



## PLG-Data and rimrock Services as Building Blocks for Domain Applications: SCIGRESS Use Case

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- Objectives
- SCIGRESS application: functionality and requirements
- PLG-Data: a simple tool for PLGrid files management
- rimrock: a robust remote process controller
- Running SCIGRESS with PLG-Data and rimrock
- Results
- Other services by DICE
- Summary

- Enable integration of third-party applications with computing and storage resources in a technology-agnostic process
- Facilitate user authentication by hiding the complexity of X509 credential proxy delegation with plain login and password
- Use API based on widely adopted protocols for better maintenance and development of integrated apps

- Molecular modeling and molecular dynamics suit for Windows, Linux and Mac
- Fully integrated GUI with predefined computational procedures
- Builders for a range of systems
- Can run ADF, GAMESS, GAUSSIAN, LAMMPS, MOPAC 2012
- Quantum docking
- Batch calculations

- Users should login with a simple login and password (preferably the same as for the PLGrid portal)
- Remote API available for
  - Preparing an execution environment
    - Transferring binaries and inputs
    - Perform cleaning tasks
    - Non-blocking operations for long-running processes
  - Job submission and monitoring
    - Stateless job submission to Zeus and Prometheus clusters

- Web-based file management service for HPC clusters
  - Files and folders upload, download and removal
  - Access rights management
- Provides REST API access with proxy certificate authorization
- Currently deployed for Zeus and Prometheus PLGrid clusters

PLG-Data

Folder shortcuts Zeus ▾

Folder shortcuts Prometheus ▾


▲ Logout




PL













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LISTING FOLDER: [MNT](#) / [LUSTRE](#) / [SCRATCH2](#) / [PEOPLE](#) / [PLGHAREZLAK](#) /

 Upload files

 New directory

Total 3 files, including 0 hidden.

Rights	Size	Modification date	Name	Type
 drwx----- 	4 KB	Mar 25 21:56	 <a href="#">j1427316831243_10534_8725_atask_1427316831558_666</a>	Dir  Delete
 drwx----- 	4 KB	Mar 25 22:05	 <a href="#">j1427317420954_10290_7383_atask_1427317421266_347</a>	Dir  Delete
 drwxr-xr-x 	4 KB	Mar 30 13:20	 <a href="#">pcs_pro</a>	Dir  Delete

## ■ Listing a folder

```
curl -X GET \  
--header "PROXY:$proxy" \  
https://data.plgrid.pl/list/people/plguserlogin/
```

## ■ Downloading a file

```
curl -X GET \  
--header "PROXY:$proxy" \  
https://data.plgrid.pl/download/people/plguserlogin\  
/graph.png
```

## ■ Uploading a file

```
curl -X POST \  
--header "PROXY:$proxy" \  
-F „file=@graph.png" \  
https://data.plgrid.pl/upload/people/plguserlogin/
```

## ■ REST APIs available for

- X.509 proxy certificate generation with user's login and password
- Remote process execution (e.g. `hostname` on Zeus)
- Remote interactive process execution (e.g. `bash`)
- Local job submission
- Grid job submission
  - With Globus middleware
  - With QCG middleware



## ■ X.509 proxy generation

```
curl -X GET \  
--header "USER-LOGIN:$userLogin," \  
--header "USER-PASSWORD:$userPassword" \  
--header "PRIVATE-KEY-PASSWORD:$privateKeyPassword," \  
https://rimrock.plgrid.pl/api/userproxy
```

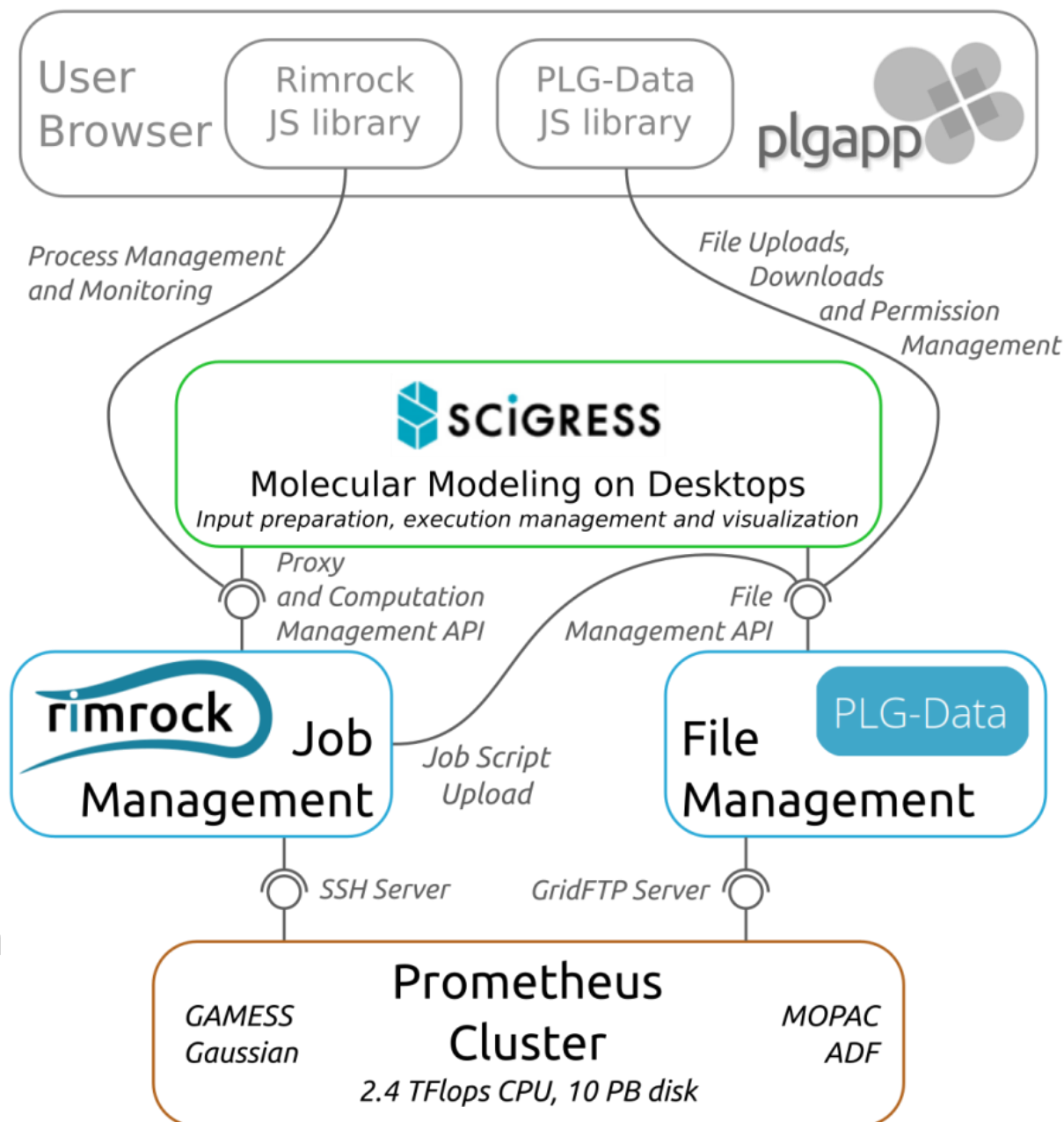
## ■ Remote process execution

```
curl -X POST \  
--data '{"host":"zeus.cyfronet.pl", "command":"pwd"}' \  
--header "Content-Type:application/json" \  
--header "PROXY:$proxy" https://rimrock.plgrid.pl/api/process
```

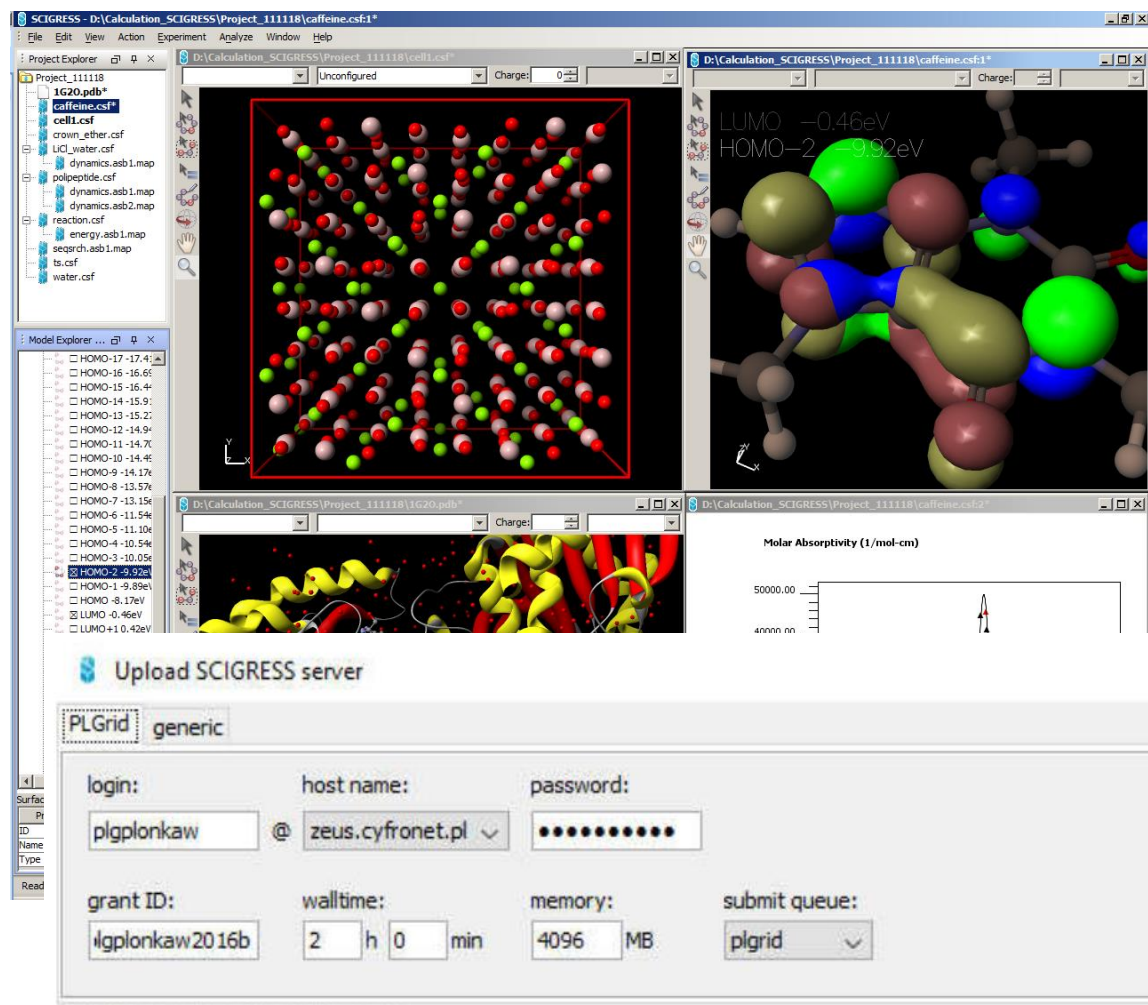
## ■ Job submission

```
curl -X POST \  
--data '{"host":"prometheus.cyfronet.pl", \  
"script":"#!/bin/bash\  
#SBATCH -A {grantid}\  
echo hello\  
next 0"}' \  
--header "Content-Type:application/json" \  
--header "PROXY:$proxy," \  
https://rimrock.plgrid.pl/api/jobs
```

- REST with JSON used for communication with PLG-Data and rimrock services
- Proxy generation and job management with rimrock
- File transfers to and from the cluster with PLG-Data
- The same APIs may be used by any desktop or web applications even directly from a user's browser



- Authentication with only login and password
  - User is not required to handle X.509 certificates manually
- Stateless job submission and monitoring
- Integration with well adopted REST/JSON standard
- A complete HPC execution environment setup through a range of operations provided by rimrock and PLG-Data



The screenshot displays the SCIGRESS software interface. The main window shows a 3D ball-and-stick model of a molecular structure within a red wireframe box. To the right, a smaller window displays molecular orbitals with energy levels: LUMO -0.46eV and HOMO-2 -9.92eV. Below these, a plot of Molar Absorptivity (1/mol-cm) is shown with a peak at approximately 400nm. In the foreground, an 'Upload SCIGRESS server' dialog box is open, showing the following fields:

login:	host name:	password:	
plgplonkaw	@ zeus.cyfronet.pl	.....	
grant ID:	walltime:	memory:	submit queue:
ilgplonkaw2016b	2 h 0 min	4096 MB	plgrid

- **plgapp** – <http://app.plgrid.pl>

A platform supporting creation of lightweight web applications built on top of HPC resources with integrated security and auxiliary services



- **DataNet** – <http://datanet.plgrid.pl>

Data and metadata management with the use of REST-enabled repositories with ad-hoc model creation for file and structured data



- **GridSpace** – <http://gs2.plgrid.pl>

A framework enabling researchers to conduct virtual experiments on Grid-based resources and other HPC infrastructures



Further details at

<http://dice.cyfronet.pl/products>

- **rimrock and PLG-Data services facilitate the process of building applications on top of the PLGrid infrastructure**
  - X.509 proxy generation API (only login and password needed)
  - File management API
  - Job management API (including process execution)
- **SCIGRESS desktop application successfully integrated with all the requirements met**
- **Available APIs can be used in desktop and web environments**
  - Direct communication between user's browser and the services also possible
- **The presented approach is generic in a sense that in the same way one may arrange access to data and execution on e-infrastructures for a large class of applications**

- DICE Team

- <http://dice.cyfronet.pl>



- SCIGRESS

- <http://scigress.com>

- PLGrid Services by DICE

- plgapp

- <http://app.plgrid.pl>

- rimrock

- <http://rimrock.plgrid.pl>

- PLG-Data

- <http://data.plgrid.pl>