

Applying Grid Technologies to In Silico Oncology

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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).

In silico oncology is an emerging interdisciplinary field aiming at mathematically describing and computationally simulating the multiscale biological mechanisms that constitute the phenomenon of cancer and its response to therapeutic techniques. Within this framework, the In Silico Oncology Group, National Technical University of Athens, has already developed a four-dimensional simulation model of glioblastoma multiform response to radiotherapy.

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.

In order for In Silico Oncology to be efficiently transferred to the EGEE infrastructure, certain aspects need to be addressed regarding its adaptation to the grid programming model. First and foremost, suitable workflows need to be developed for the coordination of the grid-enabled application components responsible for job-simulation submission and monitoring, resource monitoring, data management and result retrieval, which will provide some basic quality of service. A first approach towards grid-enabling In Silico Oncology is to execute several simulations in parallel, thus reducing the overall time that a researcher or a doctor has to wait for different simulation results. Jobs-simulations may be efficiently scheduled by the gLite workload management system, according to system loading criteria and data locality.

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)

Beyond the basic functionality described above, it is also important that further mechanisms for fault tolerance and quality of service are developed and incorporated to the application. Fault tolerance is a feature that is not supported inherently by the grid middleware at present and that is highly desirable for a grid-based application. QoS may be achieved by taking into consideration workload and resource capacity estimation, resulting in more complex scheduling patterns.

This work has been performed in the context of the research project "Development and adaptation of an in silico oncology application in grid environment"(GRID-APP). The project is funded by the General Secretariat for Research and Technology, Ministry of Development, Greece and the European Regional Participation Fund.

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

Due to the hypercomplexity of the problem, high-performance computing infrastructures are necessary. In order to simulate numerous candidate therapeutic scenarios as fast as possible, grid technologies seem to be particularly effective. In addition, as tumor response to radiotherapy is a highly non linear phenomenon, parallel executions of the simulation code for a large number of sets of parameters are highly desirable, in order to gain better insight into the dynamics of the system.

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