

## Porting a complex workflow on EGEE infrastructure: The case study of WIEN2k

Thursday 10 May 2007 14:15 (15 minutes)

**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 target community is material science. The application called WIEN2k performs electronic structure calculations of solids using density functional theory. It is based on the full-potential (linearized) augmented plane-wave ((L)APW), one among the most accurate schemes for band structure calculations. WIEN2k is used by more than 1000 institutes worldwide in academia and industry. This work aims at enabling exiting tools (w2web web portal) to be able to use EGEE infrastructure.

**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.**

This is work-in-progress and part of NA4 effort. We are using our own glite testbed based on virtual machine technology. Using our own infrastructure was necessary, because of licenses issues. Once validated, we plan to deploy our solution in Gilda, and finally on VOCE. One important step will be to show the WIEN2k community the complete integration of the glite-enabled tools into the tool (e.g. w2web web portal) they are familiar with. The key services for implementing our solution will be VOMS and the deployment capabilities based on certificate roles. Another key element for the implementation of the workflow engine is the Ganga toolkit.

**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)**

One of the missing functionalities which would simplify the development of the WIEN2K workflow is the support of loops and the ability to separate

control-flow from data-flow. Based on our experience with the ASKALON grid environment (which supports both features, but currently is not yet glite-enabled), we are trying to provide a similar but simplified solution for the WIEN2k glite porting.

**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**

WIEN2k is composed of several packages which form a complex grid workflow, including complex data-dependencies (which are separated from the control-flow), parallel sections and loops (not supported by basic job submission capabilities of glite, currently limited to a DAG for example). Our experience will give a useful input to help porting other scientific applications with similar characteristics. In addition, WIEN2k is a licensed application and existing solutions, e.g. creating a full VO per application, are not satisfactory. Institutions having already a license would like to use EGEE infrastructure, but not necessarily be bound to a VO, and at the same time, the deployed code on the Grid should not be accessible to non-licensed users. Our proposed solution is based on a combination of existing capabilities of the middleware, using certificate roles and access control.

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**Session Classification:** Workflow

**Track Classification:** Workflow