Grid computing for statistical and non-linear physics

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Grid computing is an arrangement of computer resources from multiple administrative domains to reach a common goal, complete tasks more efficiently. The grid can be thought of as a distributed system that involves a large number of files. What distinguishes grid computing from conventional high performance computing systems such as cluster computing is that grids tend to be more loosely coupled, heterogeneous, and geographically dispersed.

Since 2010, the pan-European Grid Infrastructure (EGI)[1] in collaboration with the National Grid Initiatives (NGIs) guarantees the long term availability of the generic e-infrastructures for all European research communities and their international collaborators. In this framework, the Spanish and the Portuguese National Grid Initiaves[2,3] are working hand by hand to create a large cooperative grid infrastructure, IBERGRID[4]. Nowadays Spanish researchers can access to more than 24000 cores and 20 PetaBytes of online storage just filling a form that can be found in the Spanish NGI web page[2]. IFISC[5] is member of the Grid-CSIC[6] project and shares its computational resources between all the european grid users, in particular with the IBERGRID ones.

Scientific grid has been proven to be a useful tool in some very computationally demanding fields as for example in analysis of particle physics or astrophysics data. While it has been extended to other fields such as plasma research it is still viewed as a tool associated to large projects. These large projects are the ones that can afford to have fine-tuned sophisticated interfaces for the researchers involved on these projects. Without these interfaces the access to grid using shell commands is quite cumbersome by nowadays point and click standards.

However, grid has the potential to be a key instrument for a wide variety of scientific topics which require to perform many calculations, for example to explore the dynamics as function of parameters as a typical case in nonlinear dynamics of complex systems and to perform statistics. While this high throughput computational needs are very much suitable for what grid was intended for, very few users take advantage of it because the access is cumbersome and requires a learning period that many researchers, mainly in small groups, can not afford.

To popularize grid in all scientific areas it is required to have user friendly interfaces where simple programs can be uploaded and executed in a simple way. Those interfaces should not compete with the sophisticated interfaces developed for specific applications rather they should cover the most basic aspects with suitable default options. The minimal capabilities would be submitting a job, recovering the results, monitoring the existing jobs and check the grid status (load, availability of free cores,...).

To make grid usage as common as computational clusters, user friendly interfaces are needed, and IFISC developed in the framework of Grid-CSIC project Web4Grid[7], a web interface to allow easy access to the grid infrastructure to those (until now) non-usual grid users.

By using this portal, researchers can submit applications, recover the results and monitor the status without any prior grid knowledge. After authenticating and configuring the account, job submission has been simplified: the user just uploads the application to be run and sets the parameters and the input files. All other information is the same for all the users by default but can be overwritten by each user within her own profile. When the job has benn submitted, a background script manages all the job workflow from proxy creation to results recovery and data cleaning.

FIG. 1. IBERGRID resources map.

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[1] European Grid Infrastructure. http://www.egi.eu
[2] es-NGI. http:www.e-ciencia.esngi
[3] INGRID. http://www.gridcomputing.pt/
[4] Ibergrid Initiative. http://ibergrid.eu
[5] IFISC. http://ifisc.uib-csic.es
[6] Grid-CSIC project. Ref: 200450E494. http://www.grid.csic.es
[7] Tugores, A.; Colet, P.: Web interface for generic grid jobs, Web4Grid. Computing and Informatics, Vol. 31, 2012, pp. 173–186