



GridSpace

Experiment Workbench

in the PL-Grid Virtual Laboratory

<https://wl.plgrid.pl/>

The PL-Grid Virtual Laboratory is a place where Polish researchers are able to conduct *in silico* experiments. Such experiments integrate all the research steps that can be performed using a computer into a reusable document.

While the *PL-Grid project* offers free access to computational and storage resources as well as to software packages from various fields of science, the *Virtual Laboratory* aims to make using these vast resources as simple and straightforward as possible.

The design of the *Virtual Laboratory* and the concept of its experiments were devised in close collaboration with scientists representing several domains of science, taking into account their experience and requirements.



DALTON

GAMMESS



Working with:

- computing infrastructures (Clusters, Grids, Clouds);
 - diverse software packages (Gaussian, NAMD, external Web Services, visualization tools etc.);
 - tools (libraries) available only for specific programming languages;
 - various data sources (files, databases, URLs) and storage systems (LFC, local files)
- ...may become extremely complex and tiresome.

Mathematica

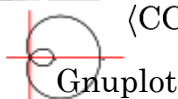
TURBOMOLE



Gaussian



<CC|CC>



Ruby

Bash



FLUENT

MATLAB

Packmol

GROMACS

NAMD
Scalable Molecular Dynamics

Solution: Experiment in Virtual Lab

- Complex, interactive workflow
- Uses preconfigured libraries (*gems*) for job submission, data access etc.
- Combines different tools, programming languages etc.
- Shareable and reusable by ad-hoc research teams

Interactive experimentation

Snippets:

scripts, config files

Gems: programs, libraries, services

Inputs:

files, URLs

Visualization:

final and partial results



Reuse

Rerun:

parameter study

Modify:

perform similar experiment

Share:

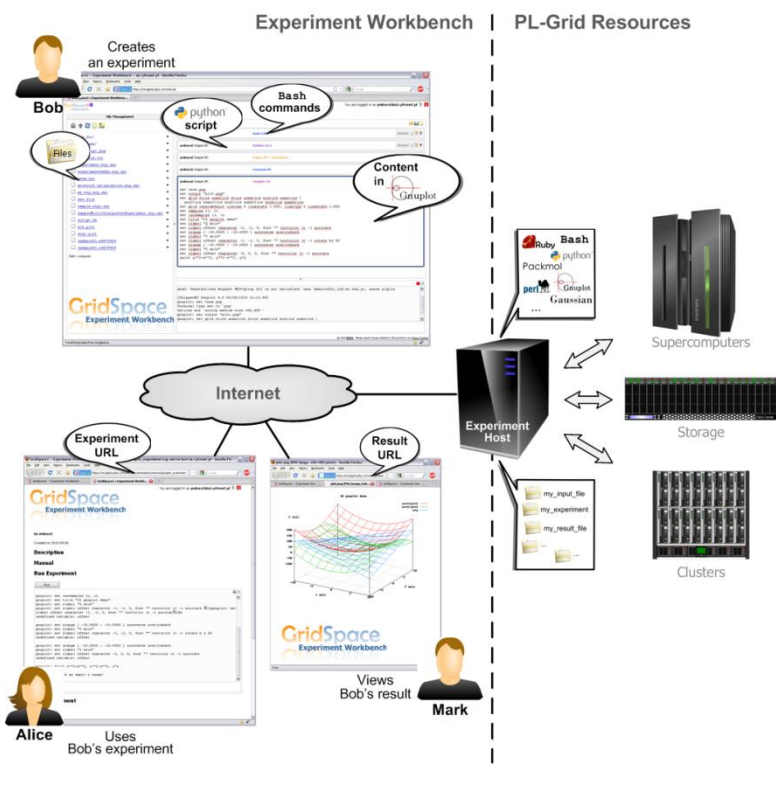
work with your team



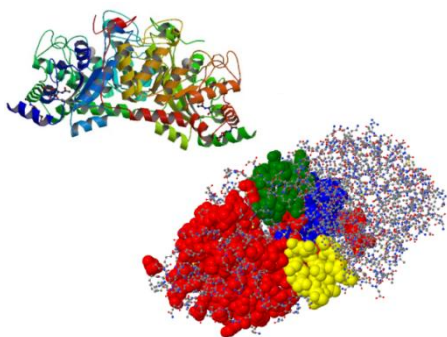
The PL-Grid Virtual Laboratory provides an Experiment Workbench - a Web 2.0 interface supporting the development and execution of *in silico* experiments. However 'virtual' they seem, the experiments created within the workbench, along with their results, persist as files in the user's PL-Grid account.

Working with the Experiment Workbench

1. Open the workbench in your browser (<https://wl.plgrid.pl>);
2. Log into one of the available servers with your PL-Grid account;
3. Start your usual work. Your files are already there. Your code snippets may play the role of scripts (in Python, Perl, Ruby etc.), bash commands or input to external applications (such as Gaussian or Gnuplot);
4. All the files you generate may be viewed with visualization tools (such as Jmol);
5. Save your work - the experiment is now visible among your other files;
6. Share the experiment with other members of your research team. Depending on the access rights you set, they may be able to modify the experiment or just execute it.



Featured Experiments



Comparison of services for predicting ligand binding sites

- Multiple services available on the Web
- Data format conversions
- Visualization scripts (Jmol, Gnuplot)
- Parameter studies performed by rerunning the experiment

Calculation of hydrophobicity profiles

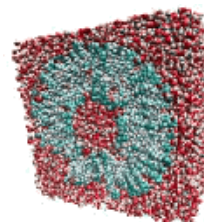
- Multiple scales, parameters, input data
- Access to PL-Grid resources (Zeus cluster at Cyfronet)
- ~ 1 Million output files to manage
- Semantic integration for metadata management

Collaboration with Prof. Irena Roterman-Konieczna and Katarzyna Prymula; Department of Bioinformatics and Telemedicine, Jagiellonian University;

Analysis of water solutions of aminoacids

- Multiple languages and libraries (Packmol, Gaussian, CCLib)
- Data format conversions
- Visualization tools (Jmol, jqPlot)

Collaboration with Mariusz Sterzel PhD and Klemens Noga; Department of Chemistry, Jagiellonian University and ACC Cyfronet AGH.



Visit us at <http://dice.cyfronet.pl/>

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