

Molecular Modelling of Complex Systems with InSilicoLab

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InSilicoLab: Idea

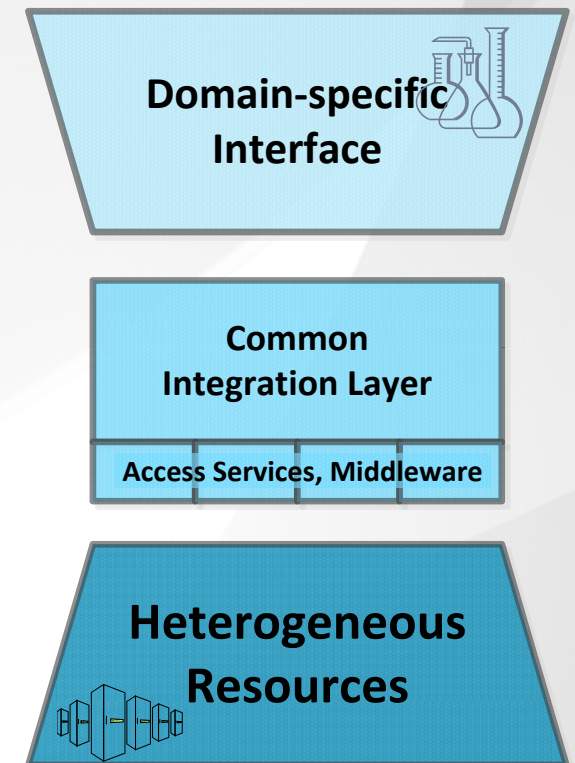
- Workspace gathering all that a researcher needs for their *in silico* experiments
 - › Enabling performing large-scale, long-lasting data- and computation-intensive experiments
 - › Facilitating categorisation and description of data
 - Enabling searches and browsing

Method: Utility

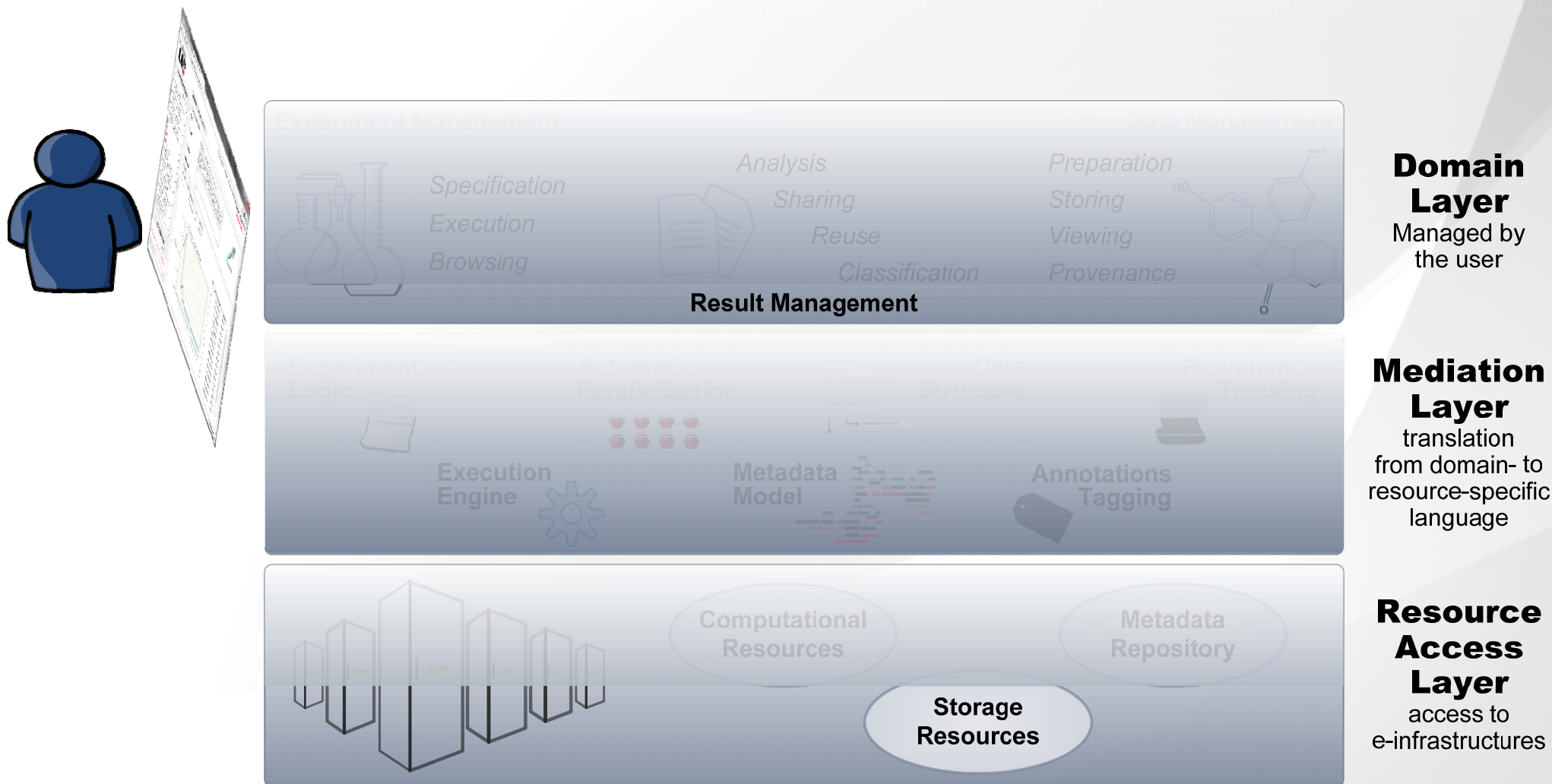
- Analysing the researchers work:
 - › Ways of working
 - › Common problems
- We intend to aid in solving **SPECIFIC** problems
- We cannot support solving **ANY** scientific problem
 - › We assume it cannot be done in a universal and comprehensive way

Architecture

- System should be optimised for problems with common characteristics, like:
 - › Large resource consumption
 - › Repeatability – experiments conducted in similar way
- It is not limited to these problems
- Architecture of the whole system is generic
 - › Ensures access to large, heterogeneous computing and storage resources
 - › Through integration layer – built on top of resource access services, middleware, etc.
 - › Presented to the user with domain/problem-specific interface



InSilicoLab Architecture – Details



How we create/integrate new experiments

- Discover a pattern in the researchers work
 - › A joint effort of the developers and the researchers teams
- Put it down as an algorithm – experiment logic
- Translate into necessary scripts
 - › Include input and results management
 - › Allow metadata attachment
- Adjust interface
 - › Input specification
 - › Result display
 - › If neccessary: new data types management

QC/MD Modelling

- Quantum-chemical modeling of complex systems often requires:
 - › Analysis of large molecular systems
 - › Preparation of large sets of input files sharing common pattern
 - › Execution of multiple computational jobs
 - › Postprocessing of output files

QC/MD Modelling

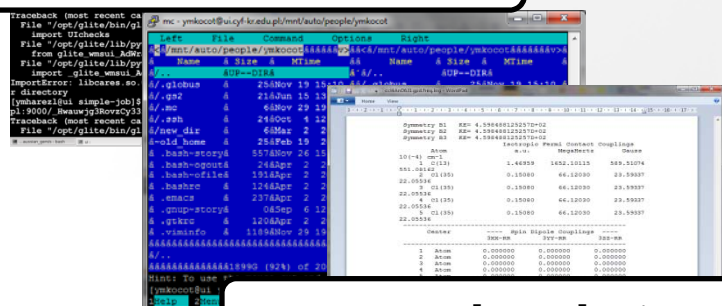
Preparation of input files



Execution and monitoring of multiple computational jobs

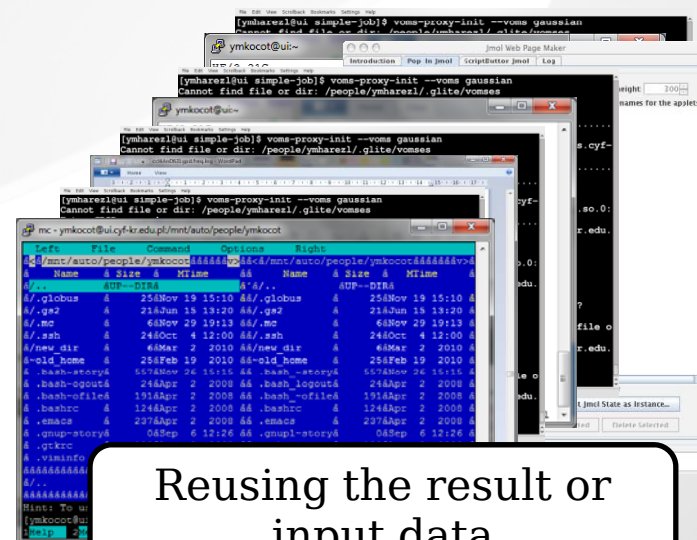


Result fetching...



... and analysis

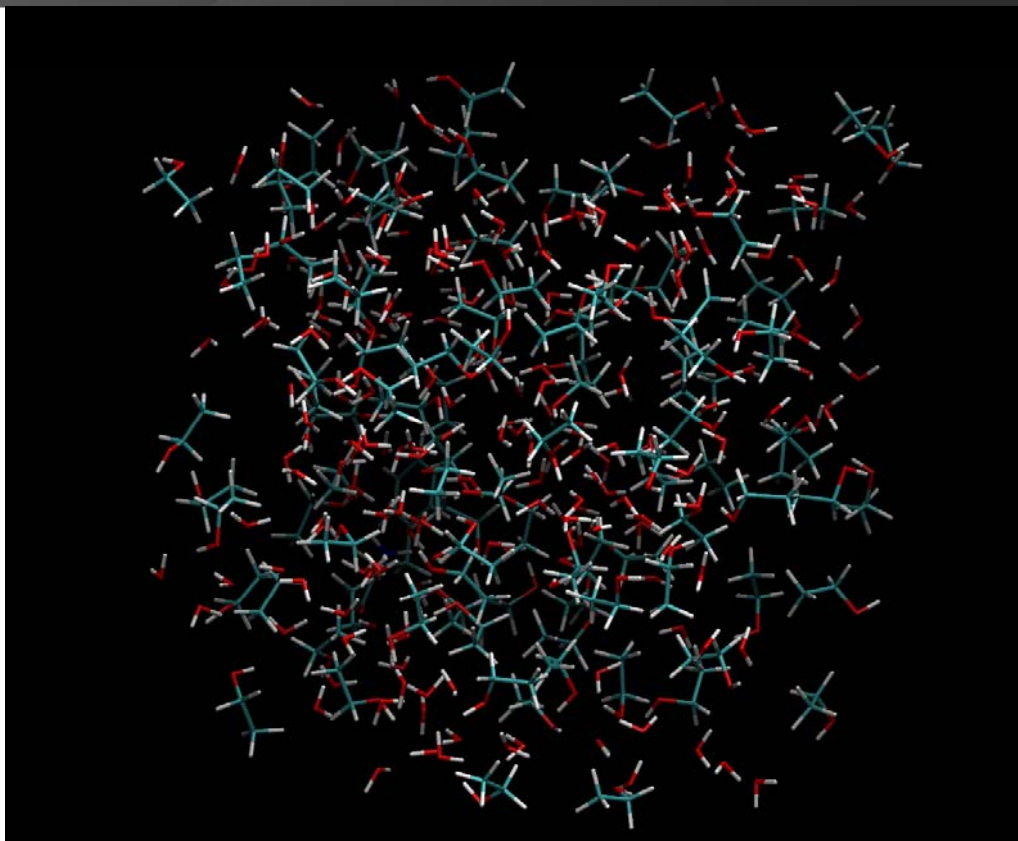
Reusing the result or input data



QC/MD Modelling: Sequential Approach

- Sequential approach to molecules in solution:
 - › Simulation of the solute-solvent system at the Molecular Dynamics level (classical or ab initio)
 - › Selection of the solute with its solvation shell and performing quantum-chemical calculations (possibly at higher level of theory) to calculate solvent effect on physical properties (energies, excitation energies, chemical shifts)

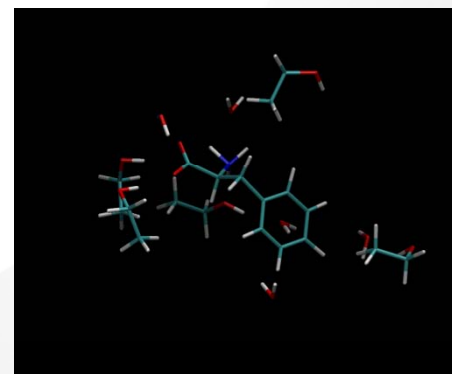
What is more... Reduction



Requires from the researcher additional effort and usually some programming skills

Reduction of the system necessary to:

- Visualize the „reaction center“
- Make the quantum-chemical calculations feasible



QC/MD Modelling: Desired Solution

- Desired features of a tool facilitating molecular modelling data manipulation:
 - › Applicability to a variety of systems
 - › Easy and flexible definition of the selectable part of the system
 - › Visualization at each step
 - › Automated preparation of series of geometries and input files
 - › Execution of QC jobs on the available infrastructure (PLGrid)
 - › Results fetching
 - › Parsing of the results and performing basic statistics

InSilicoLab for Chemistry

in silico LAB

You are identified with grid certificate issued for **Joanna Kocot - PL-Grid** [Configure proxy...](#)

Welcome | New experiment | With parameteri... | Benzene...groun... | LFC Catalogue

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 - workspace.

If you choose not to configure your proxy now, functionality. For this purpose, choose one of the workspace.

You will not see this screen if your proxy is v workspace.

Your Experiments

Menu

- Benzene
- Benzene
- Benzene
- Benzene
- Benzene
- Benzene
- Benzene
- Benzene new
- Benzene...ground state...RHF/STO-3G
- Benzene...ground state...RHF/STO-3G
- Benzene...ground state...RHF/STO-2G
- Benzene...ground state...RHF/STO-3G

Initialized experiments
Running experiments
Completed experiments
Finished with error
Experiments in preparation
Experiment templates
No filter

LFC Catalogue

- 1279701327_find.png
- 1280069308_archives.png
- chempo-experiments

Filter by name

Results

Energy Plot

Job	Energy Value [eV]	Spin Squared	Actions
1.	-24421.56997	0.0	
2.	-24421.7019415	0.0	
No.	SCF Energy [eV]	Actions	
1.	-24421.56997		
4.	-24420.1451747	0.0	
5.	-24420.2779888	0.0	
6.	-24420.2849154	0.0	
8.	-24419.1608191	0.0	
9.	-24419.1643927	0.0	
10.	-24418.4139534	0.0	
12.	-24418.5398317	0.0	

Experiment With parameterization

Oct 4, 2010 8:40:39 PM: Gaussian experiment

Experiment Status

Status: running

Jobs:

Abort all jobs

Experiment Input Data

Title Section

Link 0 Section

Route Section

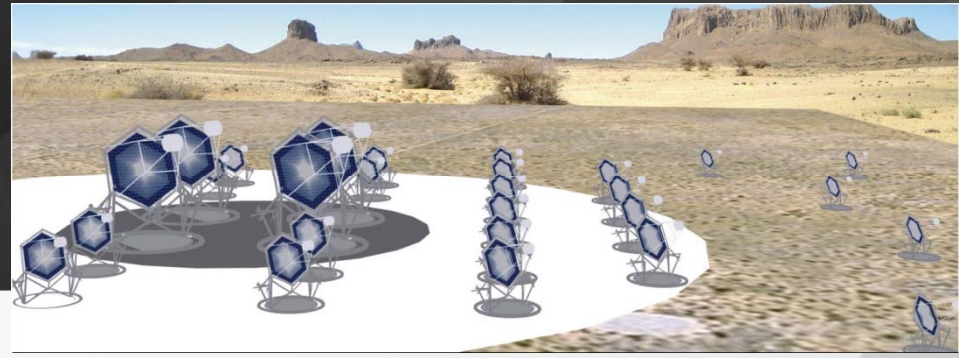
Charge & Multiplicity

Additional Parameters

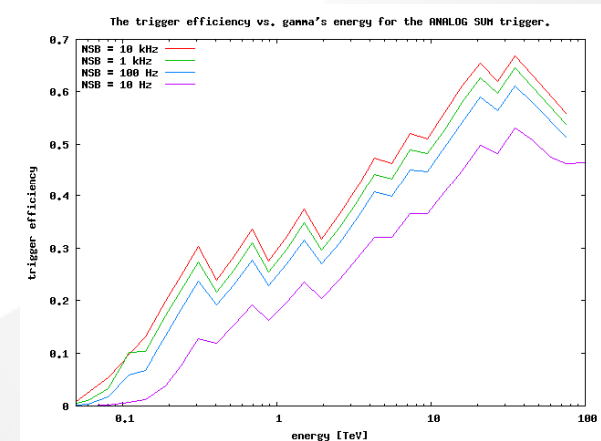
Molecules

H6C3N6O6

Other domains



- Cherenkov Telescope Array (CTA)
 - › Project for ground based gamma-ray astronomy
 - › Large international collaboration (25 countries)
 - › Scientific goal is to build telescope array:
 - 10 times more sensitive than current instruments
 - with better energy and angular resolution
 - with wider field of view and energy coverage
 - with budget ~ €190 M





- MHD code created at Centre for Astronomy, Nicolaus Copernicus University in Toruń, Poland
- Integration with InSilicoLab done by the Piernik developers
 - › Only aided by the InSilicoLab team
- Will be deployed as PL-Grid service
- <http://piernik.astr.umk.pl/>

Summary

- The *InSilicoLab* portal is a solution for researchers performing *in silico* experiments in many domains of science
 - › Specific problem support, but supports many problem classes – thanks to generic system architecture
- Validated and running in production mode for two domains (one beta-stage deployment)
 - › Will be released as PL-Grid service in March (Chemistry and in December (Piernik))
- Open for new collaborations



Thank you!

<http://insilicolab.grid.cyfronet.pl>

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