



A virtual laboratory for decision support in viral diseases treatment

# The ViroLab Virtual Laboratory

http://virolab.cyfronet.pl

Objective
The ViroLab Virtual Laboratory is a collaborative environment for research teams. It enables scientific programmers to cooperatively develop scientific experiments which combine data and processing, and which can be used by collaborating domain researchers to obtain scientific results.

## **Classes of Users**



Experiment developers combine their domain knowledge and technical skills to plan and develop new experiments.



Experiment users execute experiments to obtain scientific results and, afterwards, analyze, share and possibly publish these results.



Clinicians use specialized experiments to assist them in their daily clinical work: treating patients infected with certain viruses.

## **Experiment Pipeline**

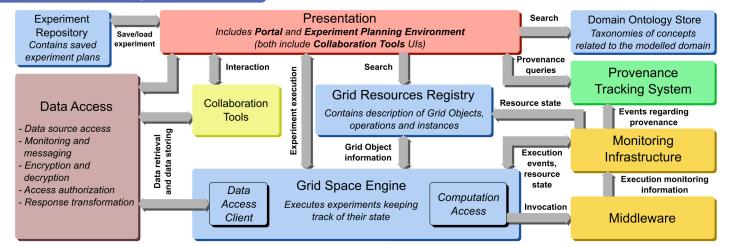


Experiment is a process that combines data with a set of activities that act on that data in order to yield scientific results.

**Developers** find and use appropriate data sources and processing algorithms to build experiments.

**Scientists**, during experiment execution, apply real data and processing power from those sources to get exeriment results.

### Virtual Laboratory Architecture



#### Capabilities

- Dedicated tools for all three groups of users
- Experiment repository that stores experiments and enables their reuse and collaboration
- Unified interface to Web Services, LCG jobs, Mocca components
- Unified access to aggregated OGSA-DAI sources and standalone remote databases
- Use history recording and provenance tracking for experiment repeatibility and evaluation
- Security based on SAML and Shibboleth solution with single sign-on and attribute-based access policy

## **Example:** Genotype to Drug Resistance

Experiment steps: acquire virus sequences for specified patient, align the sequence and detect mutations in certain region and find out what drugs are resisted by this virus.

```
patientID = 6 region = "rt"

nucleoDB = DACConnector.new
    ("mysql", "virolab.cyfronet.pl")
sequences = nucleoDB.executeQuery(
    "select nucleotides from nt sequence where
    patient_ii=#{patientID.to_s};")

mutationsTool = GObj.create("RegaDBMutationsTool")
mutationsTool.align(sequences, region)
mutations = regaDBMutationsTool.getResult

drs = GObj.create("DrugResistanceService")
puts drs.drs("retrogram", region, 100, mutatations)
```

## Virtual Laboratory Partners

ACC CYFRONET and ICS AGH, Krakow (Marian Bubak [bubak@agh.edu.pl] - Virtual Laboratory development coordinator) GridwiseTech, Krakow (Paweł Płaszczak), UvA, Amsterdam (Peter Sloot), HLRS, Stuttgart (Stefan Wesner)

P.M.A. Sloot, A. Tirado Ramos, I. Altintas, M. Bubak, C.A. Boucher; *From Molecule to Man: Decision Support in Individualized E-Health*, IEEE Computer, vol. 39, no. 11, pp. 40-46; November 2006

M. Bubak, T. Gubała, M. Kasztelnik, M. Malawski, P. Nowakowski, P.M.A. Sloot; *Collaborative Virtual Laboratory for e-Health*; eChallenges'07 M. Malawski, M. Bubak, D. Kurzyniec, V. Sunderam; *Experiments with Distributed Component Computing Across Grid Boundaries, HPDC'06* 

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