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Practical Experience from porting the Wien2k Application to EGEE

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Wien2k is a package for electronic structure calculation of crystals, used in computational chemistry. We have successfully ported this application to the EGEE infrastructure. In this talk we'll give an overview of this work, the lessons learned, and the outcome of the port.

Impact

There are two major impacts of this work: The direct impact is the completed Wien2k package, which is now available for users of the EGEE infrastructure. The Wien2k package is currently used by many research groups, which will be able to significantly speed up their research using the developed application. The second impact is the lessons learned from the porting: The described methods and algorithms are applied to the Wien2k application, but are generic enough to be re-used in further application porting.

URL for further information

http://www.dps.uibk.ac.at/

Conclusions and Future Work

The Grid Version of Wien2k is ported and provides results much faster than local execution and trivial Grid execution. The presented optimizations give an example for all Grid porting efforts.

Keywords

workflow, computational chemistry, Wine2k, application porting

Detailed analysis

Unlike parameter study applications, which are trivially parallel, the Wien2K application can be defined as a workflow of activities, with interdependencies between the activities. We have previously presented how these activities can be efficiently scheduled and executed using the worker model. In this talk we outline how the worker model can be extended with provisions for faster data transfer, thus reducing the run-time even more. We also describe the steps necessary for a user to use the Wien2k package.

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