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## The MoSGrid Community –From National to International Scale

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### Description of the Work

The task to support the international community is divided into two main parts; the security-related part and the domain-related part. The first one sets the stage for international users so that they have access to the services of the MoSGrid science gateway. In the second part, MoSGrid forges links to international user communities and further develops domain-related services.

The MoSGrid science gateway employs WS-PGRADE that is the highly flexible user interface of grid User Support Environment (gUSE). gUSE provides a large set of DCI services by which interoperation among classical services and desktop grids, clouds and clusters, unique web services, and user communities can be achieved in a scalable way. The integration of the grid middleware UNICORE into gUSE has been developed in the MoSGrid project. Furthermore, WS-PGRADE, gUSE, and the cloud file system XtremFS were extended for the use with SAML (Security Assertion Markup Language). The science gateway will be offered as open-source software. Thus, user communities working with UNICORE-based DCIs are able to make use of the MoSGrid services without any changes. Minor changes are necessary for Shibboleth-oriented infrastructures. The basic infrastructure also allows authentication via MyProxy certificates and the use of DCIs with foreign middlewares.

On top of the existing services, the MoSGrid science gateway will be extended in SCI-BUS by a semantic search for workflows and simulation results. The visualization of grid-computed results and the possibility of interaction with a 3D molecule editor based on WebGL will support the users to process the full life-cycle of data analysis within the science gateway. The collaboration with SCI-BUS, SHIWA, and EDGI facilitates the use of various European Grid infrastructures. Furthermore, additional workflows will be developed together with the communities and regular international community workshops are planned.

### Conclusions

Currently, the MoSGrid community consists of more than 100 German users. However, the MoSGrid science gateways and its infrastructure with the integrated tools and workflows as well as generated results are valuable for the international community. The design of the science gateway is open for international use and the software will be provided as open-source software.

SCI-BUS will advance a generic-purpose science gateway technology that will provide access to DCIs and their services in Europe. Additionally, life-sciences-related communities contribute to the project and partners of the communities will further develop these gateways. Several user community workshops will bring together users, developers, and providers of the science gateways. The planned collaboration with SHIWA and EDGI forges links to more related communities and opens up the possibility for the molecular simulation community to influence workflow interoperability and desktop grids on European level.

## Impact

Several communities from a number of application fields participate in SCI-BUS and COMPCHEM, Bio-science Grid, the PROSIM protein docking community, and MoSGrid represent the life sciences. Partners of SCI-BUS and SHIWA are also members of the virtual organization (VO) Life Science that is one of the first established virtual user communities. The close collaboration between these communities allows the exchange of experiences, workflows, results, and molecular structures. Thus, they can benefit from each other without spending time on calculating the same molecular simulations or repeating unsuccessful simulations. The data is sensitive and the analysis of molecular data on a large scale is time-consuming and expensive. The output of a survey in the MoSGrid community shows that 70% would share their results and molecular structures in a repository after they have published them or own a patent. We assume that researchers of the other communities would agree to share data in a repository at a similar rate.

The willingness to share tools and workflows is quite higher (nearly to 90%). Thus, the developers of services for the communities can also profit from the synergies. They can coordinate domain-related work as well as general developments for the science gateways. SCI-BUS focuses on further coordinated developments of science gateways and on offering portlet repositories whereas SHIWA concentrates on workflow interoperability, workflows, and workflow repositories. EDGI brings in new technologies with desktop grids. The participation in and collaboration with these three projects allows developers of domain-related tools and workflows to concentrate on the specific demands, whereas, general developments (e.g., security) can be completed by partners who are working on the infrastructure of science gateways. This leads to provision of advanced services better tailored to the users' needs and supporting innovation and efficiency in the scientific discovery process.

## URL

<http://chinin.informatik.uni-tuebingen.de:8080/>

## Overview (For the conference guide)

The project MoSGrid (Molecular Simulation Grid) offers a web-based science gateway supporting the community with various services for molecular modeling, docking, and quantum chemistry. Users gain access to distributed computing infrastructures (DCIs) via intuitive user interfaces for sophisticated tools, specialized workflows, and distributed repositories. Currently, the MoSGrid community consists of over 50 research groups from a number of fields related to chemistry and bioinformatics located in Germany. However, the underlying security infrastructure is not limited to national requirements. It can be easily configured for international users.

MoSGrid intends to address the international community by participating in the EU-project SCI-BUS (Scientific gateway Based User Support), collaborating with the EU-projects SHIWA (SHaring Interoperable Workflows for large-scale scientific simulations on Available DCIs), and EDGI (European Desktop Grid Initiative).

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