

WISDOM production environment

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Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

During 2005 and 2006, three biomedical data challenges were run on the EGEE grid: two on malaria and one on avian flu. These deployments, based on relevant biological needs, were successfully achieved using most of the available resources on the Biomed virtual organisation. As a total, almost 600 years of computations were achieved during these 3 deployments using the WISDOM production environment.

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

The environment is made of a set of scripts that generate the jobs, submit the files and check regularly their status while they are on the Grid through the workload management system. Given the status of the jobs, several actions are taken. The main one is the job resubmission if a job has been aborted by the workload management system, cancelled by the user or has failed because problems occurred during job run. The environment can also cancel a job automatically if the job stayed for too long in a queue; in this case the job is also resubmitted after it has been cancelled. The submission process is performed by a java multithreaded submission engine, that can submit multiple jobs on several resource brokers in a round robin. The job results are stored directly on the grid storage elements, and the useful scoring information are registered directly in a relational database.

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possible, point out the experience limitations (both in terms of existing services or missing functionality)

The grid is still a very unpredictable system and there are many single points of failure that makes the efficiency decrease as the grid become

more and more overloaded. For instance, resource brokers are still the source of a lot of troubles because they can become easily overloaded by job submissions, and are sometimes inefficient in the scheduling of the jobs.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

With WISDOM, we wanted to produce a straightforward application, “easy” to use for non grid experts, and being able to integrate any type of docking software with it.

The system was designed to deploy high-throughput experiments on the grid, and is being reengineered to offer a fully interoperable web services interface, with connections to databases to store and query, in almost real-time, the statistics and results.

One of the major added values of this new architecture is that the whole system can be easily integrated in workflow engines that just call the ad-hoc operations. The developments were focused on fault-tolerance, flexibility and scalability but several issues arose during the experiments.

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