the following one (for test purposes only):

```
# @ job_name = CFD++
# @ input = /dev/null
# @ notify_user = enrico.ribaldone@crf.it
# @ notification = always
# @ shell = /bin/bash
# @ requirements = (Feature == "DEISA")
# @ job_type = parallel
# @ total_tasks = 32
# @ wall_clock_limit= 02:00:00
# @ data_limit = 1500mb
# @ output = nlas.out.$(stepid).$(jobid)
# @ error  = nlas.err.$(stepid).$(jobid)
# @ queue

module load deisa
module load cfd++/5.1.1
export MCFD_MAXMEM=16G

EXE=r4_mpimcfd
scratch_dir=$DEISA_SCRATCH
```

```
home_dir=$DEISA_HOME
data_dir=$DEISA_DATA/2007/condotto-2005-test

cp ${data_dir}/* ${home_dir}/${EXE} ${scratch_dir}
cd ${scratch_dir}

${scratch_dir}/${EXE}
cd ..
cp -r ${scratch_dir} ${home_dir}
```

In the first phase, we worked in order to verify the correct working of distributing workload submitted different jobs by different sites. Then we were not able to verify the balancing of work load between the different core sites because the policy of the sites didn't permit to do that.

Whatever, we simulated this feature in order to verify if the solution about the license server works in a good way. To do that, we used LoadLeveler Multicluster System.

Actually, we are able to execute this kind of jobs at all the DEISA core clusters but it has been chosen to address the most part of jobs between CINECA and IDRIS as in these sites it was possible to allocate the resources requested in the time frame planned for the tests. So the activities are mainly performed at the CINECA's and IDRIS's facilities.

We worked together with SA3 to realize the solution described in D-SA3-8 [6], permitting the end-user involved in the activity to run his application and to reach the desired results.

Appendix 1: List of Abbreviations & Reference

CAA: **Computational Aero Acoustics**
Numerical technology for the simulation of aeroacoustic phenomena.

CFD: **Computational Fluid Dynamics**
Numerical technology for the simulation of Fluid Dynamic phenomena.

[1] Next 18 Months Y3

[2] D-JRA5-4 : Light Application Cases, Engineering and IT Results

[3] D-JRA5-5: Medium Application Cases, Engineering and IT Results

[5] CFD ++ ver. 5.1.1 User Manual

[6] D-SA3-8: Activity Report and Roadmap Evaluation