Contribution ID: **30** Type: **Poster**

Running a complex workflow on EGEE infrastructure: Wien2k in action

Tuesday 23 September 2008 16:11 (1 minute)

Describe the activity, tool or service using or enhancing the EGEE infrastructure or results. A high-level description is needed here (Neither a detailed specialist report nor a list of references is required).

Wien2K is a package for electronic structure calculation of crystals, used in computational chemistry. Previously we have presented issues and solutions to porting the Wien2K workflow to the gLite environment. In this session we will show a live demo of an execution of Wien2k on EGEE infrastructure, presenting show the both the user view and the internals.

Report on the impact of the activity, tool or service. This should include a description of how grid technology enabled or enhanced the result, or how you have enabled or enhanced the infrastructure for other users.

There are two major impacts of this work: The first impact is for scientists in computational chemistry: We have ported the Wien2k application to the EGEE infrastructure, while keeping the front-end intact. This allows scientists experienced with Wien2k, but with little Grid knowledge, to harness the power of the Grid to retrieve results much faster than on a single machine. The second impact is to the application porting community as a whole: We have studies several issues in-depth. We have provided guidelines on how to map application activities to Grid activities. We have shown how a worker model can reduce scheduling time while still remaining fair. We have also shown how to reduce performance overheads created during the "Gridification" of applications.

Abstracts for online demonstrations must provide a summary of the demo content. Places for demos are limited and this summary will be used as part of the selection procedure. Please include the visual impact of the demo and highlight any specific requirements (e.g. network connection). In general, a successful demo is expected to have some supporting material (poster) and be capable of running on a single screen or projector.

For this demo we are planning to show an actual Wien2k execution on the Grid - live. In particular, we will show:

The use side, consisting of the modified Wien2k web-portal to create an experiment, and the execution of the experiment on EGEE infrastructure

Behind the scenes using a specially developed visualization tool, showing where the activities are executed.

This demo requires a network connection

Describe the added value of the grid for your activity, or the value your tool or service adds for other grid users. This should include the scale of the activity and of the potential user community, and the relevance for other scientific or business applications.

The Wien2k package is well-used in computational chemistry. It is licensed to over 1000 institutes worldwide in academia and industry. The package itself is currently ported to single machines and simple parallel clusters using MPI. We have taken this package and ported it to the Grid, in particular on EGEE infrastructure. The ultimate goal is to hide the Grid from the user, and allow execution on the Grid in the same fashion that a user would execute the application locally. Along the way we have solved several issues which apply to complex workflow applications: We have defined how to identify single activities, defined when they can be combined for performance, looked into improving scheduling times, and provided support for automated deployment.

Author: Dr BERGER, Maximilian (University of Innsbruck)

Co-author: Prof. FAHRINGER, Thomas (University of Innsbruck)

Presenter: Dr BERGER, Maximilian (University of Innsbruck)

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