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Astrocomp: web technologies for high performance computing on a grid of supercomputers

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Abstract. Astrocomp is a project developed by the Astrophysical Observatory of Catania, University of Roma La Sapienza and ENEA.
The project goal is to build a web-based user-friendly interface which allows the international community to run some parellel codes on a set of high performance computing (HPC) resources. There' s no need for specific knowledge about Unix commands and Operating Systems. Astrocomp makes some CPU times, on large parallel platform, available to the referenced user .

Key words. HPC, Grid Computing, Web Based Interface

1. Introduction

Astrocomp is a portal which creates a repository of easily usable computational codes and a common database available to the community. The Astrocomp server is based on a PHP-MySQL environment. Registered users have a grant for HPC systems available to the portal and can run all the astrophysical codes of the portal. They can easily prepare jobs and submit them remotely. The portal allows the user to know in real time the job status and hardware information of an HPC system like CPU usage, memory and queue status. Astrocomp looks like a sole interface for users wishing to run parallel

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codes included in the portal; it hides HPC complexity creating a common user level.

2. Astrocomp Hardware Resources

Astrocomp resources are:
IBM SP (INAF OACT) with 24 processors on 3 nodes, 16 GByte DRAM (per node): Global Memory: 48 Gbyte.
PQE1 (ENEA) a heterogeneous parallel system composed by a general purpose MIMD (multiple instruction multiple data) platform (Meiko/QSW CS-2) coupled with 7 SISAMD (single instruction single address multiple data) platforms (APE100/Quadrics).
FERONIA (ENEA) Quadrics Alpha Linux Beowulf cluster with 40 API UP2000 nodes; Each node: 2 Alpha EV6.7/21264 processors (1.3 GFlops of peak perf.) 1 GByte DRAM 2 MByte L2 Cache QsNet interconnect ("fat tree" topology) from QSW Ltd.
SGI Origin 3800 (Cineca) is a scalable shared memory multiprocessor system.
IBM SP (Cineca) based on Processing Elements (PEs) R12000 running at 400 MHz, 6 nodes with 32 processors each and with a memory of 64 GByte per node, except one with 128 GBytes.

3. Software Resources

The Softwares running in Astrocomp are:
FLY (1) from the Astrophysical Observatory of Catania (Italy): a tree N-body parallel code for three-dimensional self-gravitating collisionless systems evolution. It is based on the tree Barnes-Hut algorithm and periodical boundary conditions are implemented by means of Ewald summation technique. Each particle evolves following the laws of Newtonian physics, and the differential equations are integrated using the numerical Leapfrog integration scheme. All the particles, having the same mass, must be included in a cubic box having fixed dimensions. The supported cosmological models are: Standard Cold Dark Matter ($OmegaTOT = 1$), Lambda Models (with Cold Dark Matter), Open Models ($OmegaTOT < 1$).
Treecode ATD (2) from the University of Rome "La Sapienza" (Italy): a parallel tree code for the computation of the gravitational interactions among the particles in a self-gravitating system. The algorithm used in this code makes such evaluation faster, reducing the computational scaling.
HSNbody[1] from ENEA - HPCN Project (Italy): a code for the direct integration of an N body problem. Given an initial distribution of stars (treated like mass-points) in a stellar system, it integrates numerically the equations of motion of the N bodies of the system and computes the force acting on each particle, due to the interaction with all the other N-1 ones.
Mara (3) from the Astrophysical Observatory of Catania (Italy): a code for stellar light curves analysis.
W3P (4) from the Astrophysical Observatory of Catania (Italy): a parallel code for 3-D structure detection of substructures in cluster of galaxies with the morphological analysis of the found objects.

4. Astroadmin: the administration

Astrocomp provides authentication and authorisation for registered users. User access can be gained compiling an on line form. The administrator accesses the portal through a reserved section : www.astrocomp.it/astroadmin. From the interface, Administrator can quickly add a new code to the portal or modify the parameters and portal behaviour towards users. Fig. 1 shows a snapshot of the web based easy to use astroadmin section. There are no limits to the variety of codes that can be included in the Astrocomp

[1] HSNbody, Mara, W3p will be available in the next future

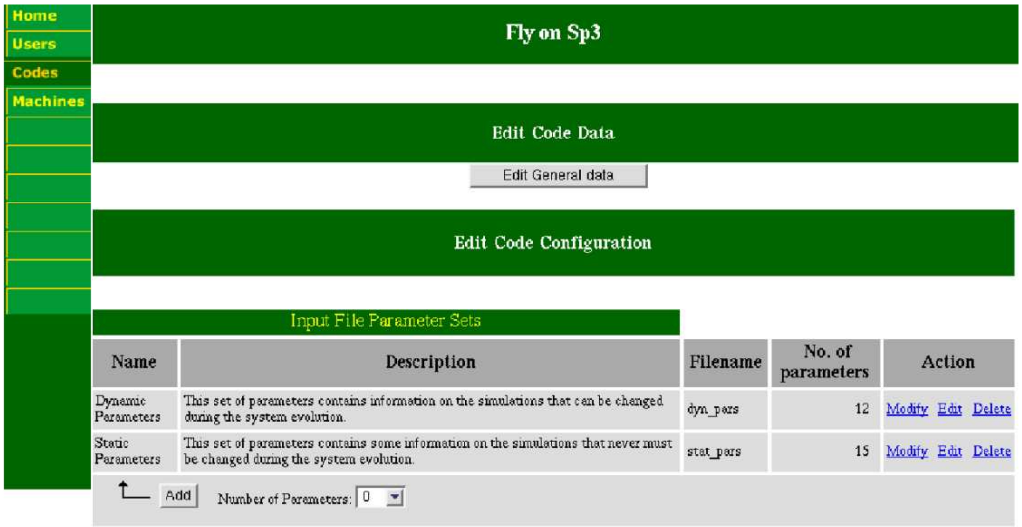

Fig. 1. The web based astroadmin section

structure; this is due to the internal code representation of the portal. Astrocomp architecture manages each code from the point of view of the user interaction as black box with some inputs such as the input files, shell scripts, or boundary files and some outputs like output files, log files. A code is an entity described by a state: Idle, Queued or Running and some properties like parameters and variables. The Astroadmin interfaces allow the Administrator to build the data structure that describes the input flow to the code entity. He must set the syntax and semantics of the parameters specifying the type, the default value, range and the hypertext shown to the user as a comment. Information given by the administrator is stored in the Astrocomp database in order to construct an internal description of the code.

5. Technologies

Astrocomp runs on Apache-Advanced Extranet Server (5): this allows you to set up connections with enormous numbers of authorised users, without bogging down the server. Apache server is run on over 6 million Internet servers (as of February 2000). It has been tested thoroughly by both developers and users. The Apache Group maintains rigorous standards before releasing new versions of the server that runs without a hitch on over one half of all servers available on the Internet. Apache is a powerful, flexible, HTTP/1.1 compliant web server, it' s highly configurable and extensible with third-party modules. The

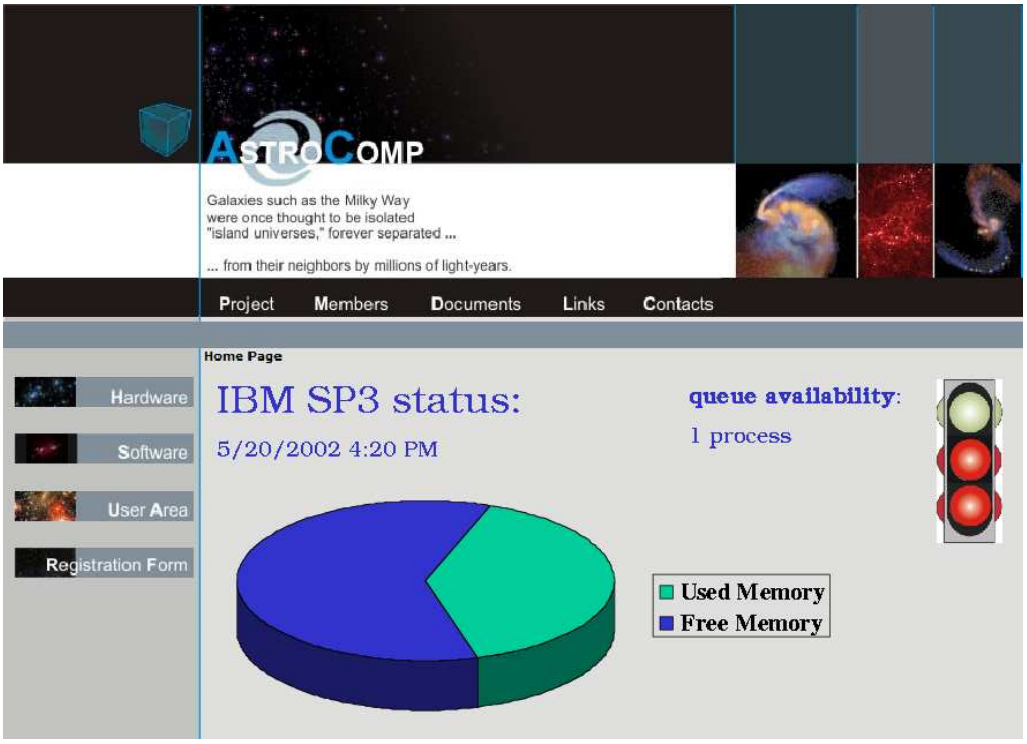

Fig. 2. Hardware resources report page

Apache server builds all the security environments that Astrocomp needs like Authorization, Authentication, and Access Control. Authentication is the process by which you verify that someone is who he claims to be; it involves a username and a password. Authorization is the process by with you find out if the person, once identified, is allowed to have the resource; this is usually determined by finding out if that person is part of a particular group or if that person has a particular level of security clearance. The Access Control is a much more general way of talking about controlling access to a web resource; Dynamical web pages are realised with server-side scripting PHP (6): (recursive acronym for "PHP: Hypertext Preprocessor") a widely-used Open Source general-purpose scripting language that is especially suited for Web development and can be embedded into HTML. Astrocomp Web structures have user specific customised and interactive content. The PHP programming language provides a powerful extension to HTML to create advanced and interactive web pages. Astrocomp has software and hardware knowledge of the systems and codes involved in the project; this is due to the presence of MySQL databases containing a description of codes properties and hardware resources. MySQL database server embodies a software architecture

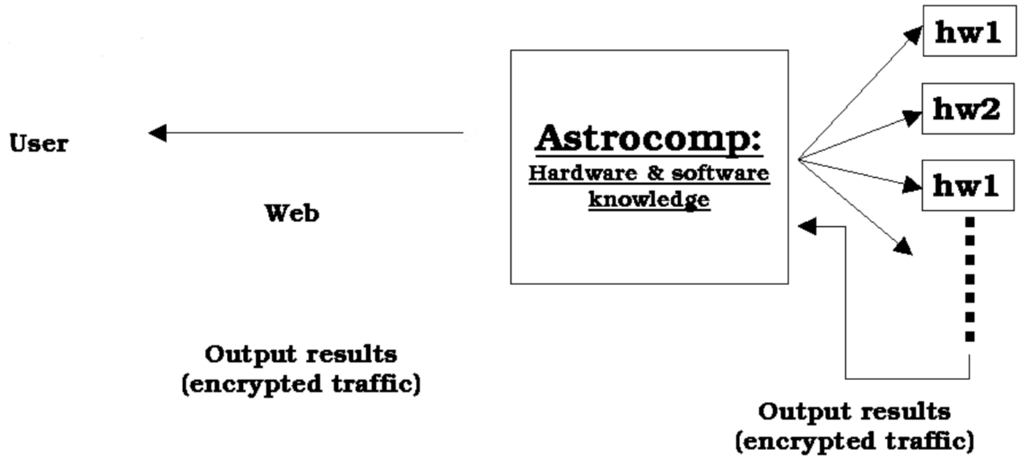

Fig. 3. Astrocomp data flow

that maximises speed. Extensive reuse of pieces of code within the software and an ambition to produce minimalist but functionally rich features have resulted in a database management system unmatched in speed, compactness and stability.

6. Astrocomp behaviour

The authorised user can access to his area. Astrocomp, who can receive real time information like CPU and memory usage from hardware resources, builds on demand report pages through PHP code. The user can take a look to the hardware status and choose an available or free platform. The PHP code allows us to build easy-to-read report pages: Fig. 2. The user can choose a code and a platform to run his job, he will compile some forms specifying the parameters and all the variables involved in the job. The complete job history for each user is stored in the MySQL database, so he can easily find his past parameters collections and simply modify them. After that Astroadmin, who owns all the sources codes, builds the input files and shell scripts, generates boundary conditions in accordance to the particular code and platform, compiles and submits remotely the source code. Data flow between HPC systems and the Astrocomp server is done by a set of PHP instructions based on ssh with the symmetric cryptography algorithm RSA for key

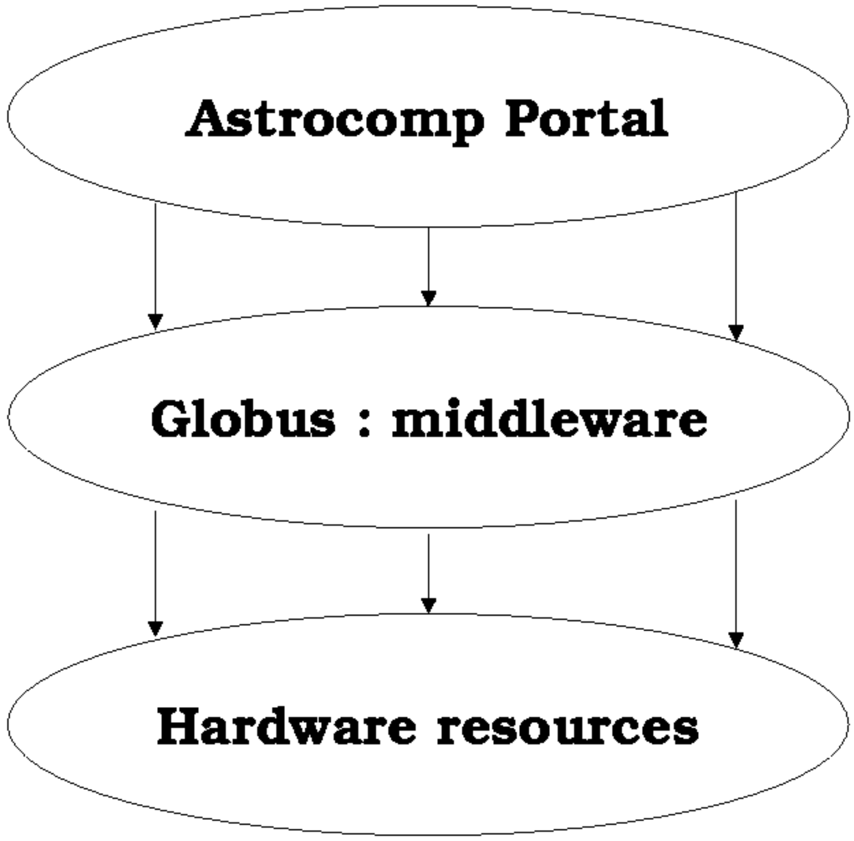

Fig. 4. Globus middleware

negotiation. Fig. 3 After job completion the PHP code allows the user to obtain a graphical representation of output data (this is useful for a quick look analysis); after that he can download every output file of his job. A constant management of software packets and the PHP code versus most cost common security bugs and attacks like buffer overflows and common exploits is actually one of the goals of the project.

7. Astrocomp Grid

The goal of the project is to manage a grid of HPC. We will use an infrastructure like Globus (Fig. 4) in order to create a middleware over the hardware resources. The Globus Project is a research and development project focused on enabling the application of Grid concepts to scientific and engineering computing. The Grid refers to an infrastructure that enables the integrated, collaborative use of high-end computers, networks, databases, and scientific instruments owned and managed by multiple organisations. A Grid provides some abstractions and concepts that let applications access across distributed area networks.

8. Conclusions

Astrocomp is a first experience of a web-based interface which allows the international community to use the codes involved in the project. It's easy to know codes behaviour and to ensue a job from the initial conditions to the graphical representation of the outputs results.

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