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Use of Scientific Software in Distributed Environments - A Practical Experience with VGE and EGEE

Thursday, 31 January 2008 11:40 (40 minutes)

The ab-initio program-suite COLUMBUS was installed within the COMPCHEM-VO in the EGEE Grid and deployed as a VGE (Vienna Grid Environment) web-service at local sites within the University of Vienna. Additionally the Molecular Dynamics package NEWTON-X was deployed as VGE web-service.
These two systems, the VGE and the EGEE, persue different philosophies, representent a bottom-up vs. a top-down approach to the problem of access to computational resources in heterogenous environments.
From the end-user's point of view both systems have their advantages and downsides, but are promising prototypes for future development.

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