Virtual Laboratory for *in silico* experiments in Computational Chemistry

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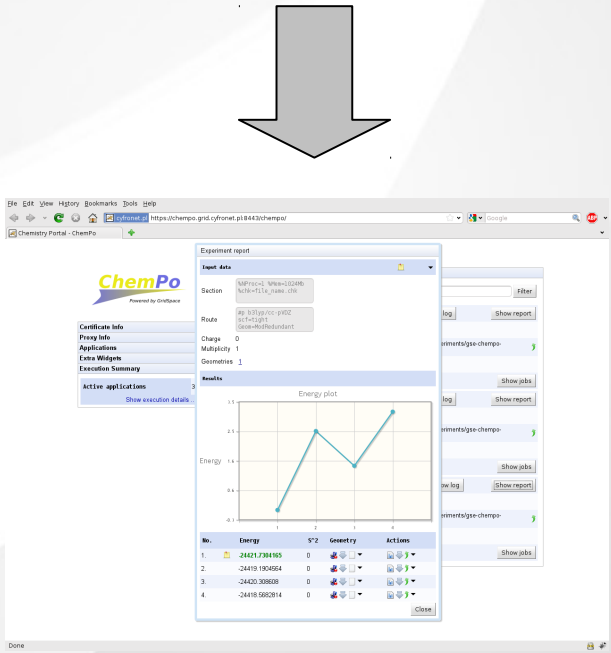
Outline

- **Computational chemistry and the Grid**
- **State-of-the-art**
- **Requirements**
- **Architecture**
- **Results**
- **Conclusions and future work**

Computational chemistry and the Grid

- Computational Chemistry uses first principles chemistry packages available on the Grid (Gaussian, GAMESS, TURBOMOLE)
- Grid is still mainly available through command line interfaces (`voms-proxy-init`, `glite-wms-job-submit`, `glite-wms-job-status`)
- Adoption to the Grid environment by non-experts is difficult
- Let us build a web-based problem solving environment facilitating the use of Grid ... but not only that

```
[ymharezl@ui simple-job]$ voms-proxy-init --voms gaussian
Cannot find file or dir: /people/ymharezl/.glite/vomses
Enter GRID pass phrase:
Your identity: /C=PL/O=GRID/O=Cyfronet/CN=Daniel Harezlak
Creating temporary proxy ..................................................
......... Done
Contacting  voms.cyf-kr.edu.pl:15001 [/C=PL/O=GRID/O=Cyfronet/CN=voms.cyf-
kr.edu.pl] "gaussian" Done
Creating proxy ............................................................
.............. Done
Your proxy is valid until Tue Mar 16 02:11:20 2010
[ymharezl@ui simple-job]$ glite-wms-job-submit -a simple-job.jdl
glite-wms-job-submit: error while loading shared libraries: libcares.so.0:
 cannot open shared object file: No such file or directory
[ymharezl@ui simple-job]$ glite-wms-job-status https://lb.grid.cyf-kr.edu.
pl:9000/_Hwauwjg3RovzCy33fWXHg
Traceback (most recent call last):
  File "/opt/glite/bin/glite-wms-job-status", line 32, in ?
    import UIchecks
  File "/opt/glite/lib/python/UIchecks.py", line 22, in ?
    from glite_wmsui_AdWrapper import AdWrapper
  File "/opt/glite/lib/python/glite_wmsui_AdWrapper.py", line 5, in ?
    import _glite_wmsui_AdWrapper
ImportError: libcares.so.0: cannot open shared object file: No such file o
r directory
[ymharezl@ui simple-job]$ glite-wms-job-status https://lb.grid.cyf-kr.edu.
pl:9000/_Hwauwjg3RovzCy33fWXHg
Traceback (most recent call last):
  File "/opt/glite/bin/glite-wms-job-status", line 32, in ?
```



State-of-the-art

- **WebMO** (*www.webmo.net*)
  - Desktop and Web access
  - Supports main computational chemistry applications
  - Does not support Grid or local queues infrastructures
- **ECCE** – Extensible Computational Chemistry Environment (*ecce.pnl.gov*)
  - Only desktop access
  - Supports main computational chemistry applications
  - Supports many queue management systems (PBS, LSF, NQE, etc.)
  - Does not use Grid infrastructures
- **CCG** – Computational Chemistry Grid (*www.gridchem.org*)
  - A virtual organization which is a part of Teragrid
  - GridChem – Java client which can be run as a WebStart application
- **P-GRADE** – Development and Execution of Parallel Applications (*www.p-grade.hu*)
  - A Grid-oriented solution

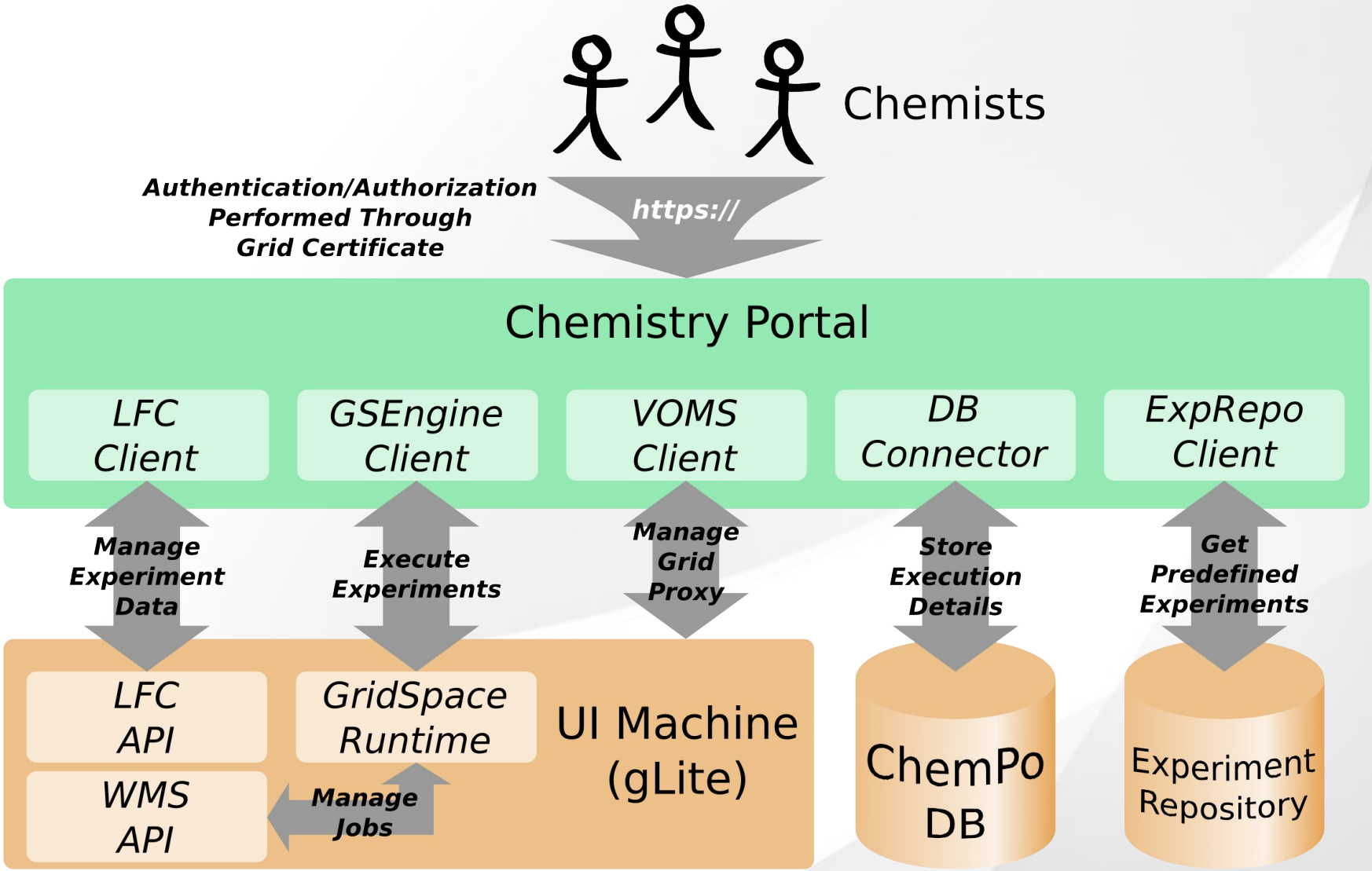
Description of the solution - requirements

- Supports *main chemistry packages*
  - Gaussian
  - GAMESS
  - TURBOMOLE
  - ...
- Is accessible through *a web interface*
  - All Grid-related operations should be embedded (proxy generation, job submission and status monitoring, LFC catalog operation)
  - Persists information about executed jobs between web sessions
- Enables *user-centric processing* rather than grid-centric
  - It should not be yet another Grid job submission tool
  - Supports inter-application geometry passing
  - Provides automated report summaries
  - Covers Grid complexity
- Supports *annotations* through user free-text tagging

Description of the solution – architecture (1/2)

- Uses *gLite* for Grid job management
  - A set of Grid APIs is used (LFC, WMS, VOMS)
- Job submission and monitoring implemented as a separate layer for *better error handling*
  - GridSpace platform used
  - Each application backed by a separate script
- *Application model* realized by using SINT (Semantic Integration Tool)
  - Basic concepts such as geometry, basic and detailed reports, input parameters, annotations are modeled
- *Interactive graphical user interfaces* are used
  - GWT (Google Web Toolkit) is used as the user front-end technology

Description of the solution – architecture (2/2)



Demo

- Demo contents
  - Getting the proxy
  - Preparing geometries
  - Running Grid applications
  - Viewing results
  - Analyzing reports
- Switching to demo ...

Conclusions and future work

- An integrated environment for planning and executing applications in computational chemistry was presented
  - *Covers the complexity of Grid* infrastructure
  - *Combines main chemistry packages* in one integrated environment
  - All this available through *an easily accessible web interface*
- Future work includes
  - Refinement of current application scripts for *better stability and performance*
  - Integration with *MyProxy server*
  - Preparation and testing of *TURBOMOLE* scripts
  - Improvement of *the web interface*

References

T. Gubala, M. Bubak, P.M.A. Sloot: *Semantic Integration of Collaborative Research Environments*, In: M. Cannataro (Ed.) Handbook of Research on Computational Grid Technologies for Life Sciences, Biomedicine and Healthcare, Information Science Reference, 2009, IGI Global

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