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Grid-based HPC astrophysical applications at INAF Catania

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Abstract. The research activity on grid area at INAF Catania has been devoted to two main goals: the integration of a multiprocessor supercomputer (IBM SP4) within INFN-GRID middleware and the developing of a web-portal, Astrocomp-G, for the submission of astrophysical jobs into the grid infrastructure. Most of the actual grid implementation infrastructure is based on common hardware, i.e. i386 architecture machines (Intel Celeron, Pentium III, IV, Amd Duron, Athlon) using Linux RedHat OS. We were the first institute to integrate a totally different machine, an IBM SP with RISC architecture and AIX OS, as a powerful Worker Node inside a grid infrastructure. We identified and ported to AIX OS the grid components dealing with job monitoring and execution and properly tuned the Computing Element to delivery jobs into this special Worker Node. For testing purpose we used MARA, an astrophysical application for the analysis of light curve sequences. Astrocomp-G is a user-friendly front end to our grid site. Users who want to submit the astrophysical applications already available in the portal need to own a valid personal X509 certificate in addiction to a username and password released by the grid portal web master. The personal X509 certificate is a prerequisite for the creation of a short or long-term proxy certificate that allows the grid infrastructure services to identify clearly whether the owner of the job has the permissions to use resources and data. X509 and proxy certificates are part of GSI (Grid Security Infrastructure), a standard security tool adopted by all major grid sites around the world.

Key words. Grid, Globus, IBM-SP, INFN-GRID, Astrocomp

1. A canonical way of buiding a grid

The configuration and installation of an INFN-GRID site usually relies on the LCFGng system (Local ConFiGuration system Next Generation) (http://www.lcfg.org 2000), developed by the Department of Computer Science at Edinburgh University. LCFG provides a configuration language and a central repository of configuration specifications and software (rpms), from which individual Linux machines can be automatically installed and configured. Changes to the central specification automatically trigger corresponding changes in the actual configuration of individual nodes. LCFGng uses XML/HTTP for transporting configuration profiles. The latest

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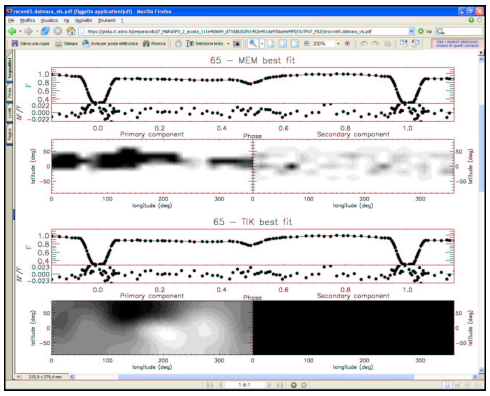

Fig. 3. Astrocomp-G: output results

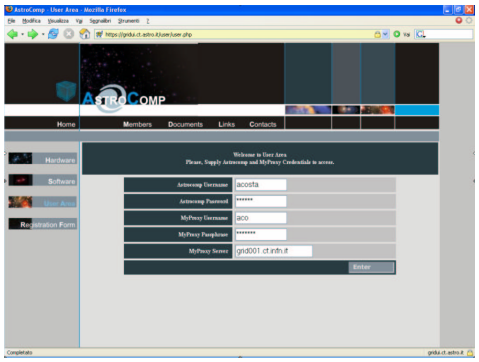

Fig. 1. Astrocomp-G: login page

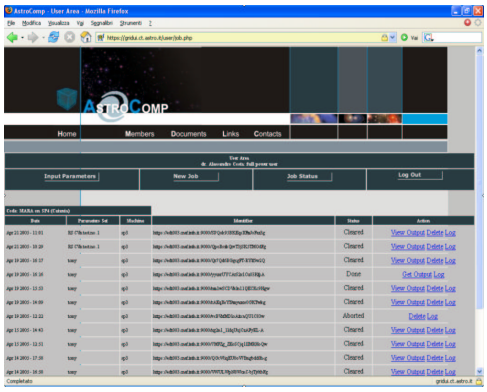

Fig. 2. Astrocomp-G: job status informations

release and its documentation is designed to be suitable for public use (under the GPL).

2. IBM SP: a new worker node

Our first goal was to find procedures to integrate an IBM SP parallel computer (8 Power 4 CPUs) into the INFN-GRID as a worker node. We cannot use an LCFG server to install an IBM SP as a worker node for at least two reasons: LCFG version of INFN-GRID initialize machines, reinstalling the OS and all needed applications The repository managed by the LCFG contains rpm packages compiled for i386 architecture and Linux Redhat 7.3: architecture and SO of target machines is definitively different. The installation must proceed in a different way.

3. IBM SP4 Configuration

OpenPBS 2.3.16 compilation and pbs_mom installation. Some slight changes has been required to the OpenPBS installation scripts. We have used "–enable-sp2" to compile special code to deal with the SP high speed switch.
IBM Grid Toolbox V3 for AIX installation (it's the IBM version of Globus Toolkit 3).
VOs user creations ex: inaf001 is the username used by our Computing Element to map the following certificate: "/C=IT/O=INFN/OU=Personal Certificate/L=INAF Catania/CN=Alessandro Costa/Email=acosta@ct.astro.it".
Population of "/etc/grid-security/certificates/" with CA certificates and Certification Revocation Lists by a cron copy from the CE.
Minor changes (mktemp command compilation and installation, creation of a list containing ssh keys of trusted hosts) on AIX 5.2.

4. Tweaking Computing Element

PBS server configuration: Add new WNs to "/var/spool/pbs/server_priv/nodes":
gridwn1.ct.astro.it np=1 lcgpro
gridwn2.ct.astro.it np=1 lcgpro
sp4.ct.astro.it np=8 ibmsp
Replace 'source' with '. ' in

"/opt/globus/lib/p/erl/Globus/GRAM/submit-helper.pl". belonging to the package: "lcg-extra-jobmanagers-1.1.6-1".
These changes have no side effects on the other linux worker nodes.

5. Astrocomp-G

Astrocomp web portal is a user friendly interface that allows to run some astrophysical parallel codes on a pool of powerful computational resources, hiding the underlying complexity of the MPP systems actually used.
Astrocomp was born by an idea of V. Antonuccio, U. Becciani (both of INAF Obs. of Catania), R. Capuzzo Dolcetta (dep. of Phys., Univ. of Roma La Sapienza) and V. Rosato (ENEA); it was developed in collaboration with Oneiros s.r.l.
We introduce Astrocomp-G, a grid-enabled portal to run codes over a computational grid. Specifically, we re-implemented the portal authentication mechanisms adopting standards currently used in many international computational grids. A user who wants to log into the portal will need, besides username/password released by the portal web master upon registration, a digital X509 certificate that will allow a proxy creation, stored by a MyProxy server (Fig. 1). It is used to authenticate users who are accessing the facilities offered by the grid. The use of proxies and X509 certificates is a key point of GSI (Grid Security Infrastructure), a standard used by all grid infrastructures all over the world.To implement the portal login and proxy creation, we made use of Grid Port 2 (https://gridport.npaci.edu 2000), a Perl toolkit designed by Npaci to aid in portal creation.To give a further level of security Astrocomp-G is accessed through HTTPS/SSL connections made available by Apache web server. Moreover, we re-engineered the job submission mechanisms of the available parallel codes to handle their running on the GRID-IT production grid. In particular, through the portal, we are able to check job status, watch logs, retrieve the output from a Resource Broker and visualize the output (Fig. 2). Because of the particular features of available applications, the portal is currently set to direct submitted jobs towards our IBM SP machine previously integrated in out testbed. The experiments have been done using MARA (Becciani et al. 2005), a parallel code for the analysis of light curves of closed binary systems.
Fig. 3 depicts the output result of a MARA job shown by the portal.

6. Conclusion

We have been able to add a Worker Node to an already working grid site without the use of a LCFGng server and without any data loss or interruptions of the mpp system and we have created a grid-enabled portal that allows an authenticate user to access the facilities offered by the grid.

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