TECHNISCHE UNIVERSITÄT DRESDEN

Zentrum für Informationsdienste und Hochleistungsrechnen (ZIH)

Generic User Management for Science Gateways via Virtual Organizations

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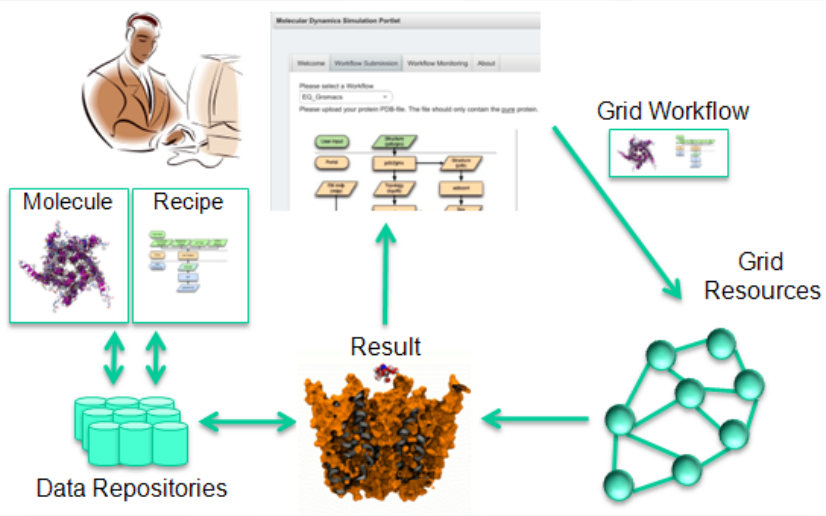
MoSGrid - Introduction

- MoSGrid Science Gateway - Simple and efficient use of complex chemical applications via a portal integrated grid infrastructure



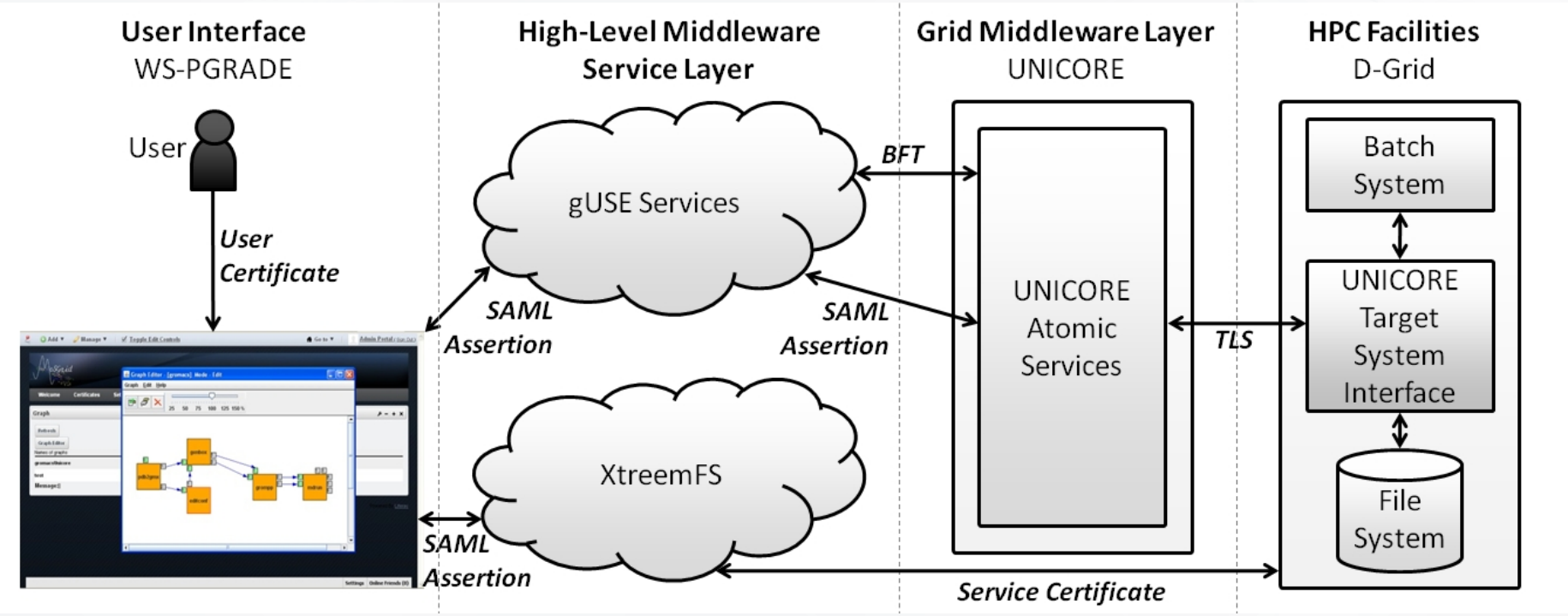
- More simple access to applications via a user friendly **Portal**
- More simple use of complex molecular simulation via **Unified Integration**
- Support work of chemists via linking of applications with **Grid Workflow Management**
- Support re-use of data and workflows via a **Data Repository**

MoSGrid - Project

- German grid project, 08/2009 – 12/2012
- Consortium members: ZIH (Dresden), Bioinformatics (Tübingen), Zuse Institut (Berlin), RRZK/Organic Chemistry (Cologne), Inorganic Chemistry (Dortmund/Munich), PC2 (Paderborn)
- Industry Partners: Bayer Technology Services GmbH, Origenis GmbH, BioSolveIT GmbH, COSMOlogic GmbH & Co. KG, GETLIG & TAR
- Associated Partners: MTA SZTAKI, Jülich Supercomputing Centre, Turbomole GmbH, Schrödinger GmbH, Oracle Germany

MoSGrid Security Infrastructure

- User certificate for creating a short lived credential and automatic login
- Credential for authentication to gUSE, XtreemFS, and UNICORE



Authentication/Authorization

- Goal: Simplify user management for users and administrators
- Use of certificate stored in browser for
  - Automatic authentication and login
  - Creation of short lived credentials (SAML assertions) for grid access
- Authorization in science gateway depends on user's VO membership
- Automatically use of VO status to activate user

Liferay

- Open source portal framework based on Java
- Widely used in grid and cloud projects
- Supports JSR168 and JSR286 portlet standards
- Highly flexible
- User management with pluggable authentication

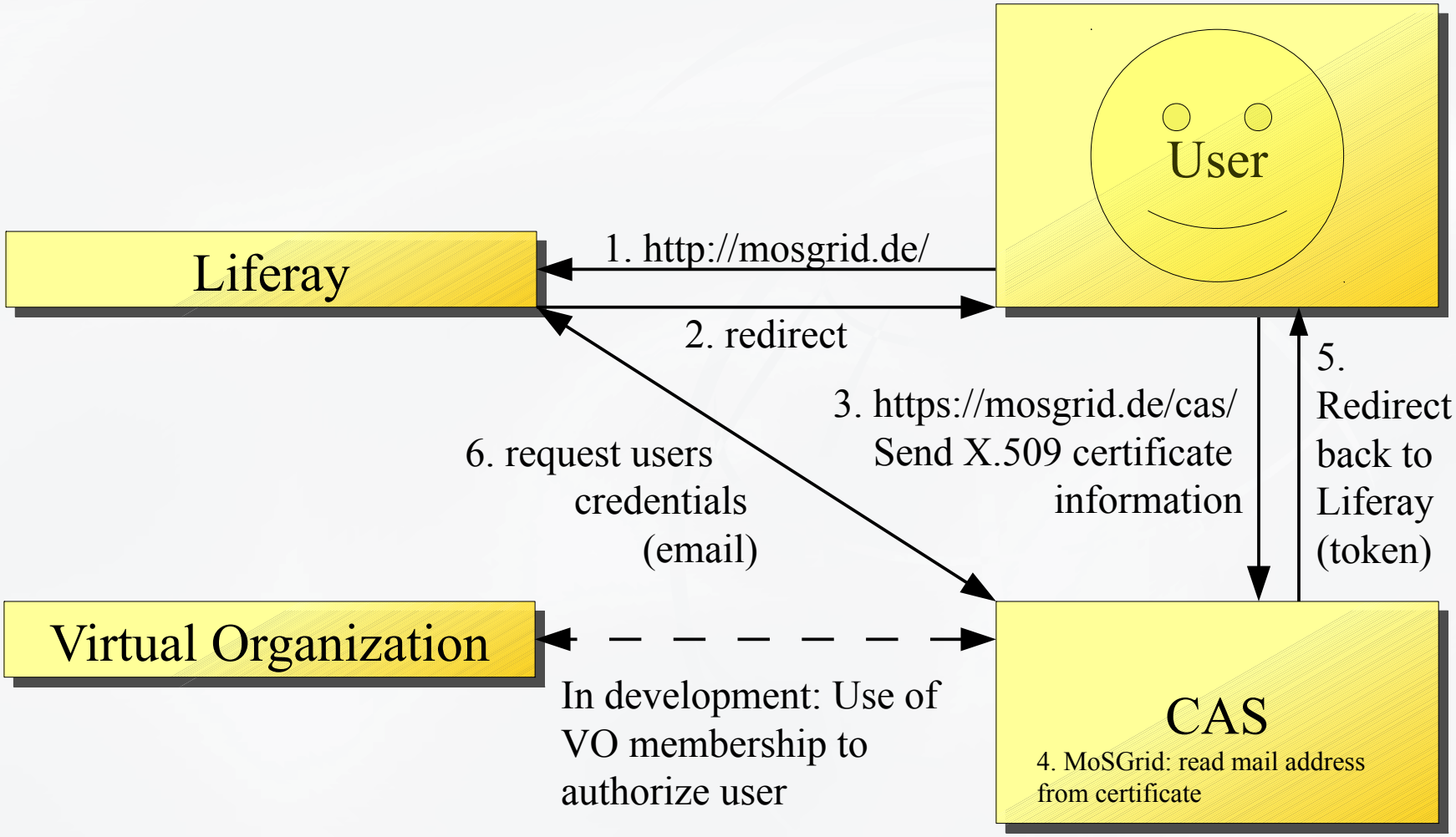
CAS

- Central Authentication Service
- Pluggable authentication
- X.509 certificate support
- Highly flexible
- Transparent Liferay integration

CAS, Liferay and MoSGrid

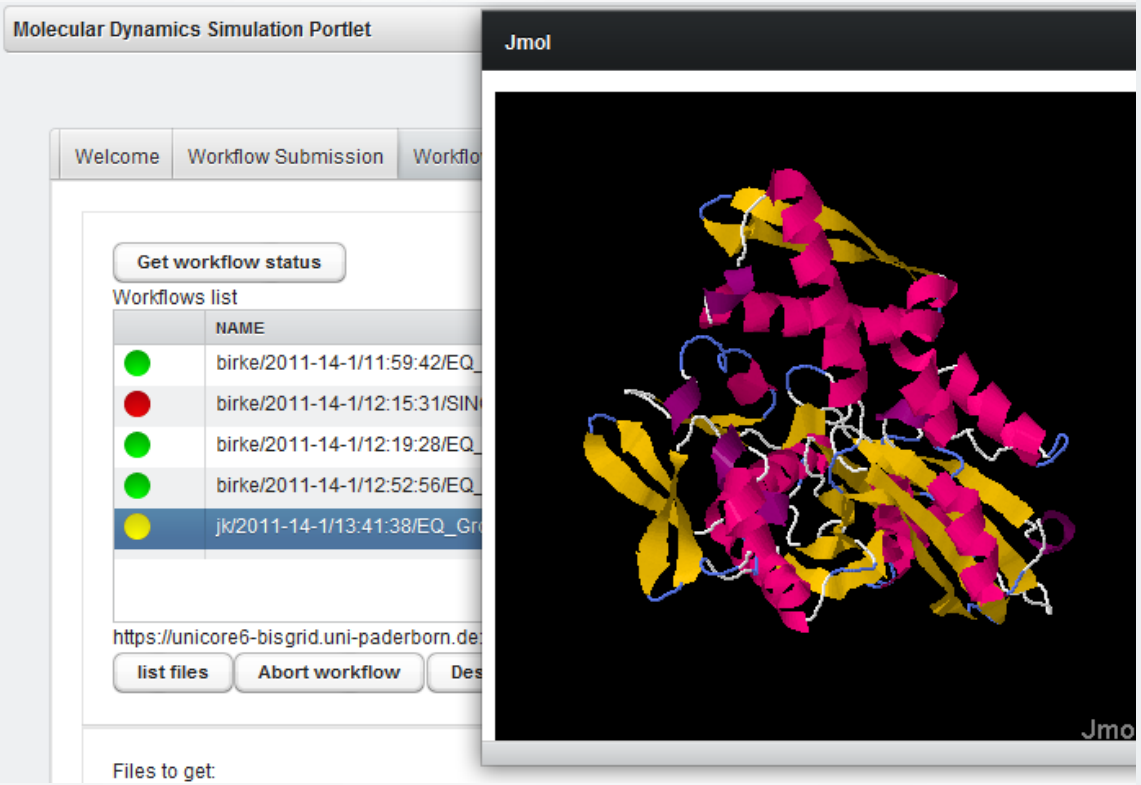
- Allows immediate authentication without login and password
- MoSGrid CAS extension: extract Email address from certificate, use as login
- Automatic access to MoSGrid area and DCIs in development:
  - Additional CAS extension
  - Support of automatic assignment to Liferay user groups based on VO
  - Evaluation of Acegi security and Liferay-API

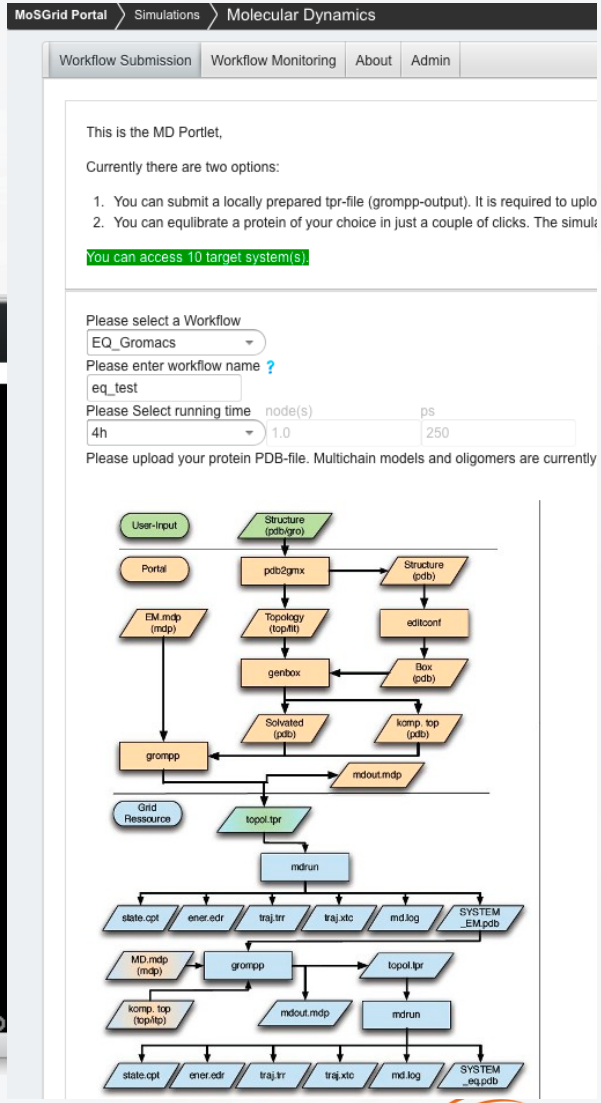
Login Information Flow



Domain Portlets – Molecular Dynamics

- Applications: Gromacs, ...





Domain Portlets – Quantum Chemistry

- Applications: Gaussian, ...

Import | Submission | Monitoring

Select an imported instance

Import
G09BASICDFT_29.05.2012_15:25

Please fill the input mask to submit your workflow

Gaussian 09 Optimisation

Functional*
BLYP

Basis Set*
D95V++

Formal charge*
0

Spin*
1

Walltime (min) [1, 10080]*
100

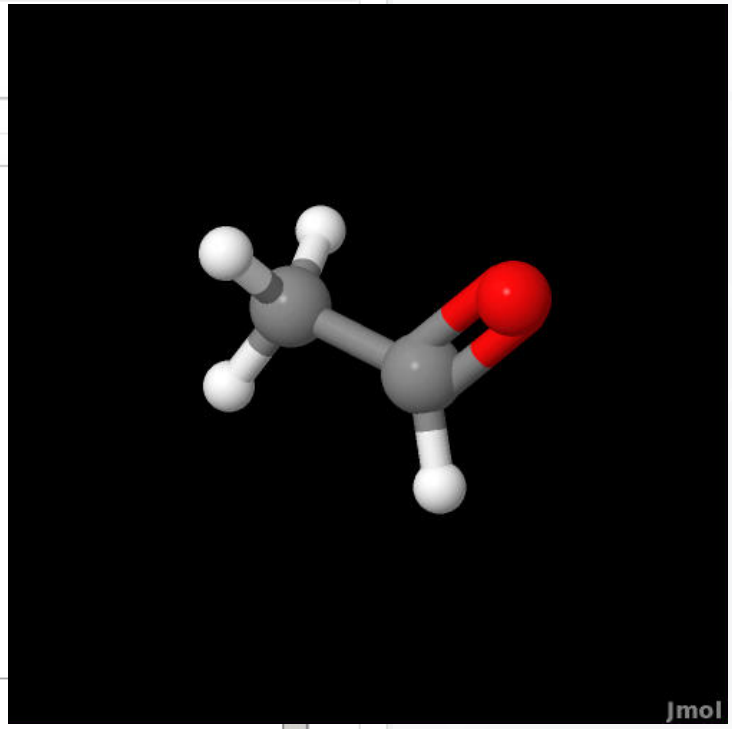
Cores [1, 8]*
8

Memory (MB) [100, 2000]*
2000

molecule structure

C	-4.84400	0.85862	0.09359
C	-3.63296	1.73879	0.02999
H	-2.71537	1.26022	-0.34931
O	-3.63668	2.91717	0.37011
H	-4.63455	0.01041	0.74987

Submit | Remove



Domain Portlets – Docking

- Applications: CADDSuite, ...

Docking Portlet

Import | Submission | Monitoring | About | ?

Select an imported instance

Import
StandardDockingWorkflow_2012-03-30-125439_29.(

Please fill the input mask to submit your workflow

PDBCutter

Filename *
1DX6.pdb
Upload PDB

PDB Model *
Model 0

☑ Chain A
☐ Chain S

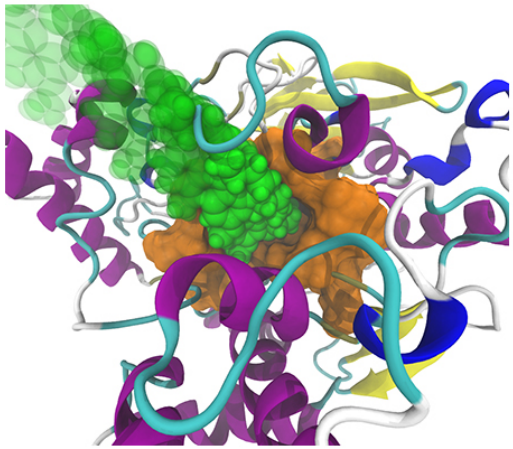
Select a protein chain from your PDB input file to act as receptor (secondary structure) including the binding pocket (orange).

Chain name of ligand *
A

Name of ligand as stated in pdb file *
GNT

Protein Chains that are to be deleted

Specifiy a reference ligand (green) by it's three letter code including the corresponding chain. It might be necessary to open the input PDB file with an editor. This information is required for the indentification of the binding site and the calculation of RMSD values.



MoSGrid Follow-up Projects

- SCI-BUS – EU project for semantic search and visualization
  - Search over workflows, results and structures
  - Workflow editor and visualization with WebGL
  - Booth in the lobby
- ER-flow – EU project to build european workflow sharing community
  - Integration of applications in SHIWA simulation platform
  - Study of data exchange between workflow systems
  - Introduction Friday Taurus/11:22

MoSGrid on Tour

All around Germany
September/October
http://mosgrid.de/ontour

Questions?

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