## User management

- based on Liferay features
- hierarchical roles

<table>
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<tr>
<th>Wiki</th>
<th>Demo</th>
<th>Workflows</th>
<th>Domain-specific pages</th>
<th>DCI settings</th>
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<tbody>
<tr>
<td>Guest</td>
<td>read</td>
<td>invoke</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>MoSGrid community user</td>
<td>read</td>
<td>invoke</td>
<td>invoke, monitor</td>
<td>read</td>
</tr>
<tr>
<td>MoSGrid advanced user</td>
<td>read</td>
<td>invoke</td>
<td>create, invoke, monitor</td>
<td>read</td>
</tr>
<tr>
<td>MoSGrid consortium user</td>
<td>create, read</td>
<td>invoke</td>
<td>create, invoke, monitor</td>
<td>create, read</td>
</tr>
<tr>
<td>MoSGrid developer</td>
<td>create, read</td>
<td>create, invoke</td>
<td>create, invoke, monitor</td>
<td>create, read, deploy</td>
</tr>
</tbody>
</table>
1. A personal account is needed to log into the MosGrid portal. Click on "Create Account" and fill out the form. It is recommended to use your official email address, that must be used later for the certificate application. The password will be displayed and mailed to you. You can now login. Please change the password to one you choose.

2. In order to get access to data and work tools and to perform molecular simulations through the MosGrid portal your account needs to be unlocked. To unlock your account please write a short note to mosgrid-contact@urz.uni-heidelberg.de. Please include the email address you entered during the account creation process.

The MosGrid Portal offers access to molecular simulation codes in the domains:
- Quantum chemistry
- Molecular dynamics
- Designing

Both experienced users and beginners will be able to perform experiments in computational chemistry through this web portal or remote grid resource provided by the academic partners of the project.

This approach randomizes the local installation of computational chemistry codes or additional software on necessary.

Submission and retrieval of compute jobs will only require:
- a modern web browser
- a valid D-Cube Certificate
- the membership in the project-based virtual organization

We appreciate your questions, suggestions and comments. Please email us at mosgrid-contact@urz.uni-heidelberg.de for all communication.
MoSGrid Community User

Web-based Science Gateways for Structural Bioinformatics
MoSGrid Community User

Web-based Science Gateways for Structural Bioinformatics

<table>
<thead>
<tr>
<th>Workflow name</th>
<th>Workflow type</th>
<th>Submitted</th>
<th>Running</th>
<th>Finished</th>
<th>Error</th>
<th>Suspended</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>gromacsWorkflow_2011-05-19-093404</td>
<td>zen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Configure, Info, Details, Submit, Delete, Export</td>
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<tr>
<td>2011-5-19</td>
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</table>

Message: []
MoSGrid Advanced User

Web-based Science Gateways for Structural Bioinformatics
MoSGrid Consortium User

Web-based Science Gateways for Structural Bioinformatics
Welcome to the Developer Wiki of the **MoSGrid** project.

Children Pages

- Certificate Portlet - Development
- Email notifications
- Incarnation Database (IDB)
- MD Portlet
- MoSGrid user roles
- Portlets with WS-PGRADE
- Theming and Layout
- Upgrade to qUSE 3.3.2
- User interface requirements
- XtremFS
MoSGrid Developer

Web-based Science Gateways for Structural Bioinformatics
Credential Management

Unicore Credential management

SAML Assertion

Browse assertion:

Keystore (.jks or .p12): Einstellungen\Sandra\Eigene Dateien\certs\gesing2010.p12
Password: *******
SAML Assertion: te und Einstellungen\Sandra\Eigene Dateien\certs\Assertion

Generate trust delegation

Upload

Message:
Credential Management

Certificate

Issuer
CN=Sandra Gesing,OU=Universitaet Tuebingen,O=GridGermany,C=DE

Time left
110 days
1:11:52

Actions
Details Delete

Message: [Press a button.]

SAML Assertion

Browse assertion:

Keystore (.jks or .p12):
Einstellungen\Sandra\Eigene Dateien\certs\gesing2010.p12

Password:

SAML Assertion:
te und Einstellungen\Sandra\Eigene Dateien\certs\Assertion

Generate trust delegation

Upload

Message:
Job and Workflow Management

grid User Support Environment

User Interface
WS-PGRADE

High-Level Middleware
Service Layer
gUSE

DCI Resources
Middleware Layer
UNICORE 6
Job and Workflow Management

grid User Support Environment

User Interface
WS-PGRADE

High-Level Middleware Service Layer
gUSE

DCI Resources Middleware Layer
UNICORE 6
gUSE Submitter

Interface GridService
- actionJobSubmit
- actionJobAbort
- actionJobOutput
- actionJobStatus
- actionJobResource

![Diagram of workflow engine and jobs](image)
gUSE Submitter for UNICORE

1. Security via SAML
2. Registry
3. Submit job
4. Upload data (optional)
5. Start job

Workflow engine

UNICORE submitter (UCC lib)

USpace

UNICORE Atomic Services

Resources

gUSE

UNICORE 6
Distributed Data Management

- XtreemFS is an object-based grid and cloud filesystem
- Replication for availability, locality, bandwidth, and latency
- Grid Security Infrastructure (GSI) and SAML support
- Easy integration in heterogenous environments
- UNICORE extension with URL scheme xtreemfs:// available