User requirements for remote accessed instruments in material science

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Abstract – The technical specification defined from instrumentation owners of suitable for remote access expencive equipment in Material Science domain are presented. The database containing all mentioned above structured information is created and used as analytical tool in this investigation. The user community requirements in several different domains for application of remote access are evaluated and analyzed. This work is one of the main parts of RINGrid project (Remote Instrumentation in Next generation Grids) under the FP-6 program of the EC that provide close collaboration of EU member states and third countries to ensure Europe's strong participation in the research initiatives conducted at the international level.

I. Introduction

There are numerous areas of science, industry and commerce that require broad international cooperation for their success. Therefore, the development and spreading of techniques and technologies that allow virtualized, remote and shared access to industrial or scientific instruments are essential progress of the society. The possibility of using scientific or industrial equipment independent of their physical location helps in the equalization and the unification of communities and subsequently opens new opportunities for industry, science and business [1]. Furthermore, it has a very important political and strategic impact, as we head towards a more unified Europe. The need to use unique and expensive equipment, which is often locally unavailable, as well as the broad international cooperation, are key issues for the success of the great number of scientific or industry tasks. This is especially important for scientific communities from countries with relatively low financial support for their research infrastructure. The systematic identification of instruments and corresponding user communities, the definition of their requirements as well as the careful analysis of the remote instrumentation synergy with next-generation high-speed communications networks and grid infrastructure will be the base for the definition of recommendations for designing the next-generation Remote Instrumentation Services. One of the main objectives in our research is to provide the critical initial infrastructure necessary to facilitate the next generation of interdisciplinary science at both national and international level, as well as in support of multi-institutional collaborative efforts. The possibility of performing research through access to grid-embedded remote instrumentation, with the utilization of next generation high-speed networks, could sufficiently increase the scientific progress and reduce the cost of the equipment use. The analyzed information includes large amount of data received from EU and non-EU institutions, which are owners and users of expensive scientific equipment. The process of identification of high-level scientific instruments with particular application in the Earth Sciences research, their ability for implementation of remote access and the approach concerning their integration in the next-generation grids is described. The users and owners community requirements for such kind of access are evaluated and analyzed. The information is implemented in database that should be used as interface between instrument OWNERS and USERS groups. The results are spread out among scientific, industrial and business groups of users in order to increase the awareness of benefits from using next generation Remote Instrumentation Systems, which are essential for the equalizing access to the European e-Infrastructure opportunities [2].

II. Database implementation

The received large amounts of different kinds of information concerning instrument specification and user requirements for remote access are collected in proper database format. The database was also planed and realized as information interface between both main groups: instrument OWNERS an instrument USERS. It could be considered as prototype of the future large databases that should contain wide structured information concerning remote accessed instruments and services integrated in the next generation grids. Due to the requirements for easier and more flexible data access, we decide to realize mentioned above database prototype using the web technology. In addition, we accepted to use free, commonly used, multiplatform compatible programming tools to create the database. Regarding that, we implemented MySQL [3] as Database Server, Apache Tomcat [4] as Application Server as well as JavaServer Pages [5] and Java Servlet [6, 7] technologies. The database structure diagram is shown on Fig. 1.

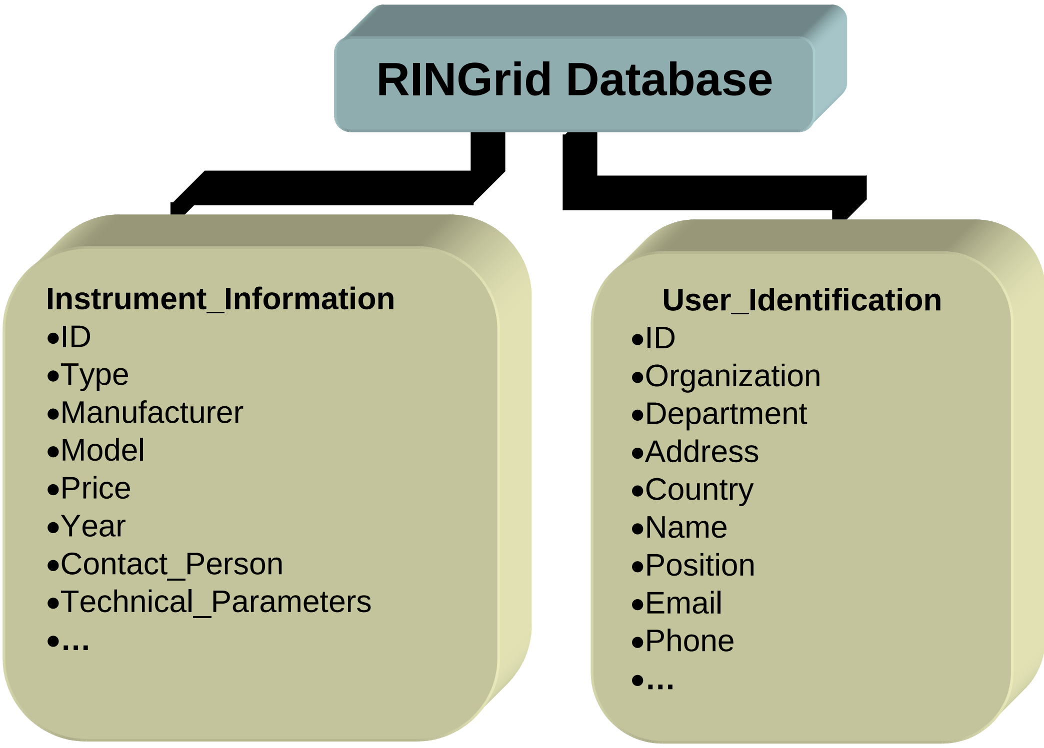

Figure 1. The database structure

The database contains two main sections – Instrument Information and User Identification. The presented database provides the following advantages, concerning instruments and users information:
- unification of the collected information;
- exhaustiveness of the data;
- flexibility of information treatment;
- possibility for statistical data processing.

The group (OWNERS) should use it in order to search proper users and user communities with potential interest to access their equipment according preliminary defined and described conditions.
The second group (USERS) can access this database in their search for suitable remote accessed instruments that fits defined from them criteria sets.

III. Examples of remote accessed instruments and their specification in Material Science

The equipment and instruments in the Material Science domain, according to received data from the user community is one of the most preferred for remote access - 57% (Fig. 2).

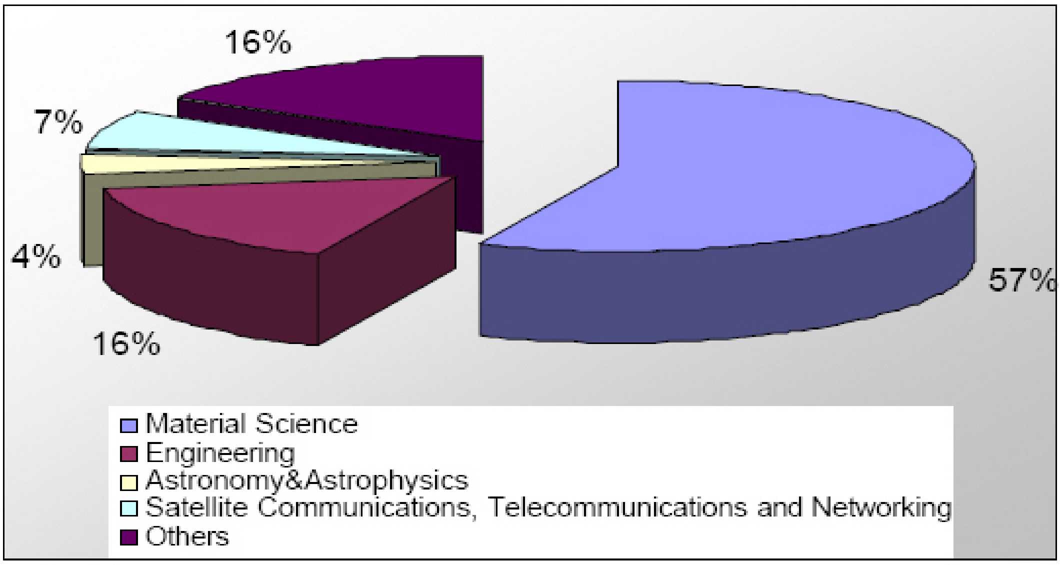

Figure 2. Distribution of equipment pointed out from different users groups

In the Material Science domain several groups of reported instruments that can be also used in the Earth Sciences could be distinguished. According remote access technical requirements they have close or similar technical characteristics for grid integration:
- Microscopes - Scanning Electron Microscopes, Transmission Electron Microscope;
- Spectroscopic equipment – IR Spectrometer, UV-Vis Spectrometer, NMR Spectrometers, Atom Absorption Spectrometer, ICP;
- Diffractometers.

Following, few examples of realized prototype models of remote accessed instruments included in the RINGrid database and widely used in the geosciences research, that have different types and levels of remote technology implementation are presented.

A. Scanning Electron Microscope (SEM)

All SEM instruments included in the RINGrid project are equipped with EDS Spectrometers which makes them suitable not only for observation of the samples by high magnification but also for quantitative chemical microanalyses. At the present, mainly researchers from different countries in Latin America – Chile, Argentina, and Brazil, use them.

In all disposed for remote access electron microscopes there is fully motorized sample stage rotation, so in this respect, the microscope is suitable for remote access. Moreover, the owners of the microscopes do not point out restrictions, regarding access to the instrument operation, access to the obtained data and about the time before transferring data to the user site, i.e. practically the user can fully take part in the analytical process.

Measurement/observation procedure – The preparation procedure of the samples is specific for each sample and it can be done by the user, if he posses the necessary technique. Nevertheless, all electron microscope laboratories are equipped with such kind of preparation technique also, so the preparation of samples can not be a problem for remote usage of the instruments. Before the measurements the microscope must be calibrated and control parameters of the analyses must be defined (accelerating voltage, beam current, counting time, elements to be analyzed to set and save in a file). The local operator does this always. In relation to the representation of measurement results two of the owners of the microscopes pointed out that the data can be transferred as numerical data and as images and one - as video

in addition. This is very important, because most of the potential users would like to watch closely the measurement process and the object that the operator sets for analysis under the electron beam.
Owner access polices description – There are no restrictions regarding access to instrument operation, observing of obtained data and time period before placing observed data in public domain.
Remote access ability – The microscope owners show that measurement process can be accessed from a remote location in real time and offline and that the user does indirectly control the remote instrument communicating by videoconference or interactive online software (i.e. LabView, VNC).
Service and infra-structure requirements in terms of computational requirements, storage requirements and requirements for streaming media (audio and video), multicasting, and requirements for interactive access to the instrument are different for particular microscope owners:

B. FTIR Spectrometer

The FTIR spectrometer included in the RINGrid project works in MIR (middle infrared) 400–4 000 cm^{-1} and NIR (near infrared) 4 000–15 500 cm^{-1} spectral ranges. It is equipped with ATR accessory from ZnSe crystal with a spectral range 15 500–500 cm^{-1} which makes it suitable for studies of thin films loaded on the supports or investigation of the surface and its distinguish from the bulk material.
Owner access polices description – no restrictions regarding access to the instrument operation, access to the obtained data and about the time before transferring data to the user site, i.e. practically the user can fully take part in and observe the analytical process. Only some preliminary knowledge about the software of Bruker FTIR instruments – “OPUS” is necessary.
Measurement/ observation procedure – There are several ways of preparation techniques, depends of aggregate state of the measured samples – KBr pellets, nujol, self-supporting pellets, KBr windows, gaseous cells. Representation of measurements results is possible in numerical data.
Remote access ability – through standard LAN interface. In real time the measurements can be accessed from the user at the remote location only through data streaming and offline but not through video streaming. The spectrometer can be operated indirectly from a remote location videoconference or interactive online software. This instrument can be accessed remotely by Remote Desktop Connection software that is part of WinOS.

C. Diffractometer

Diffractometer D5000 measures atomic spacing in crystals using diffraction of approximately monochromatic X-radiation. It can be used to characterize solid samples ranging in size from about 1 mm2 up to intact four-inch wafers. The radiation used usually is Cu Kα with a wavelength of 1.5418 A. The results are given in image form, by means of a binary graph (spectrum). The evaluated compounds and/or mineral species in the sample are reported in weight percentage. To the graph of intensity versus
angle of incidence (2 Theta), is added, in addition, the corresponding values of reticular intensities and distances (in Angstrom) of the different reticular planes (h, k, l) from compounds or present mineral species in the sample. In addition a report of conclusions is made.
Diffractometer can be used by investigations in the field of geology, mining industry, chemistry, and chemical industry. The analysis by X-rays diffraction, in powder samples, is used for the structural identification of all type of crystalline compounds of different nature: inorganic, organic and mineral.
Owner access polices description – The owner imposes some restrictions regarding access to the instrument operation – he does not allow direct users access to the instrument. In the case of services to companies the data are reserved. They are no any restrictions in respect to the period before placing observed data in public domain.
Measurement/observation procedure - There is a wide range of procedures of calibration, and parameter setting before running the experiment. . The initial conditions will vary depending on mode the instrument is in and the aim of the research, as well from the material, which will be analyzed. Moreover, some specific sample preparation is necessary prior the measurement process. The obtained by measurements results are represented as numerical data. Some safety restrictions are set up then working with radioactive materials - individuals must have specific training and must follow all the instructions and norms defined by the ones in charge of the laboratory. For preparation, mounting of the samples and for the measurement specialized personal is needed. In most cases one person does all these procedures. After sample mounting, which is manual the measurement process is fully automotive. Moreover, one sample can be analyzed

many times and several samples can be analyzed simultaneously as apparatus has the capacity to install a multiple sample holders if this is necessary.
Remote access ability – Diffractometer is connected with PC, which has standard network interface hardware – LAN interface card. Measurements can be accessed from the remote location in real time by data streaming and offline. A remote user can directly operate the apparatus. Before sending the results to the remote user, obtained row data need filtering.
Service and infrastructure requirements **–** Memory –512 Mb; Processing – 1 Gb;
Storage requirements – 20 Gb.
Network bandwidth, at which rate data need to be transmitted to remote users, is about 1 Mbits/second. There are no requirements for prioritized message transmissions, supporting critical remote control operations. After measurement offline data processing (including specialized software) is needed. The data taken by the D5000's control software are stored internally in a proprietary, binary format. To manipulate the data using anything other than Diffrac/AT it is necessary to convert them to an "interchange" format. Then it can be read into other analysis software. The needed storage space is 40 GB. No additional computational needs are pointed out.
Location of the instrument: Chili

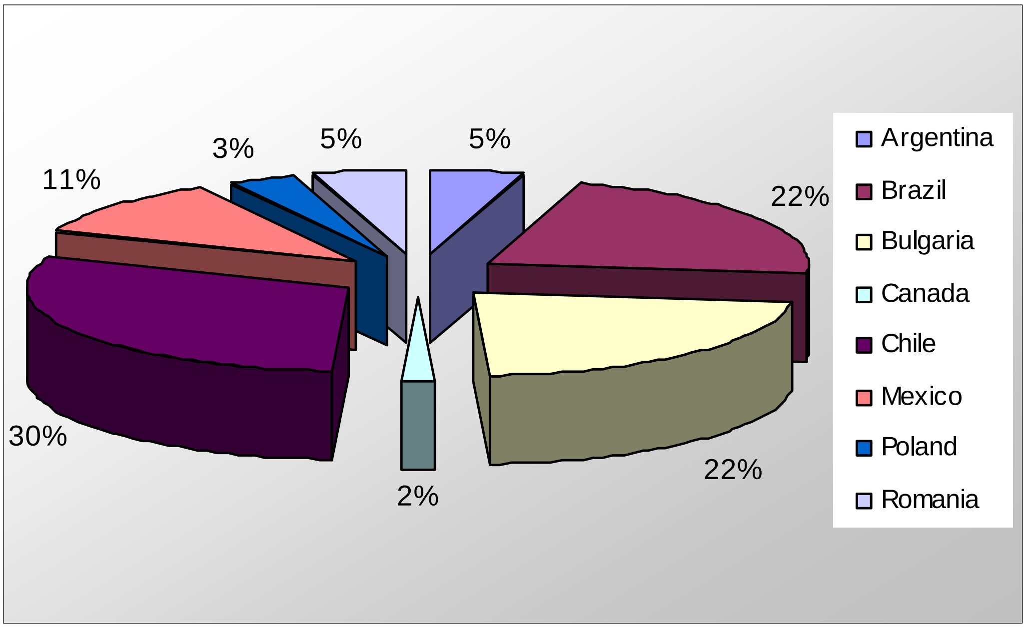

Figure 3. Country distribution of the RINGrid user community

IV. User requirements in material science

There are number of requirements pointed out from the user community in the material science. The most important of them are:
- Fast network speed
- Remote sample changing and positioning
- Full remotely control of the manipulator (for electron microscopes), including permission for manipulating remote equipments
- Visualization of the obtained data
- Preparation and pre-treatment of samples where the experiment is carried out
- Communication with the operator (audio contact)
- Use specific for the obtained results software to modelling different processes
- Possibility of following the equipment behaviour in real time
- Possibility for changing of the experimental conditions

- Possibility for preliminary training (including remote training)
- User friendly interface, easy to learn and use
- Treatment of the samples
- To test samples and conduct experiments on line
- Provide information about technical parameters of instrumentation
- Contact with an operator during the measurement
- To have same access efficiency as conventional (not remote) use**.**
- Knowledge on the instrumentation type, its software and technical parameters in advance
- Presence of operator
- Instruction of sample preparation
- High accuracy of measurements

V. Conclusions

Due to the relatively high price of the proposed instruments (in the range of 10 K-20 M Euro) as well as their geographical scattering and despite of the short time allocated for the present survey, the interest for remote access to high-level instruments from different European and non-European science communities can be determined as significant (Fig. 3).
As the remote accessible instruments are relatively new manner for scientific investigation, the users point in their practical experience several technical problems concerning the remote access – slow connection, firewall conflicts, lack of video contact with the operator of the instrument, etc. Following that, a new grid environment including remote accessed instruments as well as training centers and offline data processing services as support activities can be implemented. In this way, new opportunities for remote instrument access as well as reduction of user's and equipment owner's prices can be realized. On the Fig.4 the principal scheme of such kind of integrated environment is presented.

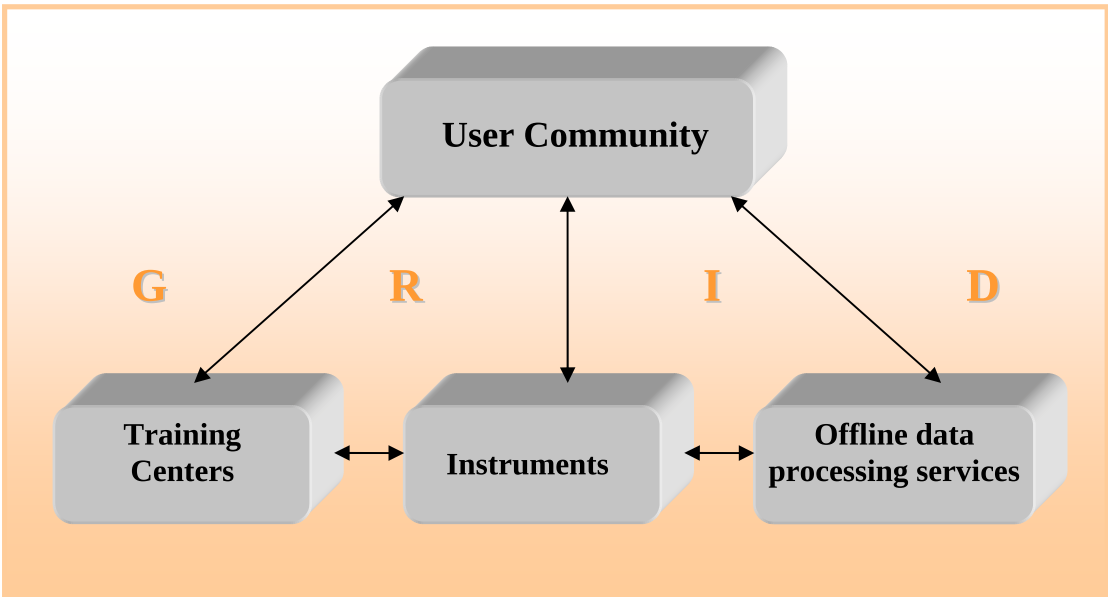

Figure 4. Schematic presentation of grid-embedded instruments and supporting services

Concerning the remote access of high-level scientific equipment, fast, reliable and secure network connections as well as user-friendly programming interfaces are requested from users of all scientific domains. Preliminary remote training activities are also highly demanded.

Acknowledgment

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