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Round-table discussion

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Abstract. These notes summarise the main topics touched upon during the Round-Table discussion held during the HPC-Grid 08 Workshop, INAF headquarters, March 12th 2008.

1. Introduction

The purpose of the workshop was predominantly to present the recent scientific results achieved by the Community, to present the new INAF-CINECA Agreement for High Performance Computing (HPC), to discuss the uses and the future developments in the GRID system in which INAF is involved, and more generally to evaluate the perspectives for Computing in Astrophysics.

The workshop was organised by INAF-SI in cooperation with the Scientific and Management Committees of the INAF-CINECA Agreement and in collaboration with the INAF representatives for the PON projects, approved by the MIUR for computational grids in the Objective 1 regions (PON 1575, Cometa Consortium, Cosmolab Consortium and University of Naples "Federico II"), with the support of the INAF Projects Department.

About forty people attended the workshop; a considerable interest was shown for the discussed subjects, not only from a scientific viewpoint, but also from a technical one.

The round table, coordinated by Giovanni Peres, had the aim of identifying the strengths and weaknesses of Italian Computational Astrophysics, and to outline the goals to pursue in the next three years.

The Community involved in computational astrophysics is composed of more than 100 scientists and is growing thanks to the new opportunities available in the field of the High Performance Computing. In addition to the use of CINECA, on the basis of the agreements active from 1997 until today, the community has also access to other national facilities (e.g. CASPUR), local clusters, new facilities created through PON funding, distributed computing using Grid technology and also foreign facilities. A big contribution to the request for computational resources is given not only by theoretical computing and numerical simulations, but also by the new prospects offered by the Virtual Observatory (e.g. cross-correlation of catalogues, re-processing of archive data and comparison with theoretical models, visualisation and analysis of complex data-sets, etc.) and by the need to reduce and analyse data gathered with new observational facilities (LBT, VST, etc.).

The discussion during the round table seemed to confirm the impression that HPC and distributed computing technologies (Grid-a-la-EGEE) are exploitable to deal with dif-

ferent and complementary issues. Conversely, of particular interest appeared to be the experiences carried out by scientists within the Cometa consortium who were able to achieve HPC-quality results through Grid technology, where computing was concentrated on local clusters having high-performance links (Grid-a-la-DEISA). It would be desirable for both approaches to merge, to simplify the interfaces for end-users.

The approach developed during the INAF-CINECA 2005-07 Agreement was to privilege few big key projects for the allocation of computing time; this tendency needs to be followed and enhanced also in the future. In addition to these key projects, there are some medium-size projects and some benchmarking and prototyping activity needing just a limited set of resources. Anyway it is worth noticing that the so-called national key projects may be defined as medium-to-small when compared with the European and US reality, and they might turn out to be not very competitive in the international scenario. Therefore, we need to pursue a national policy aimed at bringing Italy in the group of countries capable of having a HPC facility in the 100 TFlop range (as already available in France, UK, Germany, Spain, Japan), fitting the so-called Tier-1 of the EU programme for the supercomputing; the final aim should be hosting a facility at the Tier-0 level (currently, 1 PFlop) in a medium-term future. This approach would allow to start performing world-leading large-scale projects.

The Community has already contributed to this initiative preparing an astrophysics section within two different versions of a White Paper on supercomputing in Italy. We want anyhow to point out that, while satisfying the request for HPC is crucial to continue the work started in some extremely relevant sectors (N-Body simulations, magneto-fluid-dynamics, etc.), on the other hand this is not sufficient to meet the demand for computing power expressed by other components of the national community.

The computing resources available to the Community thanks to the PON initiatives in southern Italy are an important resource, also because of the collaboration aimed at ensuring interoperability among the various infrastructures set up by the projects currently ongoing. The Ministry of Education and Research (MIUR) plans to expand this collaboration to the Grid infrastructure existing in the northern and central Italy as well, and plans to ensure its maintenance (in terms of hardware, software and middleware), in order not to disperse the heritage of highly specialized know-how, which was one of the main results of the PON activity. As for the INAF Community, the investments made upon the PON infrastructure are at risk of being wasted without an appropriate investment to ensure sustainability. The next PON announcement should be able to meet this need for some time, but between the conclusion of a project and the beginning of the next one there could be a gap that should be covered in some way (e.g. through a INAF partnership). Furthermore, it should be noted that the use of the infrastructure by the INAF Community also provides a special kind of know-how, intermediate between the middleware and the application, which can not be assured by PON financing.

Exploitation of the Grid technology is very promising, particularly in the presence of real HPC experiences obtained on the Grid, in addition to the more traditional experiences of data analysis and low-data-interchange computing. The number of applications of astrophysical interest that use the Grid infrastructure is quickly growing: on this topic the Italian community has an indisputable leadership role, recognized at European level (EGEE). But it would be important to iron out the difficulties that a potential user of HPC and Grid systems finds in moving his/her application from one infrastructure to the other. It is understood that the optimisation of an application on a specific computational infrastructure requires an investment of human resources in any case; however, the joint EGEE-DEISA initiative to create a coherent interface for the exploitation of both infrastructures is relevant and should be carefully monitored. It is anyhow important to create and manage a subset of the Italian Grid infrastructure dedicated to astrophysics to have shared resources to offer to the other grid partners and, especially, to avoid problems and bottlenecks when the CERN experiments

for which the Grid itself was initially proposed will be eventually active.

The EU strategy for the computer infrastructure (e-infrastructures) foresee different overlying layers: starting from the network infrastructure, passing through the grid and data infrastructures, and through the integration of generalized and domain-specific applications, a knowledge infrastructure can be achieved, which is expected to be the basis of the scientific progress during the coming decades. From this viewpoint, it becomes essential to work so as to achieve an effective interoperability among several infrastructures and an integrated utilisation of a series of facilities for the understanding of astrophysical data, observed or simulated (visualisation, data mining,...). In this area the work performed at international level for the Virtual Observatory can be located. This work is often invisible (and this is right, since we are talking about an infrastructure), but it includes a series of software tools that are becoming part of an astrophysicist's daily life.

Only if we follow these strategies in the field of HPC, Grid and Virtual Observatory it might be possible for our community to remain competitive world-wide. In any case, to reach this competitiveness level, the creation of teams (both through the collaboration among already-existing groups, and through the involvement of new young scientists) having proper critical mass is needed, in order to allow e.g. to analyse the simulation results, to obtain scientific results, or to keep the technical competence about infrastructures. It is therefore indispensable to have the capability of attracting young researchers, to meet their expectations in terms of career development, and to create and maintain the needed know-how.

INAF has not shown so far the will to support significantly the coordination and development of e-infrastructures. But in this way the investments made to obtain pixels from the instruments could be thwarted by the lack of investments aimed at processing and understanding the scientific meaning of those very pixels.

We suggest that the Scientific Council and the Information Systems Unit work together within INAF, each according to its own competence, in order to define a strategy that, from scientific needs, defines and plans the necessary resources for supporting suitably computational astrophysics in Italy.