



Domain-oriented services and resources  
of Polish Infrastructure for Supporting  
Computational Science in the European  
Research Space – PLGrid Plus

# InSilicoLab for chemistry

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ACC Cyfronet AGH

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**INNOVATIVE ECONOMY**  
NATIONAL COHESION STRATEGY

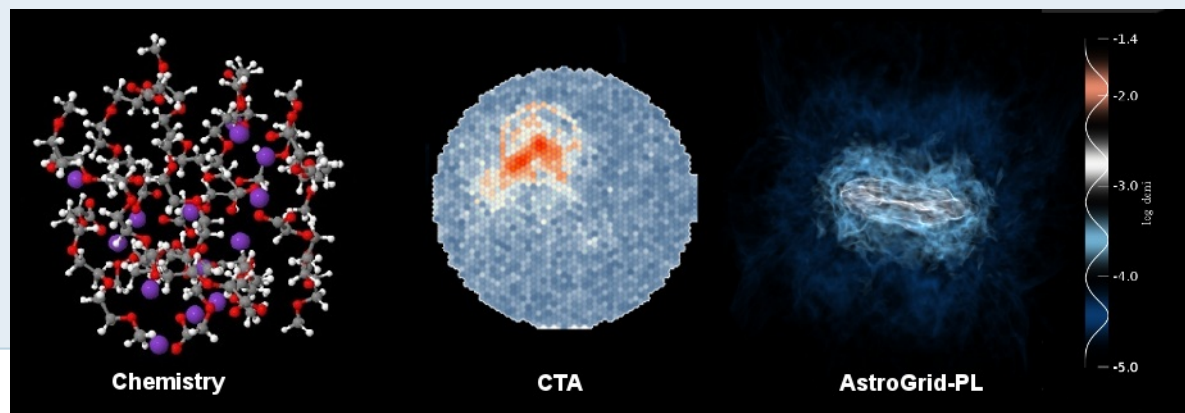
**EUROPEAN UNION**  
EUROPEAN REGIONAL  
DEVELOPMENT FUND



- InSilicoLab
  - features
  - technological background
- Grid accounts
  - grid certificates
  - Virtual Organisations
- Hands-on
  - grid certificate management
  - Quantum-Chemistry calculation
  - Trajectory Sculptor
  - experiment “workflows”

InSilicoLab - <http://insilicolab.cyfronet.pl>

- InSilicoLab - framework of application portals
  - enable execution of large-scale, long-lasting data- and computation-intensive experiments
  - support the management of complex calculations
  - automate repetitive cycles of calculations
  - enable joint analysis of results from massive parallel computations
- Scientific domains
  - quantum chemistry
  - Cherenkov Telescope Array (CTA)
  - multihydrodynamic for astrophysics



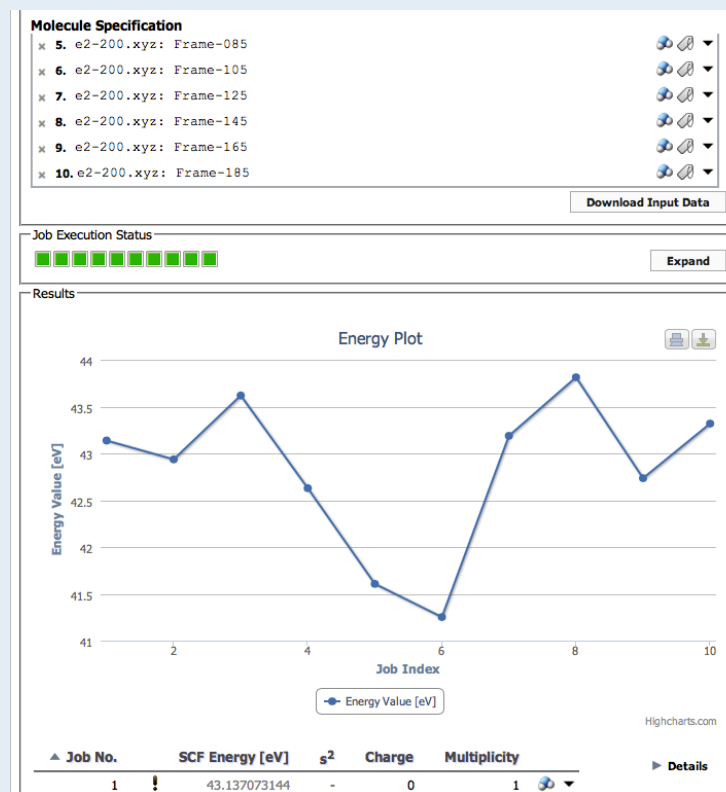
InSilicoLab - <http://insilicolab.cyfronet.pl>

- Complete workspace in **web browser** for Chemist who wishes to perform Quantum Chemistry calculations
- Assist with
  - preparing input to various QC applications
  - performing computations on grid infrastructure
  - controlling complex and recurrent jobs
  - collecting output files
  - analysis of obtained results (also from many calculations at once)
- Main features
  - automatic parallelization
  - automatic results analysis
  - data categorization and visualization (JMol)
  - easy reuse of input and results in new experiments
  - automatic conformation scans (prototype)



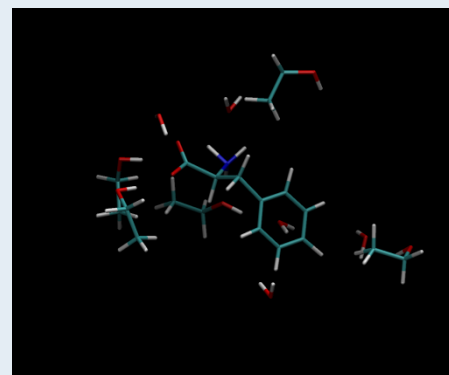
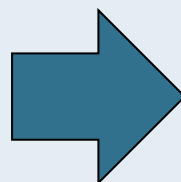
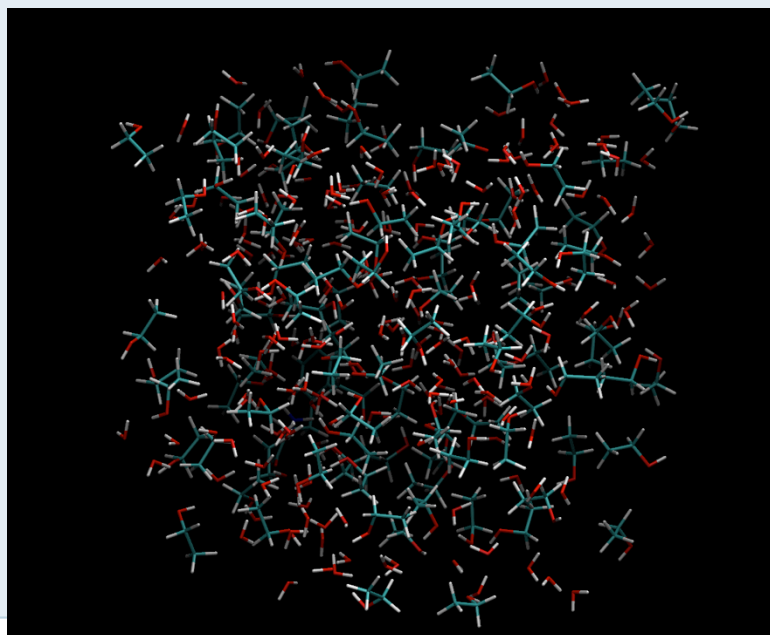
**in silico**  
**LAB**

- Two types of experiments
  - Quantum chemistry calculations
  - Trajectory Sculptor
- **Quantum chemistry calculations**
  - QC applications – full integration
    - Gaussian
    - GAMESS
    - TUROBMOLE
  - automatic results analysis
  - simultaneous multiple geometry runs

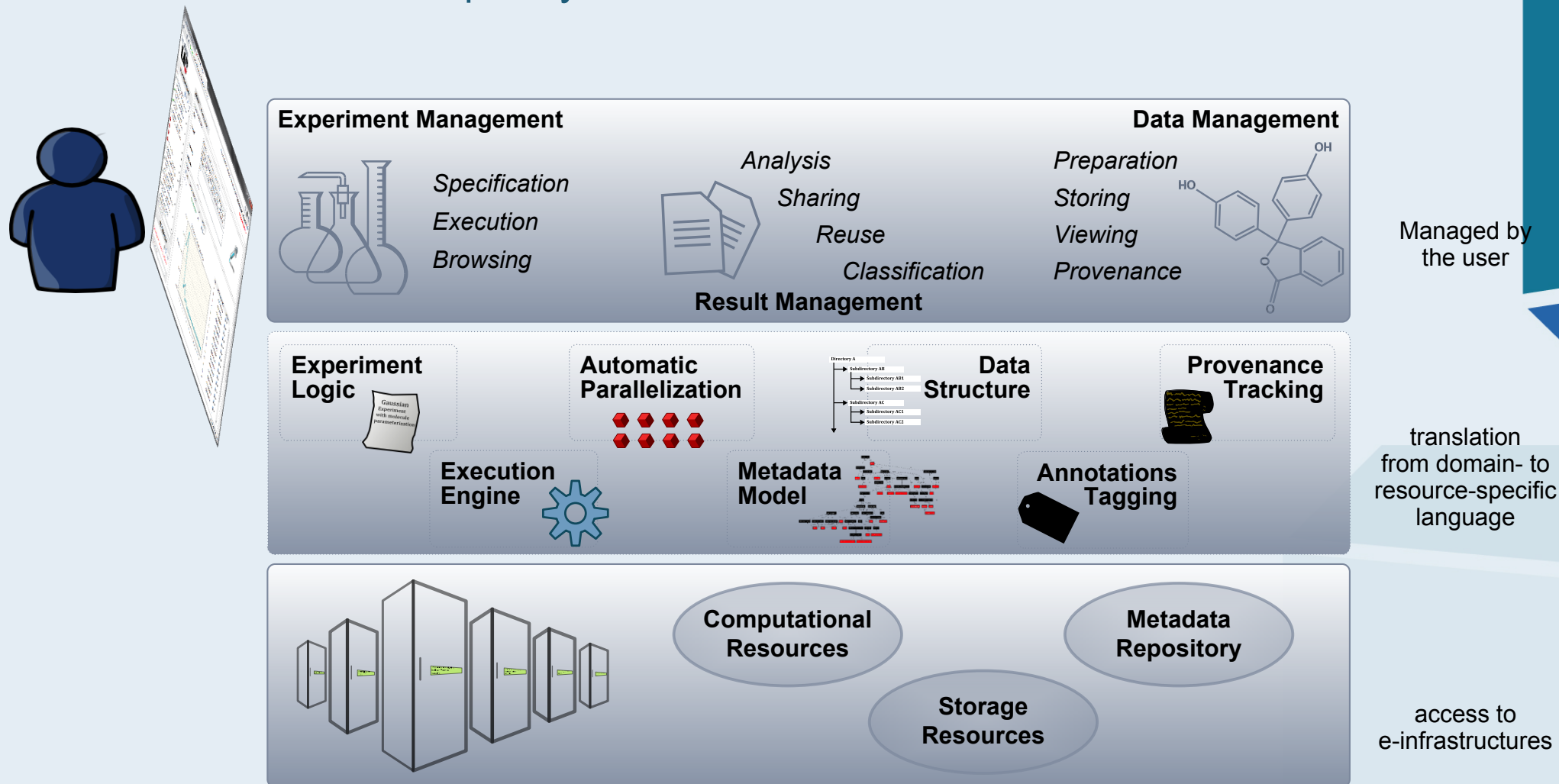


InSilicoLab - <http://insilicolab.cyfronet.pl>

- **Trajectory Sculptor** - advanced tool for manipulation of Molecular Dynamics trajectories
  - automatic extraction of relevant parts of the input structure (based on user choices)
  - automatic processing frames chosen by user
  - results easily reused in quantum chemistry calculations



## InSilicoLab hides complexity of e-infrastructures



## Technology used

- Server
  - Java (jSAGA)
  - Ruby
- Middleware
  - gLite
  - DIRAC
- Computing Node
  - Quantum chemistry software packages
  - Python (cclib, lxm2)
- Web portal
  - Google Web Toolkit
  - jmol





# Team



9



Joanna Kocot  
(leader)



Tomasz Szepieniec



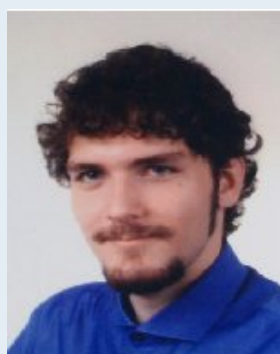
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# How to use InSilicoLab?



10

## What is necessary to use InSilicoLab?

- Grid certificate (X.509 standard)
  - both PEM and PKCS#12 (.p12) formats supported
  - have to be installed in web browser
- Virtual Organisation membership
  - VOs available: gaussian, vo.plgrid.pl
- Some knowledge about Quantum Chemistry
  - familiarity with input formats of QC packages which user want to use (but we're working at Experiment Wizard and Quantum Chemistry Advisor)



## User identification and authentication

- Needed by all grid services to authenticate user and secure communication
- Protected with password (analogy: ATM card and PIN)
- Must be kept secure and not given to any other person
- Could be obtained from **certification authority (CA)**
- Certification authorities (CA) available in Poland
  - PL-Grid CA (<https://plgrid-ca.pl>)
  - Simple CA (<http://plgrid-sca.wcss.wroc.pl>)
- Most of grid services use short lived **proxy** certificates generated from user long term certificates due to security reasons
  - standard proxies are “fire & forget” type
  - **MyProxy** mechanism allows user renewable longer-time proxies
- Certificates could be used to sign and encrypt e-mails

- Dynamic set of individuals or institutions defined around a set of resource-sharing on established conditions
  - research teams working on human genome, HEP (ATLAS, CMS, ALICE, etc.) projects
  - group of users using same computational software packages (e.g. Gaussian)
- Each member has to have grid certificate and sign up it to VO
- VOs available for chemists in InSilicoLab:
  - gaussian (sign up via <https://voms.cyf-kr.edu.pl:8443/voms/gaussian/>)
  - vo.plgrid.pl (sign up via <https://portal.plgrid.pl/web/guest>)

## Grid certificate web browser import

- To access InSilicoLab web portal user needs to have valid grid certificate installed in web browser (or use PL-Grid OpenID)
- Import procedure (in Firefox)
  - use certificate in PKCS#12 (.p12) format
  - Linux: Edit → Preferences → Advanced → Security → Manage certificates → Your certificates → Import  
(pl: Edycja → Preferencje → Zaawansowane → Szyfrowanie → Wyświetl certyfikaty → Użytkownik → Importuj)
  - (Windows): Tools → Options → Advanced → Security → Manage certificates → Your certificates → Import  
(pl: Narzędzia → Opcje → Zaawansowane → Szyfrowanie → Wyświetl certyfikaty → Użytkownik → Importuj)
  - type in certificate password
  - done!
- Accounts on local computers: login: confXX, password: conf\_XX;  $X \in \{01, \dots, 26\}$

# Hands on: portal structure



14

GUI

Tabs

User manual

The screenshot shows the InSilicoLab Portal interface. On the left is a sidebar with 'Your Experiments' (a list of experiments with checkboxes and a 'Filter by name' box) and 'LFC Catalogue' (a file tree showing 'experiments' and a 'Filter by name' box). The main area is titled 'Welcome to InSilicoLab Portal' and contains a 'Welcome' tab, a 'Workspace' section with 'Actions' (Configure your proxy, Create a new experiment, Manage your experiments, Manage your LFC files), and a 'User ID & proxy management' section. A 'Report a problem' link is at the bottom right. Red arrows point from text labels to specific UI elements: 'Tabs' points to the 'Welcome' tab; 'User manual' points to a link in the top right; 'Create an experiment' points to the 'Create a new experiment' action; 'Workspace' points to the 'Workspace' section; 'User experiments' points to the 'Your Experiments' sidebar; and 'File catalogue' points to the 'LFC Catalogue' sidebar.

in silico LAB

Your Experiments

Menu

- ✓ dye
- ✓ method2/basis2 // method1/basis1 test 2
- ✓ method2/basis2 // method1/basis1 test
- ✓ Opt/Freq test
- ✓ RDX ground state
- ✓ B3LYP/cc-pVDZ geometry optimization
- ✓ RDX ground state
- ✓ B3LYP/de2-SVP geometry optimization
- ✓ RDX ground state
- ✓ B3LYP/cc-pVDZ geometry optimization
- ✓ RDX ground state
- ✓ B3LYP/cc-pVDZ geometry optimization
- ✓ testing no of proc - 4
- ✓ testing no of proc
- ✓ RDX ground state
- ✓ MP2/de2-SVP geometry optimization

Filter by name

LFC Catalogue

~

experiments

Filter by name

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Report a problem

Welcome

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Welcome to InSilicoLab Portal

To take advantage of the full portal functionality (including job submission and LFC directory management), it is required that you have a valid proxy configured. You can configure it now - using the left panel, or do it later at any time - by clicking the "Configure proxy..." button in the workspace.

If you choose not to configure your proxy now, you can still access the portal and work with limited functionality. For this purpose, choose one of the options right panel below.

Actions

- Configure your proxy
- Create a new experiment:
  - Quantum Chemistry experiment
  - Trajectory Sculptor
- Manage your experiments
- Manage your LFC files (only with valid proxy)
- Just close this tab

You are logged in as **Klemens Noga**

User ID & proxy management



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## Example experiment

### Tabs

in silico LAB

**Your Experiments**

Menu

- ✓ dye
- ✓ method2/basis2 //
- ✓ method1/basis1 test 2
- ✓ method2/basis2 //
- ✓ method1/basis1 test
- ✓ Opt/Freq test
- ✓ RDX ground state
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- ✓ RDX ground state
- ✓ MP2/de2-SVP geometry optimization
- ✓ RDX ground state
- ✓ MP2/de2-SVP geometry optimization

Filter by name

**LFC Catalogue**

~

experiments

Filter by name

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Welcome RDX ground stat... Opt/Freq test method2/basis2 ... dye

Experiment dye

Started 2013-06-21 at 03:47:43

Status Completed

Identifier 1371779263636

LFC directory /grid/vo.plgrid.pl/insilicolab/c.PL\_\_o.GRID\_\_o.UJ\_\_cn.Klemens\_Noga/experiments/experiment-1371779263636

Experiment Input Data

Load prepared input

Title Section semiempirical single point energy

Link 0 Section %mem=512mb

Route Section pm3

Charge & Multiplicity 0 & 1

Additional Parameters

Molecule Specification

1. e2-200.xyz: Frame-005
2. e2-200.xyz: Frame-025
3. e2-200.xyz: Frame-045
4. e2-200.xyz: Frame-065
5. e2-200.xyz: Frame-085
6. e2-200.xyz: Frame-105

Download Input Data

Job Execution Status

Results

Energy Plot

Energy Value [eV]

Report a problem

Input data

Jobs status

Results

User experiments

File catalogue

## Certificate upload and proxy creation

- Open **Configure your proxy**
  - upload your .p12 certificate
  - choose your favourite VO
  - check MyProxy box (for long renewable proxy usage)
  - type in passphrase
  - hit “Generate proxy” button
  
- You are ready for *in silico* experiments!



## Simple QC Gaussian run

- Create new **Quantum Chemistry experiment**
  - upload rdx.pm3.gjf
  - view uploaded molecule geometry
  - upload another conformation (i.e. rdx.aae.xyz or rdx.all.xyz)
  - check data consistency
  - click “run” .-)
  
- After while
  - check which conformation has got lower energy
  - view optimal geometry
  - download detailed Gaussian log file
  - reuse lower energy structure to optimize geometry using B3LYP/cc-pVDZ

## Trajectory Sculptor run

- Create new **Trajectory Sculptor experiment**
  - upload MD trajectory from md.2-200.xyz.b2z
    - Periodic Boundary Conditions with 44.7302 Å box
  - preview selected frame
  - find molecules in mixture
    - solute's atoms are in 1-38 range
    - there are 3 types of solvent molecules
      - Acetonitrile (atoms sequence CNCHHH)
      - perchlorate anions (atoms sequence ClOOOO)
      - lithium cations (Li)
  - preview findings
- propose trimming conditions
  - you could use different metrics for different solvents
  - use closest molecule metrics due to obtain electro-neutral structure (i.e. 20 acetonitrile molecules, and one of each iones; syntax: 20;1;1)
- preview findings

## Trajectory Sculptor run cont.

- define frames range to be processed (there are 200 frames in MD file)
- reuse obtained trimmed frames in QC experiment (i.e. PM3 single point in Gaussian)
  - review obtained results
  - reuse selected frames using better QC method

<http://insilicolab.cyfronet.pl>

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