

General Conception of the Virtual Laboratory

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Abstract. In the paper some theoretical considerations about virtual laboratory (VL) aspects are discussed. Possibilities of the VL system creation to control many laboratory apparatus in a remote way are considered by the authors. The main research goals on which the authors want to focus their attention are: laboratory framework and dynamic measurement scenarios.

1 Introduction

Virtual Laboratory (VL) is a heterogeneous, distributed environment, which allows scientists all over the world to work on a common group of projects [1]. This environment should allow conducting experiments with the usage of physical devices, doing simulation using the computational application, and communication between users working on the same topic. Similarly to typical laboratory tools and research techniques depending on the specific field of science, virtual laboratories can benefit from some collaboration techniques as tele-immersion, but they are not mandatory.

Research work of the authors is focused on virtual laboratory aspects [2] which have significant influence on creating a general system which will allow taking control on many different devices. In the virtual laboratory system there are many factors which are significant in our work. The most important of them are: laboratory framework and dynamic measurement scenarios.

The Virtual Laboratory system is developed in Poznań Supercomputing and Networking System in collaboration with the Institute of Bioorganic Chemistry and Radioastronomy Department of Nicolaus Copernicus University.

2 Virtual Laboratory Framework

In the virtual laboratory architecture we can distinguish four layers (see Fig. 1). The first of them is the Access layer. Originally it consists of tools which enable access to the laboratory resources and for presentation stored data. The most important modules are:

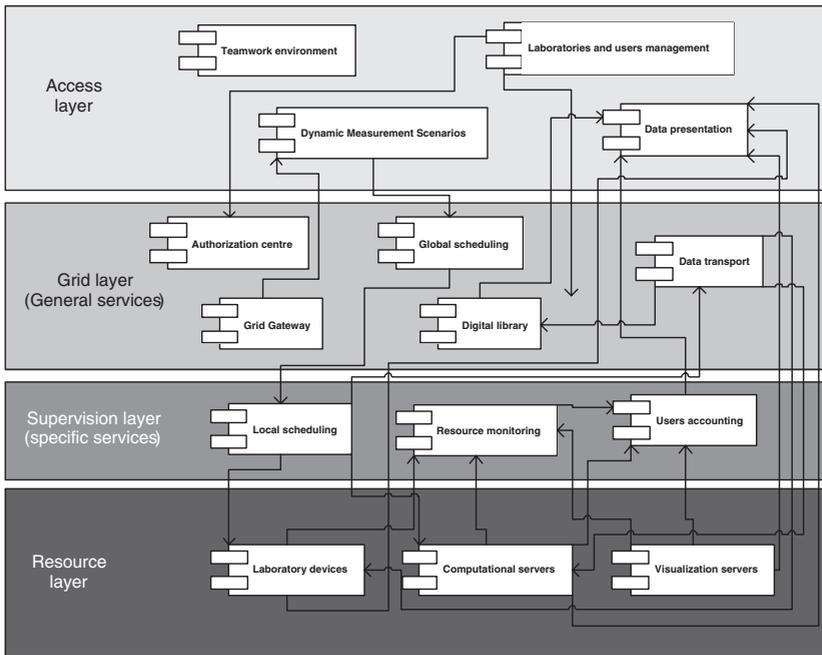


Fig. 1. The framework of virtual laboratory architecture

- Dynamic measurement scenarios - assure control and execution of the operations (experiments) chain, which is submitted by the user,
- Users and laboratories management - tools for creating new laboratories profiles, new users accounts, management of the access rights to devices, digital library and communication media,
- Data presentation tool - presentation experiment results collected in the data management system, on-line visualization tool and accounting data looking through,
- Users communication tools - allow users to communicate with one another

The second is the Grid layer where services which we can call general were accumulated. They are required in most laboratories instances. There are also connections with the outside grid services e.g. with Globus services [3]. The most important are:

- Authorization centre - granting (or not) access to many virtual laboratory resources, certificates management,
- Global scheduling - responsible for choosing the appropriate laboratory device and load balancing when possible,
- Digital library - storing experiments results and electronic publications,
- Data transport - responsible for download and upload data from/to destination machine,

- Grid Gateway - communication with the grid broker (e.g. GRMS [4]), sending computational tasks to the grid and receiving experiment tasks from the grid systems

On the supervision layer specific services are gathered. These services have to be implemented taking into consideration a given device and their specification. Usually it consists of:

- Local scheduling - tasks scheduling on a given device taking into consideration parameters and priority
- Resource monitoring - resources using control, tasks actual state control
- Users accounting - information about the used resources

Finally we can define the Resources layer which consists of devices to experiment execution and also the necessary software:

- Laboratory devices - laboratory apparatus and software for experiment execution
- Computational servers - also software for pre- and post-processing computation
- Visualization servers - also visualization software

3 Dynamic Measurement Scenarios

The experiment process execution in many types of laboratories consists of very similar stages. The given experimental process is often recurrent and must be executed many times by some parameters modification. In this situation the measurement scenarios conception seems to be very useful.

The conception of the dynamic measurement scenarios allows defining the process of an experiment in any way, from pre-processing, through executing the experiment, to the post-processing and visualization tasks. Users are also allowed to add their own module as a part of the scenario. Defining the measurement scenario allows to spare a lot of time during computation. The user does not have to wait for the end of a given process stage to submit another one. It is made automatically.

Initially, we divide the experiment execution process into four steps: preprocessing (data preparation to use as an input source), experiment (executed on real device), postprocessing (output data processing) and visualization.

This simple task's execution chain we call a static measurement scenario (SMS). It allows connecting particular stages only between themselves. Here, the execution path is specific and the user can not manipulate it.

To increase the possibility of the jobs scenario the dynamic measurement scenario (DMS) was defined. In the DMS model, besides the definition of the tasks execution sequence, we can also define some extra connections (e.g. loops, parallel connections), conditions on the connections and different lengths of the execution paths. In fact, DMS allows to define many SMS models in one scenario. Thanks

to the possibility of the conditions defining on the connections paths the real path is determined during execution and can depend on computational results.

To properly define the dynamic measurement scenario the system has to have knowledge about connections which are enabled. In case of the laboratory type where the processing software is well known, it seems to be easy. The case will be more complex when we want to define the DMS model for a wider range of virtual laboratories.

To solve this problem we defined a special language which determines the following conditions: names of the connected applications, a condition (or conditions) connected with a given path, an additional condition which has to be met to pass a given path, e.g. when special conversion between application is needed and in the end a list of input or output files for applications.

An expertise from a particular discipline is necessary to define rules for DMS. It can be done by a laboratory administrator together with a domain expert.

4 Conclusions

The universal virtual laboratory framework allows to spare a lot of human energy and money during the development stage. It is possible to build many different types of laboratory systems which provide and adapt functionality to specified needs. Designers of a new laboratory have to focus their attention only on a few aspects connected with adaptation to a new data set, and a specific scheduling algorithm.

To proof our assumptions and as an exemplary implementation it is planned to make the NMR Spectrometer (Bruker Avance 600) and radiotelescope (diameter 32m) available to the Grid users [5].

References

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