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A WSRF-based Computational Gateway to the EGEE Infrastructure for the Simulation of Cardiac Electrical Activity

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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).

The understanding of cardiac electrical behaviour is essential to comprehend the genesis of cardiac arrhythmias and to develop new therapeutic methods based on the use of antiarrhythmic drugs. Computer simulations are an essential tool, as the mathematical models that predict ionic currents and propagating wavefronts have reached a high level of electrophysiological detail. However, these simulations are both computationally and memory intensive, producing a large amount of simulation data.

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.

We have deployed a WSRF-based Grid metascheduler (GMarte) that enables biomedical experts to access a computational infrastructure, composed of different clusters of PCs within our research group. This provides transparent access to computing power for users. However, the multi-user support of the metascheduler combined with large cardiac studies can often overload these computing resources. Therefore, we plan to provide a computational gateway to LCG-2, so that those simulations that can not be executed in our Grid are automatically delegated to a Resource Broker for its execution on a production Grid. This would require coordinated data staging to Storage Elements, using the functionality provided by a File Catalog to manage different replicas of simulation data. The usage of MyProxy is ideal to automatically renew the proxy for long simulations. Also, the Logging & Bookkepping service is fundamental to integrate the lifecycle of tasks within our metascheduler.

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 application is MPI-based, thus requiring parallel executions on LCG-2 resources.
In addition, it uses MPI-2 I/O techniques for parallel I/O, what demands a shared
file system among all the worker nodes. On the other hand, the application is complex
enough to try an in-place compilation before execution. Thus, we are producing
statically-linked self-contained executable files which we expect to be able to run.
We would be interested in using Java APIs to interact with LCG-2 services.

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

The electrical activity enables to analyse the influence of certain drugs to heart
diseases as well as the influence of different cellular parameters to the electrical
activity. Moreover, cardiac case studies are inherently composed of lots of
independent multi-parametric jobs, and the Grid is the appropriate infrastructure to
accelerate their execution.
On average, we have estimated a requirement of 96 CPUs per day producing a total
amount of data in the order of 120 GBytes. This would include research lines that
investigate the genesis of reentrant activity under acutely ischemic (phase Ia)
conditions, and the effects of antiarrhythmic drugs such as lidocaine or pinacidil.
Potential user community is composed by cardiac electrophysiologists interested in
using detailed cellular models to study effects on electrical activity. In addition,
this activity fits within the goals of the Virtual Physiological Human by providing
an effective simulation tool for action potential propagation.

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