





A virtual laboratory for decision support in viral diseases treatment

Development and Execution of Collaborative Application

http://virolab.cyfronet.pl

Objectives

ViroLab virtual laboratory should provide an advanced collaboration space for the end user (scientist)

and the experiment developer. There is a need for high-level experiment plan notation, to express complex collaborative applications. It should be supported by tools facilitating

clear development, release, execution and result mangement practices.

Grid Object abstraction

Grid Object Class (🛜

Grid Operation

Grid Operation

Grid Object Implementation

Grid Object Instance

Implemented as

Published as

Data

Access

Client

Grid

Application

Optimizer

Grid

Operation

Invoker

script

Experiment

Experiment script is a piece of program in a computer language that the virtual laboratory execution component is able to interpret. The script defines the main steps in experiment process and the

control flow between those steps.

Data

Access

Service

Remote

Relational Data Base

Data sources

Grid Operation

Grid Operation A - C

Grid

Resources

Registry

Computational

resources

Grid Object Class

Published as

Grid Object Instance

Experiment Script

Development:

- high-level scripting language (JRuby)
- easy access to remote databases
- Grid Object abstraction: focus on "which" computational functionality is required, not "how" to access it

Collaborative Experiment Development

Experiment sharing:

- storing scripts in SVN system, to allow creating experiments by many developers

Commit

- clear releasing process

Grid Object Class - a group that has similar functionality with regard to its domain operations.

Grid Object Implementation - realization of Grid Object Class in concrete technology (e.g. WS, MOCCA)

Grid Object Instance - an implementation that is deployed and can be accessed by the Invoker

Data

Data

7

кеsources dentification

Available

Tech

specific info

Invocation

Result



- web application for browsing and executing experiments

Experiment Repository

Commit feedback

Browse experiments **Running experiments:** - single-click experiment

execution - Interaction between

experiment and user

PROToS Provenance System

Query for provenance data

Gathering results:

- dedicated renderers for script input and output parameters
- important experiment data are automaticaly stored in provenance system
- easy provenance data search

Update experiment execution Execution (reauest

Scientist

Generate provenance data

Experiment

results

Operation Invoker

Grid result = dr_system.drs(100, mutation)

= DACConnector.new(

mutation = rdb.executeQuery(

"mysql","virolab.cyfronet.pl",
"test","testuser","")

"select mutation from patients

dr_system = GObj.create(

Resource choice

dr_system = GObj.create(

Invoke

operation 9

'org.virolab.DrugRankingSystem')

where patient_id = patientID;"

'org.virolab.DrugRankingSystem')

'retrogram', region,

GSEngine

Developer activities

Scientist activities Experiment script execution

Feedback:

- easy communication between end user and developer
- scientist feedback is very important for creating new versions of experiment scripts

Authors

Tomasz Gubala (2,3), Marek Kasztelnik (3), Maciej Malawski (1), Marian Bubak (1,3)

(2) Informatics Institute, University of Amsterdam, (1) Institute of Computer Science AGH, al. Mickiewicza 30, 30-059 Krakow, Poland Kruislaan 403, 1098 SJ Amsterdam, The Netherlands

(3) ACC CYFRONET AGH, Krakow, ul. Nawojki 11, 30-950 Krakow, Poland

P.M.A. Sloot, Ilkay Altintas, Marian Bubak, Charles A. Boucher: From Molecule to Man: Decision Support in Individualized E-Health; IEEE Computer Society, vol 39, no.11, pp. 40-46, Nov., 2006

Tomasz Bartynski, Marian Bubak, Tomasz Gubala, Maciej Malawski: Universal Grid Client: Grid Operation Invoker; Proceedings of International Conference of Parallel Processing and Applied Mathematics (PPAM'07), Gdansk, September 2007, LNCS (to appear).

ViroLab EU-IST 027446

Coordinator: Prof. P.M.A. Sloot Universiteit van Amsterdam www.virolab.org























