Effective integration of scientific instruments in the Grid

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Abstract

The paper presents a framework for Virtual Laboratory (VLab). Authors focus their attention on the application structure, which can make it possible to remotely use very expensive devices. It is important that this structure is universal and can be used with every device and every simulation. Therefore the framework is a critical issue in that concept. To prove the concept we plan to put into practice the Virtual Laboratory of Nuclear Magnetic Resonance Spectroscopy (NMR), which bases on this general structure. Another significant issue is to handle remote facilities like other Grid resources. This assumption generates new requirements concerning e.g. resource scheduling and global accounting.

1 Introduction

Virtual laboratories are now in the scope of activities of research groups and companies which are working on new solutions for remote access to very expensive laboratory devices. The Virtual Laboratory (VLab) project is developed by Poznań Supercomputing and Networking Center in collaboration with the Institute of Bioorganic Chemistry. The main goal of VLab is to create a framework for building many different types of laboratory. Another purpose is defining all accessible remote facilities treated as simple resources in the Grid infrastructure. It is possible thanks to the VLab broker which is connected with the Grid resource broker. Each job directed to the real laboratory facilities is treated as any other Grid task. Another issue concerns a concept of dynamic measurement scenarios. It allows defining the process of 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.

The Virtual Laboratory is not only a set of mechanisms to submit, monitor and execute jobs. It is also a possibility to give access to the resources of the digital library, communication, and e-Learning systems. A digital library allows users to store and share experiment results and bibliography concerning a given scientific discipline. Thanks to the communication systems, scientists from geographically distant places can work together without moving from their mother institute. The e-Learning system is very useful as it gives users necessary knowledge about theory, terminology and using a specific laboratory device (e.g. spectrometer). Usually the end user is obliged to use High Performance Computing (HPC) and High Performance Visualization (HPV) resources in the experiment process. The calculations are done before (pre-processing) and after (post-processing) the real experiments. This makes it crucial to answer the question how to efficiently manage remote facilities. To fulfil the requirements we introduced a new approach. The novelty is to use measurement (experiment) scenarios that can be defined by the end user specifying what kind of computations and experiments will be done as well as the coupling between specific calculations. It gives full HPC/HPV support for the experiment with all the critical demands concerning interactivity, response time, deadline of finishing computations, etc.

As an exemplary implementation it is planned to make the NMR Spectrometer (Bruker Avance 600) and radio telescope available to the Grid users [6,7,8].

The research and development is done under projects no. 6 T11 0052 2002 C/05836 co-funded by the Polish State Committee for Scientific Research (KBN) and Silicon Graphics and 4 T11F 010 24, funded by KBN [16].

2 Functional assumptions

The **Virtual Laboratory** is a heterogeneous, distributed environment which allows scientists all over the world to work on a common group of projects correlated with remote facilities. This environment should allow conducting experiments with the usage of physical devices, doing simulation using the computational application, and should allow communication between users working on the same topic. Virtual Laboratories can benefit from such collaboration techniques as tele-immersion, but they are not mandatory.

We can distinguish two types of experiments: real and computational. By the real experiment we understand an experiment which is executed on a real facility. However, by the computational experiment we understand simulation of a real experiment or computation on a computational machine.

In order to meet these goals the Virtual Laboratory should specify some requirements. The most important requirements follow:

- The possibility to conduct experiments (real and computational)
- The possibility to compare results achieved in real experiment and simulation, which may help to properly adjust the simulation parameters
- Reservation of time for experiments execution, especially for experiments that require supervision or can be observed by more people.
- Communication with laboratory administrators, which might be necessary to run some specific experiments
- Sharing experiment results – the result should be stored in a database and available for other scientists (with the possibility to restrict access rights)
- Integration with HPC and HPV resources (Grid environment) to support the pre- and post-processing analysis
- Communication with other people working on similar problems (collaborative applications).

3 Main VLab research

The main goal of this venture is to create a framework for the laboratory, which will be remotely accessed via the network. This framework must be flexible enough to adapt to?many types of laboratories, which in fact means many types of labour equipments and specific demands coming from the end user. It will be accomplished thanks to the modular architecture of VLab (Figure 3).

All accessible facilities and machines will be defined as resources in the Grid infrastructure. Within the scope of the VLab project a universal broker, which will be connected with the Grid resource broker, will be created. In this way every job directed to the real laboratory facilities can be treated as any other Grid task [5,11,12].

A very important idea in this approach is the concept of dynamic measurement scenarios. It allows users to define the experiment process in any way, from pre-processing through executing the experiment to post-processing tasks. Users can also add their own modules as parts of the scenarios.

Another element of our research is taking into consideration the human factor. Many types of real experiments cannot be executed without human support. The scheduling module should take into consideration e.g. working hours or minimizing human work by scheduling similar jobs side by side.

The testbed infrastructure supporting our research and development is shown in Figure 1. The infrastructure gives HPC and HPV support with computational resources geographically distributed on many sites. The proof of the concept will be done for the NMR spectrometer (Bruker Avance 600) and radio telescope. The remote facilities and HPC resources are connected by dedicated channels of 1 Gb/s extracted from the national network PIONIER.

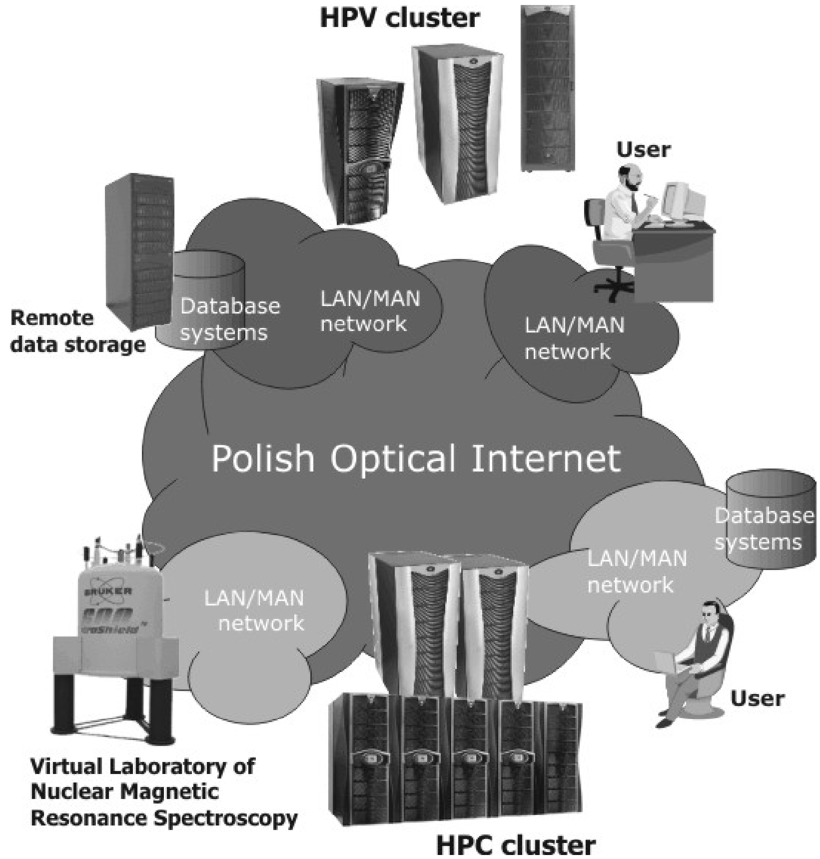

Figure 1 Testbed infrastructure of Virtual Laboratory

4 Networking issues

The available network connections are very important for delivering high-level service quality. We have to deliver a high-speed network from the end user to the HPC and HPV resources and a good quality connection to remote facilities. In addition, the required throughput depends on the amount of data sent between computation sites. The technology we are going to use, e.g. parallel and distributed visualisation, is strongly dependent on the networking layer. For testbed purposes (Figure 1) we have defined dedicated 1 Gb/s connections based on fibre optic cables delivered by the Polish Optical Network PIONIER (Figure 2), coupling the HPC centres in Poznań and Kraków, and end users in Łódź, Gdańsk and Wrocław [16].

Another example we can mention is the virtual laboratory for radio astronomy, which we are trying to realize with the Department of Radio Astronomy of the Nicolaus Copernicus University in Toruń, member of the VLBI consortium (Very Long Baseline Interferometry), connecting several radio telescopes. We would like to entirely automate the process of defining and executing the VLBI experiment. In the virtual laboratory the user only needs to specify necessary observation parameters. Parameters distribution to radio telescopes, recalculating them to appropriate radio telescope values, launching observation on time, data transporting and correlating and post-processing execution can be performed automatically. This example generates higher network bandwidth demands and needs to assure special data transfer caches. The amount of data transferred in one experiment is in the order of dozens of TB.

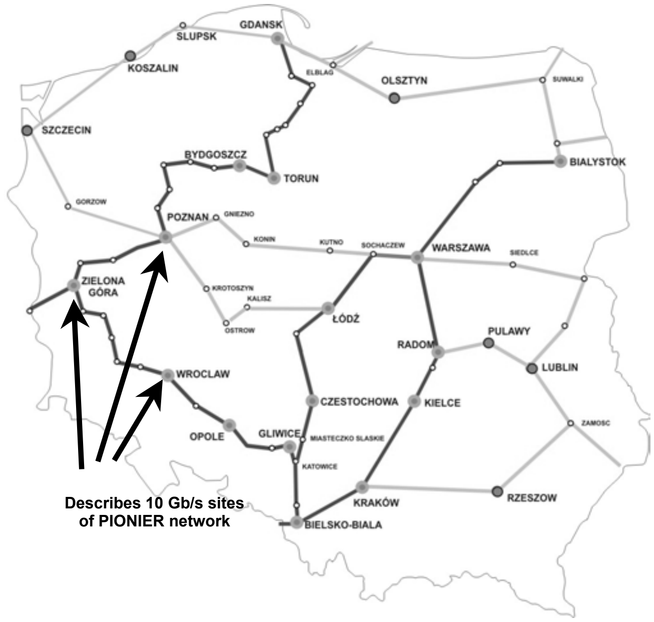

Figure 2 The topology of the Polish Optical Internet network PIONIER

The circles depict the currently installed 10 Gb/s sites. The PIONIER network technology gives the possibility to define dedicated networks for R&D purposes, as those described in the paper.

5 System architecture

Each part of VLab has a modular construction. It allows increasing the system flexibility by adding new modules, easily changing the existing modules into others with biggest possibilities without changing the architecture and any rebuilds or recompilations. To make it possible we defined a unified access interface between modules.

All modules can be divided into two types: general and specific modules. General modules can be used in any type of laboratory. Specific modules are built for a given type of laboratory. The construction of general modules allows to accept many types of jobs whose parameters and results descriptions are standardized. Specific modules which know the given application or experiment type are responsible for standardization.

Thanks to this solution the existing implementation can be adapted to any other type of laboratory, by exchanging some specific modules only.

The VLab approach was integrated with the existing Grid middleware software, which makes simple integration of HPC and HPV infrastructure possible (Figure 3).

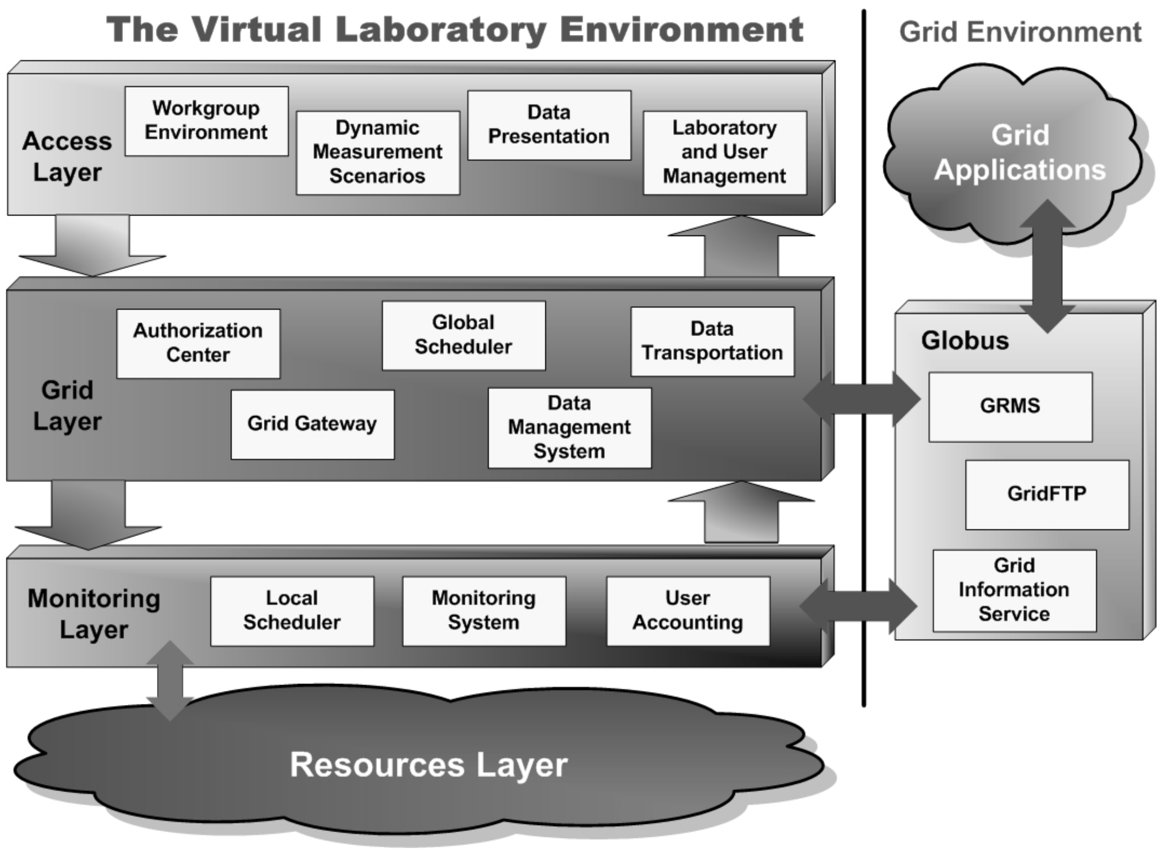

Figure 3 Virtual Laboratory architecture integrated with the Grid approach

The concept of the general framework and most important for the virtual laboratory will be discussed next. In the virtual laboratory architecture we can distinguish four layers. 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:

- Dynamic Measurement Scenarios – assure control and execution of the operations (experiments) chain which is submitted by the user,
- Laboratory and User Management – tools for creating new laboratories profiles, new users accounts, management of the access rights to devices, digital library and communication media,
- Data presentation – presentation of experiment results collected in the data management system, on-line visualization tool and accounting data looking through,
- Workgroup environment – allows users to communicate between themselves and communicate users with lab technicians

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. The most important are:

- Authorization Center – granting (or not) access to many virtual laboratory resources, certificates management,
- Global Scheduler – responsible for choosing the appropriate laboratory device and load balancing when possible,
- Data Management System – storing experiments results and electronic publications,
- Data Transportation – responsible for download and upload data from/to the destination machine,
- Grid Gateway – communication with the grid broker (e.g. GRMS [15]), 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 Scheduler – tasks scheduling on a given device taking into consideration parameters and priority
- Monitoring System – resources using control, tasks current? state control
- User Accounting – information about the used resources by the user

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,
- Network facility – also with QoS software

Resources in the Grid

The objective of the VLab project is to create a framework for laboratories to define all accessible remote facilities treated as simple resources in the Grid infrastructure. The VLab broker is connected with the Grid resource broker. Each job directed to the real laboratory facilities is treated as any other Grid task. Users can submit an experiment as any other computational job and do not need to care how it will be executed. After some time they can only obtain experiment results (Figure 3).

Dynamic Measurement Scenarios

Experiments executed in the science laboratories are complex and consist of many stages [20]. Usually it looks as follows: a scientist prepares a sample and/or input data (e.g. parameters) which will be measured/computed. Next he/she uses laboratory devices to achieve data which are the processed by a specialized software. Processing can include the visualization stage if it is needed to assess the results. In case of undesirable results some measurement stages should be repeated. At each stage the scientist decides which way the research should go next. As we can see, the experiment process execution may consist of very similar stages in many scientific disciplines (laboratories). The given experimental process is often executed recurrently by some parameters modification. Obviously, the presented scenario is typical but we realize that scholars can have more sophisticated needs [21].

Thus, we can define a graph which describes the execution path specified by a user. Nodes in this graph correspond to experimental or computational tasks. Edges (links) correspond to the path the measurement execution is following. In nodes we have a defined type of application and its parameters. In links the passing conditions which substitute decisions made by the user are defined. These conditions are connected with applications and let us determine if the application is finished with the desired results (if not, the condition is not met). This execution graph with specified nodes and links (with conditions) is called the Dynamic Measurement Scenario (DMS). The term "dynamic" is used, because the real execution path is determined by the results achieved on each measurement stage. All of these parameters can be written down using a special language: the Dynamic Measurement Scenario Language (DMSL).

Thanks to DMS it is possible to synchronize task-flow in the system. Moreover, thanks to the advance scheduling process which takes into consideration human-factor, we enable interactive task execution in the measurement scenario.

Digital Science Library

The Digital Science Library (DSL) is used to store and share experiment results, publications and manage computational data between scientists. DSL bases on the Data Management System (DMS) developed under the Progress project [18]. Except for the functionality mentioned before, DMS provides proxy to other databases and data accessed from the Internet. The next function is mirroring the whole or a part of the external database.

DMS consists of three logical layers. The highest layer is the Metadata Management. Inside this layer there is a repository. You can think of the repository as a place where metadata is stored. The Metadata Management is responsible for storing and manipulating metadata. The data is described with attributes and access rules. In fact, the metadata is stored in an object database in the property=value format. This format meets the requirements of the Dublin Core (DC) standard, the Content Standard for Digital Geospatial Metadata (CSDGM) standard or the Resource Description Framework the XML standard. The second layer consists of the Data Broker and the Mirror & Proxy. The Data Broker is an interface between the user and DMS. The user can be grid computational software or a special software client DMS i.e. a computational web portal. The Data Broker can also arrange several replicas of data. The mirror and Proxy is responsible for accessing and mirroring external databases. The main purpose of this module is to grant access to various external objects in a uniform way. The lowest layer is the Data Storage. This layer is responsible for the physical storage of data. This module can store data in several ways: in computer file systems, in databases or on tape storage systems. The described structure is shown in the figure below.

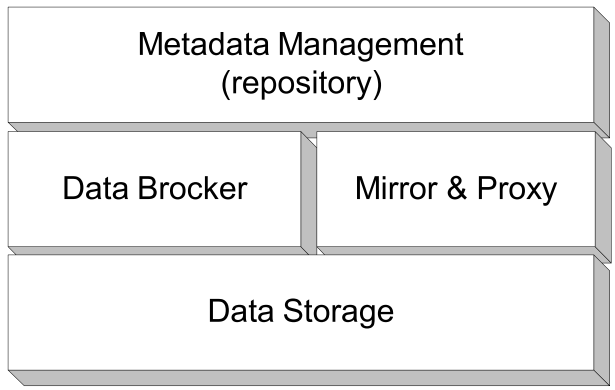

Figure 4 Logical architecture of the DMS

Security

Jobs which are executed in the Virtual Laboratory system should ensure an appropriate security level. These jobs often consist of data which are very important for a particular scientific unit or company that may be misused [7,10].

Our project plans building a multilevel security system. Access to every level is determined to specific users with appropriate rights. The system has several access zones which are designed for? people who administrate and use the Virtual Laboratory: application server administrator, laboratory administrator, physical device administrator, computational system administrator and user.

The security level development is done according to the Global Grid Forum Security Group recommendations, especially in the range of communication protocols.

Global accounting

The Grid economy approach requires a global accounting system which is able to report all resource usage. There is still lack of such system, which delays the introduction of a production Grid environment [9].

Users who use the Virtual Laboratory should be accounted for experiments and simulations. All accounting data will be stored in an information system. The stored data will refer to:

- In case of real experiment: device working time, used components (e.g. samples in spectroscope);
- In case of simulation or computation: processor time, operating memory, disc capacity, network interfaces load (an amount of transferred data).

It is also expected to store information about the total time spent in the system by a user (from login to logout time) and about applications used by the user (e.g. communication applications, experiments results library, etc.).

The global accounting system will collect all standard accounting data (delivered so far by each Unix accounting system) and specific data received by the management module of a remote facility.

Interfaces standardization

Building a universal virtual laboratory architecture requires designing and creating the standardized module interface. Thanks to this solution the laboratory administrator (creator) can adapt the laboratory structure to particular laboratory needs by selecting appropriate modules. It is also possible to write their?own modules with standardized interfaces.

Besides defining one unified interface there is also a need to define an appropriate communication protocol which meets all laboratory types requirements. The datagram which will be sent between particular modules should have a unified (in some range) construction. Its structure should enable flexible adaptation to different types of laboratories, type of transferred data and ensure inviolability of transferred data. The data construction transmitted between modules has a diverse construction due to the different nature of laboratory experiments executed on particular devices. Obviously, some data are recurrent. Thus, the virtual laboratory datagram has been divided into two parts: general – with data appearing in every communication independently of the laboratory type and specified (so-called binary content) with data dependent on the experiment data structure. In Figure 5 a communication datagram structure is presented with a detailed general part.

Parameters description:

long	datagramId
int	validTaskId
long	userId
int	groupId
char*	inetAddress
long	operationId
int	operationStatusId
int	contentId
long	contentSize
int	datagramNumber
int	datagramCount
binaryContent	

Figure 5 Communication datagram structure

- DatagramId – unified in the system datagram ID, created when the datagram is generated,
- ValidTaskId – datagram concerns task ID, verified during the communication process – according to the active task table
- userId, groupId – user and group ID, in VLab the system group corresponds to laboratory group, data are used on the authorization and authentication stage
- inetAddress – destination IP address for the datagram,
- operationId – operation ID, describes the type of executed operation (and indirectly datagram content), destination module for datagram and communication type (synchronous, asynchronous)
- operationStatusId – the current status of operation described by operationID field,
- contentId – a detailed description of binary content, used in connection with operationID field,
- contentSize – size of binary content (in bytes)
- datagramNumber, datagramCount – the next datagram number and total number of datagram which consists of the whole communication,
- binaryContent – class-defined binary content of datagram;the content is coded in the DIME standard; class definition:

unsigned char*	__ptr
int	__size
Char*	id
Char*	type
Char*	options

Figure 6 Binary content structure in communication datagram

Parameters description:

- __ptr – data bytes pointer

- __size – data sequence length
- id – DIME attachment unique identifier
- type – attachment type (e.g. application/octet-stream)
- options – optional field (currently unused)

VLab cooperation

The Virtual Laboratory also grants access to communication mechanisms. It enables an interactive exchange of experiences, comments and knowledge between scientists. Users can use standard communication mechanisms like: short messages, discussion forum, chat, audio and video. It is also possible to use these mechanisms by a number of users simultaneously and thus create discussion groups. Access to these groups will be limited by special rights only for given users, so communication confidentiality will be ensured.

Not only the communication between users is allowed. The user can also communicate with the device administrator (lab technician) when he/she needs additional information for setting up and executing remote experiment. This kind of contact also is valuable when the user needs anadditional description for some special parameters for a given device which is not directly mentioned in the available documentation. In case of experiments where access to sample is needed, communication with a lab technician allows providing information to the user about the sample condition and user can instruct the technician on how to proceed with the sample before the experiment. Advanced users can suggest the administrator how to set up manual parameters (parameters which can be tuned up only manually by the technician) on a laboratory device. As we can see, the cooperation between the user and the lab technician is needed and sometimes essential.

6 Virtual Laboratory Workflow

To illustrate the complexity of job-flow management in the virtual laboratory system, a very simplified workflow is described. We want to base our description on the NMR measurement scenario. We should mention that the NMR spectrometer is a device which needs human interaction to control because of its nature. It causes that the virtual laboratory workflow depends on the human factor.

Firstly, the user has to define the measurements scenario. Usually the NMR scenario consists of three stages: experiment, post-processing and visualization. Next, the scenario description is sent to the Scenario Management Module (SMM) where is decomposed and every job is sent to modules in proper sequence. Experiment tasks are sent to the Global Scheduling module, and computational tasks are sent to the GRMS module via Grid Gateway.

On the global scheduling stage an appropriate laboratory device is chosen for the job. Additionally, user rights and accessible devices are checked.

In the next step the job goes to the Local Scheduler module where it is scheduled according to the given algorithm and priority. The job is sent to the Job scheduling module only when the previous job has been finished.

Every NMR experiment can be divided into two parts. The first one needs some operator's activity which includes preparing the sample, characterizing probe type and mounting it into magnesium, next inserting the sample inward and manual probe tuning to appropriate frequency. The second part of this type of experiment is automated and can be executed remotely.

At this stage we can use specialized software to control the experiment: VNMR for Varian spectrometer or XWIN-NMR for Bruker spectrometer. This software is made? available to the user using Virtual Network Computing (VNC) [20]. Commands like choosing working directory and sequence impulses, modifying sequence parameters can be done remotely, without direct access to the spectrometer. When experiment is finished, all results are sent to the digital library.

The post-processing task is sent to the Grid Gateway where it is transformed into the Globus format and sent to the GRMS module. GRMS make a decision basing on the job description where to run the computation. If the job needs user interaction, the VNC software is used again. Before computation the spectrometer data are transferred to the server, and when post-processing is finished, the output data are transferred back.

Execution of a visualization task is very similar to the post-processing stage. Only on the scheduling phase will the job be probably directed to other device, better adapted to visualisation needs. Also, the interactive work will be executed more often.

After every execution stage the accounting data are transferred to the Accounting module. The above-described workflow in the Virtual Laboratory is presented in Figure 7.

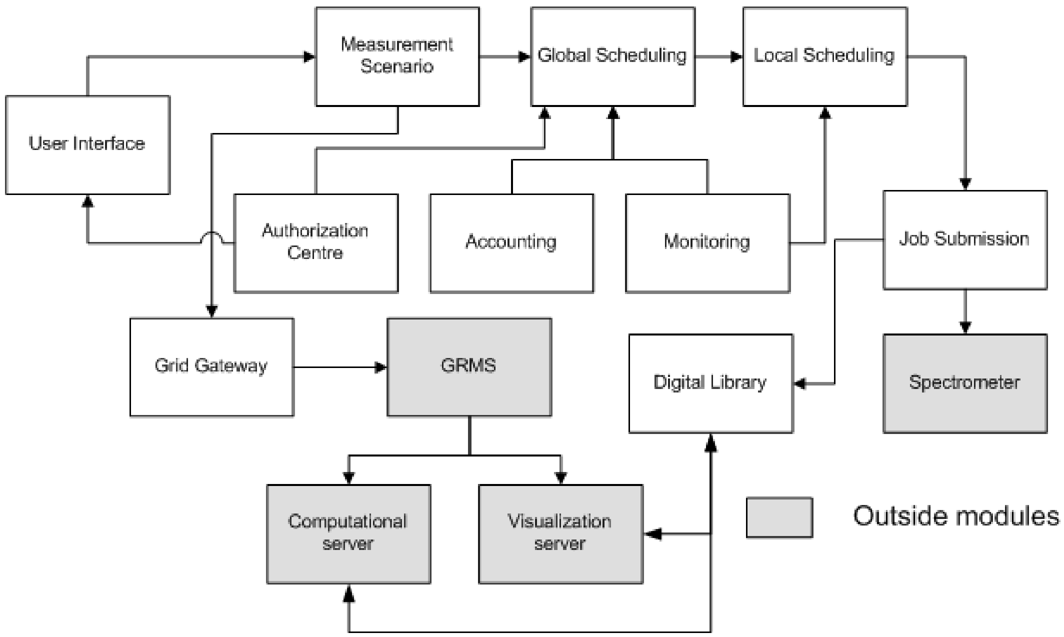

Figure 7 Simplified virtual laboratory workflow

7 Conclusions

Virtual laboratories are undoubtedly the technology of the future [18,19]. They are perceived as a remedy to problems connected with access or buying costs of expensive and rare devices. Current technologies connected with VL are in their first stadium of development. New services are created, which allows running simple experiments that can be managed by changes in a limited parameter pool.

The structure of virtual laboratories should not be limited only to a toolkit, which allows conducting an experiment, but it should also contain virtual collaboration tools for users from different parts of the world, who are working on the same problem. The first step could be a simple tool as chat, later it would be developed into tele-immersive applications.

There is lack of a universal toolkit for creating virtual laboratories [11,12,13]. Developed solutions are assigned just to specific tasks and their structure is strongly conditioned by problems for which they are created. There is a demand for the creation of a universal structure which could be adapted to specific types of laboratories.

A properly deployed VLab system will equal chances for many scientific groups to access very expensive labour equipments. It makes the eScience vision in eEurope closer.

The work is done under project no. **6 T11 0052 2002 C/05836**, called **SGIgrid - High Performance Computing and Visualisation with the SGI Grid for Virtual Laboratory Applications** is realized in co-operation with Academic Computing Centre Cyfronet AGH - Kraków (the lead partner), TriCity Computing and Networking Centre in Gdańsk, Wrocław Networking and Supercomputing Center, Technical University in Łódź and ATM S.A. (Warsaw).

The R&D tasks in project no. **4 T11F 010 24** are done with the Department of Radio Astronomy, Nicolas Copernicus University in Toruń (Poland).

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