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A Science Gateway for Molecular Simulations

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Overview

Nowadays, scientists in multiple research areas like material science, structural biology, and drug design are supported by invaluable molecular simulation tools. These tools allow analyzing increasingly complex chemical structures on high-performance computing facilities. However, the lack of graphical user interfaces, the limitation of the usability of the tools and the complexity of infrastructures demands intuitive user interfaces. The project MoSGrid (Molecular Simulation Grid) addresses these issues by combining an easy to use portal-based infrastructure with expert knowledge on the correct use of complex methods. The emerging portal will support users in all stages of the simulation process with easy access to data repositories storing information about molecular properties and the possibility of creating, editing and invoking workflows. The project integrates the UNICORE 6 grid middleware and the cloud file system XtreemFS into the workflow-enabled grid portal WS-PGRADE.

Impact

The emerging science gateway offers a single point of entry to the whole process of analyzing data for molecular simulations facilitating UNICORE 6 infrastructures. It will support multiple molecular simulation tools, workflows on molecular simulations and repositories which store the information on structures, workflows and simulation results. The supported tools are selected via a survey in the MoSGrid community including about 100 working groups in the fields of computational chemistry and bioinformatics. Workflows and results can be exchanged in the community via a global repository. Workflows can be created, re-used and changed by the community and additional knowledge will be obtained by cross-referencing different result data files. Compared to similar existing activities like ProSim, G-FLUXO, the e-NMR portal and projects based on EnginFrame, the MoSGrid science gateway will offer a larger scale of tools and methods and will support the possibility to refer to molecules and results in a global repository under an open source license.

EnginFrame is also a workflow-enabled grid portal with existing projects for molecular simulations but under a commercial license model for non-academic users. ProSim and MoSGrid can benefit from each other. ProSim offers workflows and workflow templates for carbohydrate recognition in a portal on top of WS-PGRADE with access to several grid infrastructures. Users could re-use workflows of ProSim in the MoSGrid science gateway and the ProSim portal could offer carbohydrate recognition in UNICORE 6 infrastructures. G-FLUXO provides Gromacs workflows based on P-GRADE (the first generation of WS-PGRADE) and visualization of simulation results. The workflows and the visualization could be integrated into the MoSGrid science gateway. The e-NMR portal offers also multiple molecular simulation tools with access to a number of grid resources but does not offer a repository of results.

Description of the work

MoSGrid is an interdisciplinary project which aims to facilitate molecular simulation tools in grid infrastructures via a science gateway. This science gateway is based on the workflow-enabled grid portal WS-PGRADE

which is the highly flexible graphical user interface (including a graphical workflow editor) of the grid User Support Environment (gUSE). gUSE is a virtualization environment providing a set of services including a workflow engine, so-called submitters (Java-based applications), a workflow storage, an application repository, monitoring and logging. Submitters implement the grid service interface of gUSE and exist for classical service and desktop grids, clouds and clusters, unique web services. MoSGrid added a submitter for UNICORE 6 using the UCC (UNICORE Commandline Client) libraries. The submitter enables to invoke jobs of WS-PGRADE workflows on UNICORE 6 infrastructures and additionally the invocation of existing UNICORE workflows via WS-PGRADE.
Besides the extended workflow features of WS-PGRADE, MoSGrid has been developing intuitive portlets for predefined basic workflows for the most popular molecular simulation tools within the MoSGrid community. Furthermore, users will be supported by repositories which store information about initial structures for the simulation process, parameters of workflows like used molecular simulation tools and resulting structures. The repositories will allow external referencing of simulation results and will be available replicated in XtreemFS via the science gateway.
In general the authentication process for grid infrastructures relies on X.509 based certificates. In MoSGrid WS-PGRADE has been extended for the use of SAML (Security Assertion Markup Language). The user is enabled to create an assertion file from his X.509 certificate via an applet. The certificate remains on the user' s computer, solely the assertion file is stored on the science gateway server and handed over to the UNICORE infrastructures.

URL

http://mosgrid.informatik.uni-tuebingen.de:8080/

Conclusions

The emerging MoSGrid science gateway will support the users of molecular simulation tools in grid infrastructures. At the current stage of the prototype, the UNICORE 6 integration for WS-PGRADE workflows and the SAML extension is operational. Furthermore, there are archetypical workflows available for quantum chemical simulations with Gaussian and molecular dynamic simulations with Gromacs in single portlets.
Next steps include the definition of workflows for the MoSGrid community and the uptake of the Application Specific Module (ASM) for WS-PGRADE in the developed portlets. Latter will serve as templates for further portlets on additional tools. The portlet developers do not have to become acquainted any more to the UNICORE integration in detail and the users are enabled to monitor their different workflows on one page. Furthermore, the repositories based on XtreemFS will be integrated into the science gateway. Hence, XtreemFS will be extended for authentication with SAML.

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