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# Gridification of Computation Chemistry WIEN2K Workflow Application

*discussion during EGEE Conference October 2007, Budapest*

*present: Alex, Hurng-Chun, Kuba*

WIEN2K has been ported to Ganga by Alex. Each workflow activity (node) is a grid job submitted by Ganga. The files are passed around in the sandbox or via SE depending on their size. The application itself is automatically installed when the job reached WN. In the Ganga implementation of WIEN2K the workflow is hardcoded. It consist of five steps and a loop. Two of the steps are parallel jobs. The loop goes from the end of the second step to the begining of the first step. Contrary to more general ASKALON framework, the Ganga WIEN2K workflow couples the control and data flows. In ASKALON data flow may be independent of the control-flow which allows to sometimes optimize the data transfer (by prestaging the data on the WN). In ASKALON the Grid submission is based on Globus.

Alex is to send the WIEN2K Ganga implementation so that the possibility of using DIANE may be evaluated. If feasible then we should start with something simple for the concrete WIEN2K application. The timescale interesting for Alex is the end of EGEE-II (March 2008). If this is successful, feasible and interesting we could continue to do something more generic for ASKALON later.

-- JakubMoscicki - 06 Oct 2007

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This topic: ArdaGrid > WIEN2K

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