RINGrid contract no. 031891

WP2

Deliverable 2.3.

Formal Specification of requirements defined by potential end-users and instrumentation owners

Document Filename:	RINGRID_WP2_D2_3-2007-03-10 Formal_specification_of_requirements_defined_by_potential_end_users_and_instrumentation_owners
Work package:	WP2
Partner(s):	CLMC, TUI, UNAM, CLARA
Lead Partner:	CLMC
Document classification:	Public

Abstract:

This document describes formal specification of requirements defined by potential end users and instrumentation owners. The analysis is based on structured information received from IIFs and UIFs. The created in D2.2 task database (DB) containing all mentioned above data is used as analytical tool in this task. The user community requirements for remote access are evaluated and analysed. Deliverable D2.3. defines also the base for research and development concerning other work packages of the RINGrid. The user communities indicated in this issue are subjected to future project activities. The preliminary WP6 group's determination based on the received till now information in WP2 is done.

Delivery Slip

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Approved by	Norbert Meyer	PSNC	2007-04-13	

Document Log

Version	Date	Summary of changes	Authors
0.1	2007-02-28	Draft version -1	Valentin Ganev
0.2	2007-03-10	Draft version -2	Valentin Ganev, Yuri Kalvachev
0.3	2007-04-04	Draft version -3	Valentin Ganev, Yuri Kalvachev, Lubomira Macheva, Jana Harizanova
0.4	2007-04-11	Draft version -4	Valentin Ganev, Yuri Kalvachev, Lubomira Macheva, Jana Harizanova, Jesus Cruz, Romeo Ciobano
0.5	2007-04-13	Final version	Yuri Kalvachev

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1. Introduction

The opportunity of accessing expensive and sophisticated equipment plays a significant role in the scientific communities. This opportunity is very important also for research and development of industry sectors. The possibility of carrying out research through access to grid-embedded remote instrumentation, with the utilization of next generation high-speed networks, will even out their chances for the scientific progress. That is why the focus of RINGrid project is put on the creation of new possibilities for remote-instrumentation-based cooperation among scientists from different countries, working in the same or closely related scientific domains.

In D2.1 we pointed out the first and very important step in reaching this goal - collection and systematization of detailed information about expensive, rare and high-level scientific instruments suitable for the implementation of the idea of remote access and sharing the instruments with other groups of potential users in order to achieve optimization of equipment utilization. After that a database with the collected already information was created and thoroughly described in D2.2. This product could be considered as prototype of the future databases that should contain structured information concerning remotely accessible instruments, potential users and services integrated in the next generation grids.

The goal of this deliverable is the identification of user communities, which will benefit from the access to scientific instrumentations and the correlation of their requirements with the requirements of instrument owners. The diversity of user communities is very helpful in creating a solid base for obtaining reliable guidelines and recommendations. Till now, Instrument Information Forms (IIF) and User Identification Forms (UIF) containing detailed information about instruments and users were collected trough PDF- or/and web-based forms.

The process of collection of instrument and user information is considerably time consuming, but a very important task serving as basis for other workpackages. Very important point is that our survey includes international cooperation between European and Latin American countries (Mexico, Chile and Brazil) and this geographical diversity is substantial for investigation of user communities situated in different cultural and political environments. Important issue is the dissemination of the knowledge about the possibilities, which gives the remote access to the scientific instrumentations among potential users. Investigation of user requirements has crucial significance for the successful implementation of the idea of remote access. Only taking into account these requirements, it is possible to increase the awareness of benefits from using the next-generation remote instrumentation system among scientific and industrial communities of users.

2. Identification of user communities and their requirements

The process of identifying remotely accessed instruments and their potential user communities draws special attention to a number of specific fields of application, including: material science, astronomy and astrophysics, ecology, engineering and industry. The identification of user communities and their requirements for remote access usage of scientific equipment is complex process that includes the following steps:

- preliminary determination of target users groups (by IIFs);
- creation of specialized tool (UIF) for information collection;
- dissemination of the UIFs;
- systematization and analysis of the received information.

2.1. Description of the process of information collection

The preliminary determination of the target group of users was based on the information received by IIFs. The collected information for instruments suitable for remote usage already had their own user communities that accessed the instruments conventionally (i.e. no-remote), so this information was concerned as starting point for next more detailed survey. Furthermore, the majority of instrument owners have interest to use in their research other equipment (i.e. they are also users of high-level instruments) and in this case they are potential source of information regarding specification of requirements for remote access too.

As a next step, a specialized tool UIF (see Appendix I) for collection of information was created and disseminated among science community. The received in this way data were directly recorded in the created as a result of D2.2. task database and no additional data conversion was needed. In this way we simplify the analytical activities and reduce the time of information systematization.

All the WP2 partners were involved in finding the instrument owner and user communities by using their working contacts and collaborations and encourage both groups to fill in the IIFs and UIFs.

2.2 Creation and dissemination of User Identification Form

In order to identify the potential user communities interested in a usage of remote accessible instrumentations the User Identification Form was created as the most appropriate tool for collecting further information. This form consists of three main sections:

A. GENERAL

B. EXPERIENCE WITH REMOTE ACCESS EQUIPMENT

C. FEEDBACK.

The first section comprises details, connected with:

i) basic information about the user – position, affiliation, contact information;

ii) research field in which user works, years of experience and conventional scientific equipment, which he usually use.

The second section is the most important for analysing of User requirements. In this section the users should answer if they have used expensive or rare scientific equipment remotely, if they intend to do this and the circumstances under which, they will be interested in using remotely accessible instruments. Other group of questions in this section gives the answer how close is the user to the idea of remotely accessible instruments:

- about their belonging to an existing user group working on expensive scientific equipment;
- about availability of a national remote access equipment initiative to scientific instruments in their country;
- if user institution provides some equipment for remote access or has plans to do this.

The third section gives the possibility for some additional feedback.

Similarly with IIF, this way of collecting of the information is convenient for the next work, because of:

- unification of the collected information;
- exhaustiveness of the data;
- flexibility of information treatment;
- possibility for statistical processing of the collected data.

2.3. *Description and analysis of the information collected through UIFs regarding the end user requirements*

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 of science communities for remote access to these high-level instruments can be determined as significant. In the short period provided for information collection by UIF tool (about a couple of months), more then 60 UIFs from European and non-European researchers from different institutions and research areas are received. The majority of them are with sufficient experience in the corresponding fields of their work (37 Professors, 17 Researchers and 6 Graduated and Postgraduate Students), so the collected information is concerned as relevant. The data regarding country and regional distribution of researchers participated in the UIF surveys are presented on Figs.1 and 2.

In most cases the forms are filled in after personal contacts with the researchers where some details and objectives of the idea for remote accessible instruments are explained and discussed.

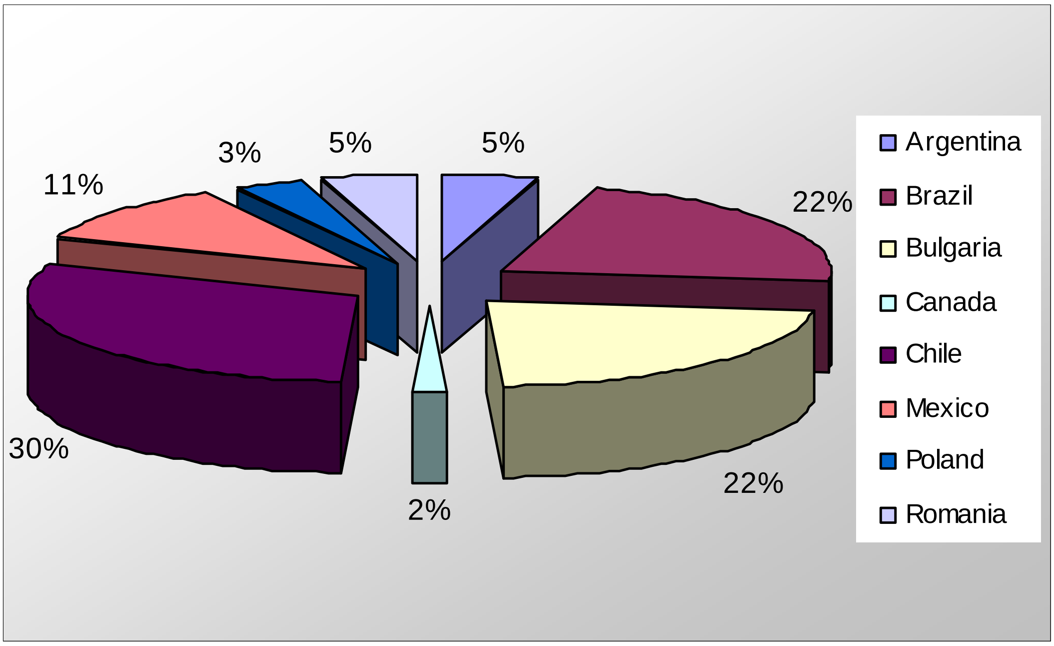

Figure1. Distribution of the received UIFs by countries

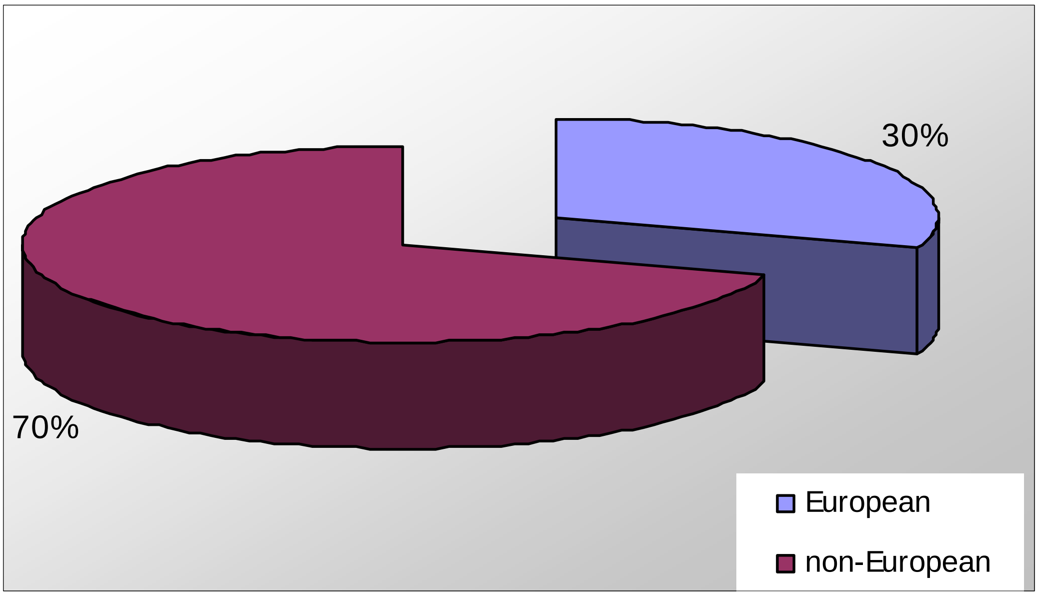

Figure 2. Distribution of the received UIFs by regions

The received data show that users' interest for remote accessed instruments can be defined in few domains shown on Fig.3. As was pointed out in D2.1 the number of the preliminary identified domains is considerably reduced. The reasons of this is that the plotted on Fig.3 domains cover larger scientific fields, which use the same instrumentation. A good example along this line is material science, which includes Biology, Chemistry, Physics, Geology, Ecology and interdisciplinary sciences. Furthermore spectroscopy can not be perceived as a separate domain according the RINGrid project purposes.

As is seen on Fig.3 the leading field of interest of the users is Material Science, followed by Engineering, Earth and Computer Sciences. In fact, almost all of the pointed instruments in Material and Earth sciences can be used in both fields, so these groups can be combined for large number of investigation purposes.

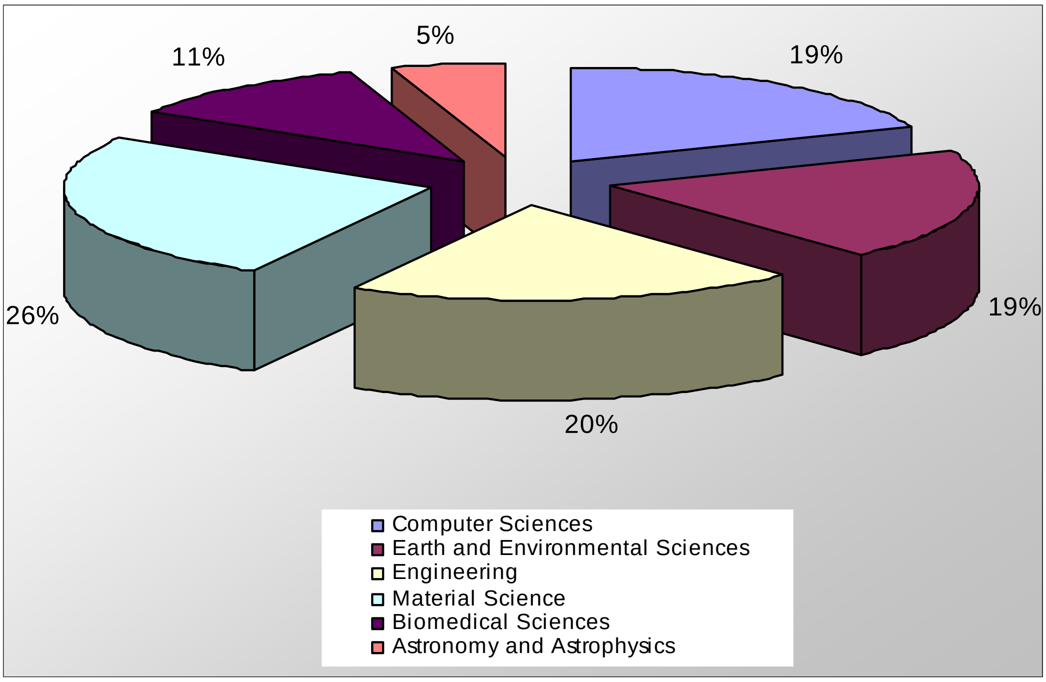

Figure 3. Distribution of received UIF by research fields

According to the classification referring to the instrument cost, described in our D 2.1 report (p.15-16), the expected access distributions are presented on Figs.4 and 5.

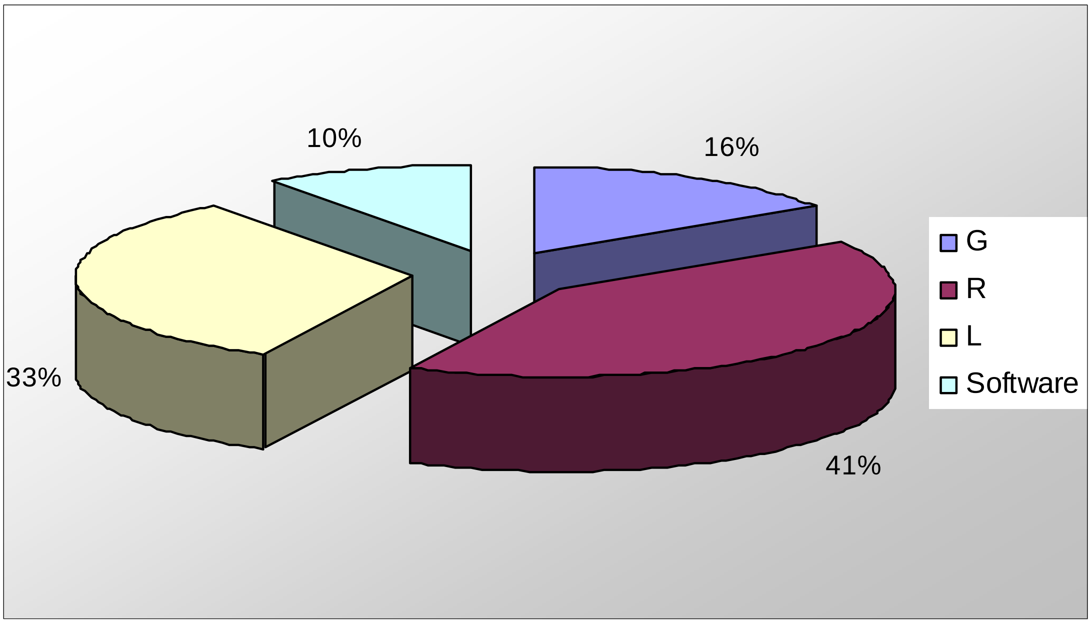

Figure 4. Distribution of the instruments used not remotely till now (Question 12 – Appendix 1)

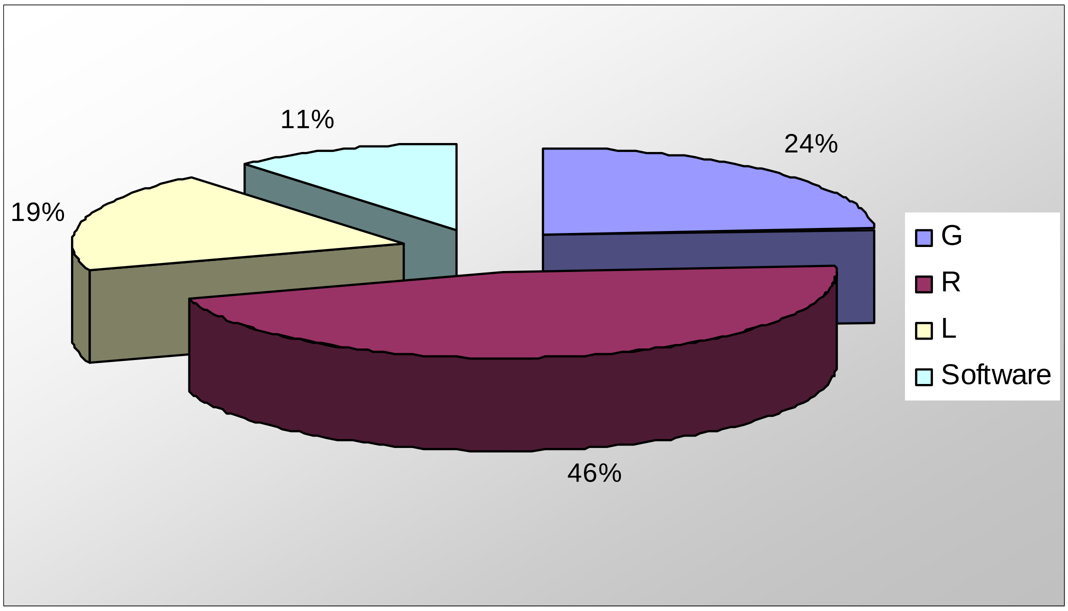

Figure 5. Distribution of instruments by the intention of users (Question 14 – Appendix 1)

They show that the R-group (Regional) of instruments followed by G-group (Global) and L-group (Local) is preferred from users for future scientific investigations. In most cases for particular user, all three groups of instruments are checked in the UIF. It could be explained by the reason that the preparation of experiments for large-scale facilities (G-type) in most cases needs preliminary use of R, L or of both types of equipment.

On Fig.6, circumstances under which the user will be interested in using remotely accessible instruments are pointed out. The preferred form of remote access to instruments is the "scientific collaboration" and no dependence regarding particular research field is find out.

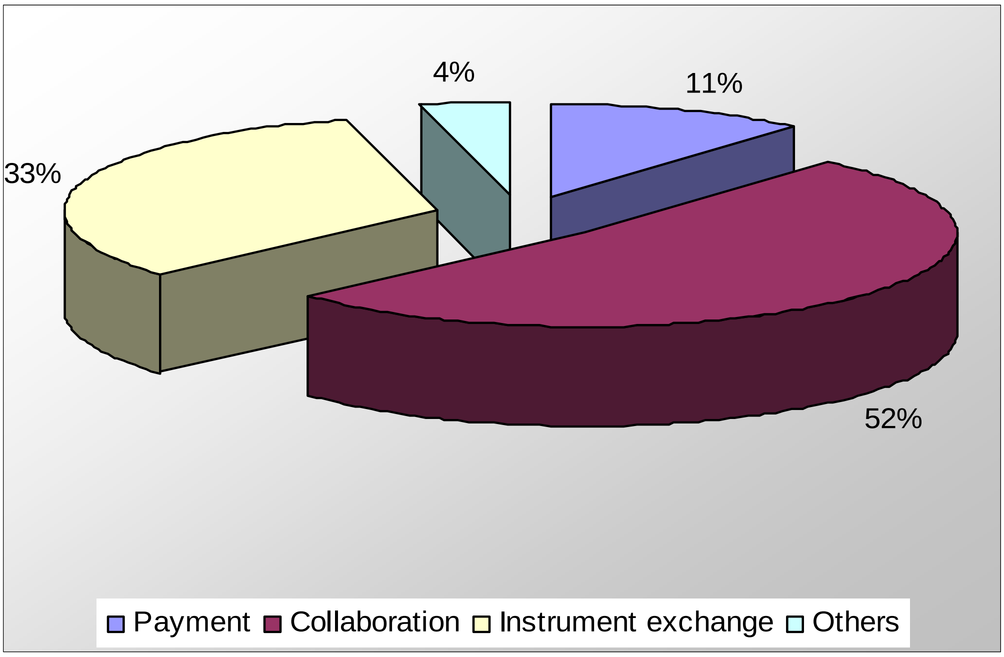

Figure 6. Presentation of the circumstances under which the researchers prefer to use remote accessible instruments

As the remote accessible instruments are relatively new manner for scientific investigation, the users point in their answers several technical problems concerning the practice of remote access – slow connection, firewall conflicts, lack of video contact with the operator of the instrument. From 17 interviewed researchers, which already have used remotely some kind of scientific equipment only 5 answer that they have found no problems.

The significant part of the experience for remote usage of instruments comes from remote software usage based on cluster technology. In small number of cases, the remote access technology is partially implemented in the fields of astronomy and material sciences (i.e. in some telescopes and synchrotron beamlines). Despite the lack of considerable amount of experience, different technical requirements for remote instrumentation access depending on users' domain of application are find out. In the field of material science, the adequate sample manipulation from remote site is leading, while in astronomy the possibility for transfer of large amount of visual information in real time is preferred. 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. Following that, a new grid environment including remote accessed instruments as well as training centres and offline data processing services as support activities can be implemented. On Fig.7 the following principal scheme is proposed.

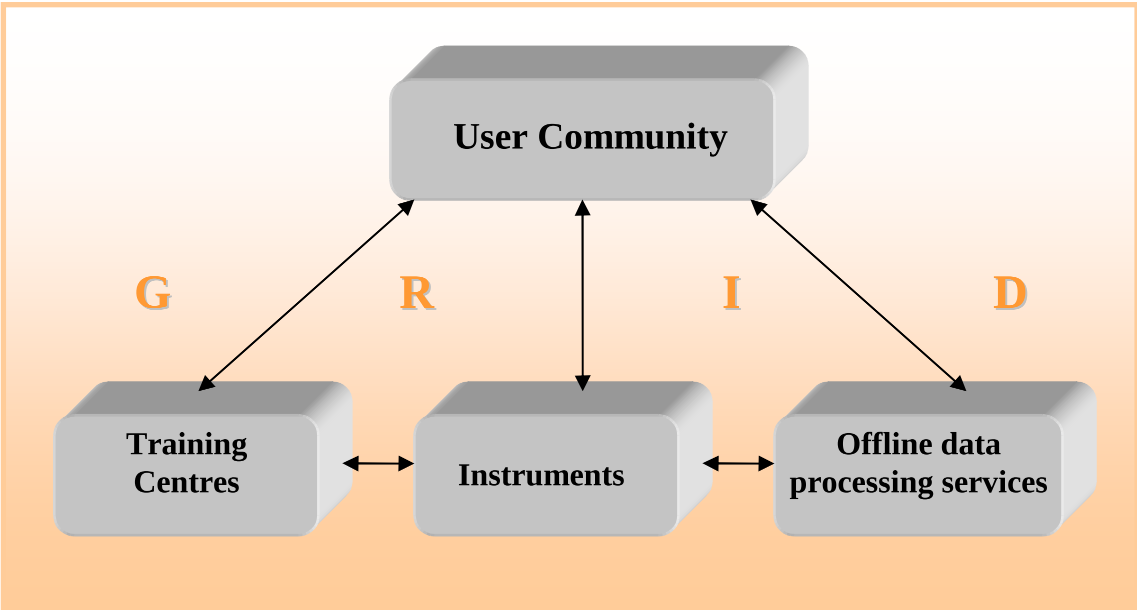

Figure 7. Schematic presentation of grid-embedded instruments and supporting services

Other information relevant to requirements for remote accessed instruments is received from other sources (i.e. other projects, personal contacts with researchers in different fields, etc.) is also taken into account and they do not contradict with data and analysis presented above.

3. Data correlation and analysis of the information from IIFs and UIFs in respect to the requirements of instrument owners and end users

After systematization of the information about the expensive and rare scientific instruments and their owners and users, suitable for introducing the idea of remote access to expensive instruments, assessment of the collected information that meet the expectations of users and owners was done. This is crucial to the success of the Project as well for the creation of worked remote instrumentation systems. For achieving this goal we analyzed all the collected information related to the possibilities for remote usage of the instruments:

- data about technical parameters of the collected instruments, concerning the main way of equipment use;
- restrictions of the owners connected with the access to the instrument;
- all technical details connected with the measurement process - sample preparation and manipulation during the experiment, measurement conditions, and representation of the results;
- possibilities for remote access as well as the level to which the instrument can be operated remotely, including the way of communication with the operator of the instrument (if any), as well as requirements for visualization renderings;
- infrastructure requirements for data processing and data transfer to the user site.

Scientific communities as potential and actual users of remote instrumentation systems have a substantial influence on the project outcome, as they are the most important source of potential requirements and suggestions concerning remote access to various types of scientific instrumentation. The requirements of the users are taken into consideration, depending from one side on the peculiarities of their research, and on the other site on their already gained experience.

The correlation and analysis of the information from IIFs and UIFs is done in the particular domains by groups of instruments.

3.1. Assessment of the specifications and requirements of instrument owners and end users for the Material Science domain

The equipment of Material Science domain is one of the most preferred by the users - 57% as can be seen from Fig. 8.

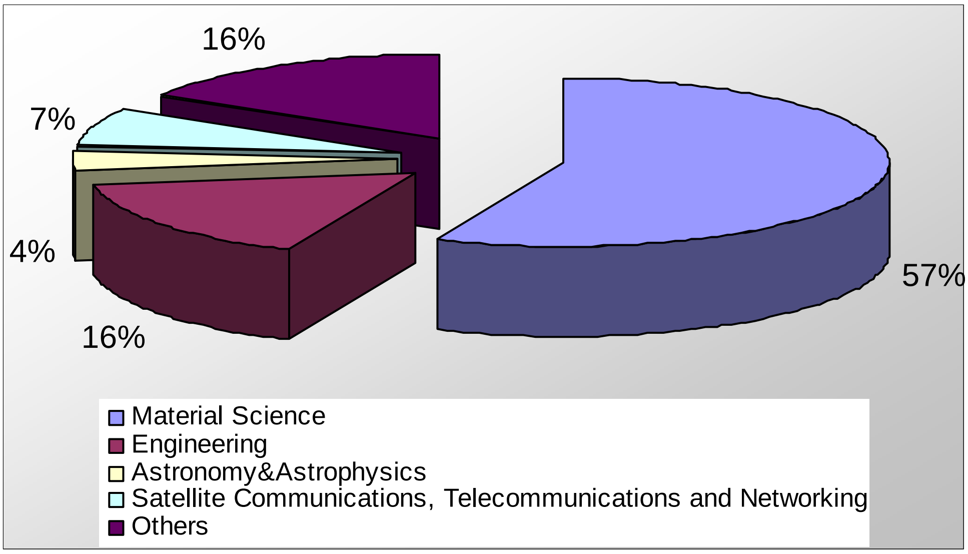

Figure 8. Distribution of equipment pointed out from different users groups

In the Material Science domain several groups of instruments could be distinguished which requires similar sample preparation as well similar technical conditions of analysis, representation and transfer of the obtained results.

- Microscopes - Scanning Electron Microscopes, Transmission Electron Microscope, Laser Scan Microscope;
- Spectroscopic equipment – IR Spectrometer, UV-Vis Spectrometer, NMR Spectrometers, Atom Absorption Spectrometer, ICP (Inductively Coupled Plasma Spectrometer), Gas Chromatograph.

3.1.1. Microscopes

Scanning Electron Microscopes

All scanning electron microscopes 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. The disposed for remote access electron microscopes are with different analytical possibilities and equipped with different software, so that they can be used also for chemical mapping, high resolution crystallographic analysis, phase identification, texture analysis, orientation and deformation mapping. This enable they use in a broad research areas – inorganic chemistry, chemical physics, solid state physics, geology, biology, civil engineering, electric engineering, microfabrication, archaeology, numismatics, quality control in metallurgy, ceramics, and glasses. At the present, some of the microscopes are used by researchers from different countries in Latin America – Chile, Argentina, and Brazil.

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. This is also the wish of the users they pointed out in the UIFs.

All owners indicate that it is impossible to use the microscopes in configuration with other equipment situated in another location. Principally this is not necessary for this group of microscopes. It makes sense only for Transmission electron microscope studies, but in these cases TEM- studies are leading and the samples should be prepared in a different way.

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 operator does this always, even though the remote user can do it if the system is fully automotive.

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.

In all cases specialized personal is required:

- for the measurement process;
- for preparing the sample and its mounting.

Remote access ability – Most of the potential users point out that they want to observe the measurement process. In this connection all 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 telephone, videoconference or interactive online software (i.e. LabView, VNC). One of the owners does not permit directly operation of the microscope by a remote user, possibly because of high cost of the instrument.

Service and infra-structure requirements in terms of computational requirements, storage requirements and requirements for streaming media (audio and video), multicasting, requirements for interactive access to the instrument are different for particular microscope owners:

- Memory – from 512 to 1024 Mb;
- Processing - 1-3 Gb;
- Storage requirements – 1- 80 Gb;
- Requirements for streaming media (audio and video) are: high priority QoS;
- One user at time can access streaming media produced by observations;
- Web cam needed.

Other requirements - offline data processing and storage space requirements referred only to instrument owners – in all cases specialized software is needed and only one of the owners has pointed out that 40 Gb are required storage space for the obtained information.

In all cases by dataset loss the measurement must be repeated.

Transmission Electron Microscope

The placed at disposal transmission electron microscope is equipped with holders allowing single and double tilt of the sample stage and can operate by low temperature that is important for some kind of samples that can be destroyed under the electron beam (i.e. biological). The microscope is equipped with TV-rate Camera with Image transfer, as well as with multi scan CCD camera. The availability of EDS Spectrometer allows the chemical composition of unknown phases (substances) to be determined. All devices with which the microscope is equipped allow its usage in inorganic chemistry, chemical physics, geology, solid-state physics, biology, catalysis, studying semiconductors and thin films etc.

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.

Measurement/ observation procedure – The owner requires the samples to be prepared by the user, because it is specific for each sample. All measurement parameter settings are controlled by analogical interface. Measurement procedure, sample preparation and mounting the sample must be done by specialized personal. The manipulation of the samples (insertion and ejection) can be done manual, but the movement of the sample is automatic. More than one experiment can be performed in one sample. All measurements are performed in vacuum.

Representation of measurement results – It can be done as numerical data as well as images.

Remote access ability – The PC connected with the microscope has standard network interface hardware – LAN interface card. It is point out that measurements can be accessed from the remote location in real time by data streaming, video streaming and offline. A remote user can not directly operate the microscope, but the user can indirectly control the remote instrument through communication by telephone, videoconference or interactive online software.

Following *Service and infrastructure requirements* are point out:

- Memory –1024 Mb;
- Processing - 3 Gb;
- Storage requirements – 80 Gb;
- Requirements for streaming media (audio and video) are: high priority QoS;
- One user at time can access streaming media produced by observations;
- Web cam needed;

The requirements for visualization renderings are - online for interactive analysis; offline for prioritized message transmissions, and for supporting critical remote control. Network bandwidth at which rate data need to be transmitted to the remote users is 8 Mbits/sec.

For analyzing of the obtained results, the images can be offline processed and appropriate Image Software program can be used. No additional requirements are indicated. In case of dataset loss the measurement must be repeated.

Confocal Laser Scan Microscope

The microscope is provided with three lasers (488, 583 and 633nm) with system of processing and analyzing images. It is used for obtaining high resolution images and 3-D reconstructions of medical science (microbiological objects in transmitted light and fluorescence - normal cells and histological pathological weave cuts), in imunocitochemistry for studying molecules marked with fluorescent antibodies, in pharmacy, agronomy and chemistry. In confocal fluorescence, it is possible to make determinations of molecules dynamic and obtain series of images through time with a resolution of 1.5 milliseconds. Also it is possible to determine the distribution of substances in different planes from the cells by means of the obtaining of series of images in different optical cuts, having the possibility of integrating a single images and obtaining a three-dimensional reconstruction that can be animated.

Owner access polices description – Except training before using the microscope no other restrictions are put from the owners. As other microscopes Laser Scan Microscope can not be used in configuration with other equipment situated in different location.

Measurement/ observation procedure – There is a wide range of setting procedures before the measurement/observation - moving the filter block, mount the sample, focus, and center your specimen in the eyepieces, setting parameters from LSM software. Microscopic observations and analyses require preliminary special preparation technique to be used. The preparation of the samples, their mounting and the measurement process requires specialized personal. Sample mounting as by first examined microscopes is manually and all other manipulations are automatic. They could be performed several experiments in one sample but not simultaneously at the same time.

Representation of measurement results – In contrast to the Scanning and Transmission electron microscopes by Laser Scan microscope the observed results can be represented in several ways – as numerical data, as images, as video, and in a complex manner.

Remote access ability – The network connection of the microscope is realized as by Scanning and Transmission microscopes. In real time the measurements can be accessed from the user at the remote location only by data streaming and offline but not by video streaming. The microscope can be operated indirectly from a remote location by telephone, videoconference or interactive online software, but it the user will not have the ability to operate directly the instrument. The row data are filtered before sending to the remote site.

Service and infrastructure requirements – the requirements for realization of remote usage of the Laser Scan Microscope are not high:

- Memory –512 Mb;
- Processing - 1 Gb;
- Storage requirements –20Gb;
- Requirements for streaming media (audio and video) are not pointed out;
- One user at time can access streaming media produced by observations;

As no visualization is foreseen no requirements for visualization renderings are described. The requirements for the network bandwidth at which rate data need to be transmitted to the user site are 1 Mbits/sec. Storage space expected to been allocated for obtained row data is 20

GB. The owner of the microscope points out that dataset loss can be quite critical, therefore data replication are expected.

3.1.2. Spectroscopic equipment

IR 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. Solids, liquids, pastes, films, gases can be investigated with the instrument at room temperature and normal pressure. This method gives information about bond vibrations in the molecules, so with it investigation of bond types and functional groups in the molecules can be done, as well as qualitative and quantitative analysis of the samples. This makes the instrument applicable in all fields of industrial and scientific chemistry, biology, ecology, geology, mineralogy, catalysis, petrol chemistry, pharmacy, food, dyes, pigments, etc.

Owner access polices description - At the present, researchers in Bulgaria in the field of mineralogy and catalysis use this instrument. It is equipped with software so in this respect the spectrometer is suitable for remote access. Moreover, the owners of this spectrometer do not point out any 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, but it is easy for operation and user friendly.

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 – 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 by telephone, videoconference or interactive online software. This instrument can be accessed remotely by Remote Desktop Connection software, that is part of Windows OS.

UV-Vis spectrophotometers

The disposal UV-Vis spectrophotometers (Cary 100 and Cary 1E) are produced by company Varian. The instruments work in wavelength range 190-900 nm with limiting resolution 0.189 nm and wavelength accuracy 0.02-0.04 nm. The equipment is double beam, dual chopper, ratio recording PC-controlled spectrophotometer, which is equipped with Czerny-Turner monochromator and R928 photomultiplier based detector system. The sources of light are tungsten halogen visible light and deuterium arc for ultra-violet light. The fields of application of the instrument are organic and inorganic chemistry, chemical physics, material science, and solid-state physics. The Cary 100 is the new analog of Cary 1E.

Owner access polices description - At present the instrument (Cary 100) is used in the field of geology and mineralogy. The owners of this spectrophotometer do not point out any restrictions, regarding access to the instrument operation, access to the obtained data and about the time before transferring data to the user site. The user can fully take part and observe the analytical process.

Measurement/ observation procedure – Calibration and initial instrument checking procedure is automatic. Measurements parameters setting are controlled by PC with Windows program (DOS for Cary 1E) interface Cary WinUV Analysis Pack. Sample must be fit in the sample holder. The single measurement takes 20 minutes and representation of measurements results is in numerical data and can also be presented graphically.

Remote access ability – In real time the measurements can be accessed from the user at the remote location through data streaming and offline. The spectrophotometer can be operated indirectly from a remote location by telephone, videoconference or interactive online software. This instrument can be accessed remotely by Remote Desktop Connection software, that is part of Windows OS.

Gas Chromatograph

Gas chromatograph included in the RINGrid project is produced by company Varian. The model is GC-3800, produced 2000 year. The instrument is PC-controlled, equipped with flame ionization detector which works in the temperature range – from – 99 to +450° C. The temperature in the column compartment is program controlled. There is an electronic control of pressure and flow rate. Detected concentrations are up to 10^{-8} M. With such instruments qualitative and quantitative analysis of liquid and gaseous mixtures can be made and can find an application in many fields of industry and science – control of quality of processes, analysis of organic compounds, presence of ionic traces in natural water, food insecticide remainders, plastics, analysis of stable volatile compounds, hydrocarbons, perfumes, etc.

Owner access polices description - The owners of the Gas Chromatograph point out restrictions, regarding access to the instrument operation – knowledge of the efficient use, base knowledge of the method. For the data generated by experiments of the user, the limit will be the one established by the grid structure. For the data generated previously by the owner of the equipment, which can be required with intentions of comparison or using of reference, the access will be defined to criteria of the owner.

Measurement/ observation procedure – The equipment has a preliminary calibration. If the experiments require reference parameters, this needs to be executed previously and to obtain required data. The samples should be placed in the instrument. The single measurement takes 30 minutes and representation of measurements results is in numerical data and can also be presented graphically.

Inductively Coupled Plasma Spectrophotometer (ICP)

The producer of disposed ICP spectrophotometer is Jarrel Ash and year of manufacture is 2 000. It is suitable for determination of concentration of over 70 chemical elements in solids and liquids – organic and inorganic. Capacity is analysis of 18 samples simultaneously. The equipment can find very wide area of application – analysis of ground, water and air samples, characterization of alloys, kinetic of solid reactions.

Owner access polices description - The owners of the ICP Spectrophotometer mark restrictions, regarding access to the instrument operation – knowledge of the efficient use, base knowledge of the method. For the data generated by experiments of the user, the limit will be the one established by the grid structure. For the data generated previously by the owner of the equipment, which can be required with intentions of comparison or using of reference, the access will be defined to criteria of the owner.

Measurement/ observation procedure – The equipment has a preliminary calibration. If the experiments require reference parameters, this needs to be executed previously and to obtain required data. The samples should be placed in the instrument. Once the sample is placed in the instrument, the manipulation is completely automatic. The single measurement takes 30 minutes and representation of measurements results is in numerical data.

Nuclear Magnetic Resonance Spectrometers (NMR)

Two of NMR spectrometers included in the RINGrid project are relatively old – produced 1990 (Varian Unity 300) and 1991 (Bruker AC-250P). With Bruker AC-250P NMR spectrometer analysis of nuclei between the frequencies of resonance of 31P and 109 Ag as well as 1H and 13C can be done. Varian Unity 300 NMR spectrometer is equipped with two probe heads – indirect detection 1H with range 31P-15N and broadband 1H. Both probe heads can work in the temperature range -150 +200° C.

Other two NMR spectrometers are produced by Bruker and they are from the series "Avance". They are high performance digital spectrometers. Their probe heads give possibilities to work in large range of elements and temperature and they are with automatic matching and tuning. All disposed NMR spectrometers are suitable for investigation of liquid samples. The fields of application of these instruments are organic chemistry, physics, biological science, pharmacy, and dye industry.

Owner access polices description - The owners of the NMR spectrometers indicate restrictions, regarding access to the instrument operation – the users must be trained and authorized to use the instruments. For complex experiments specialized supervision is required. The user can fully take part and observe the analytical process.

Measurement/ observation procedure – There is a wide range of preparation procedures with different types of solvents depends from complexity of experiments. The measurements results are presented in numerical data and manipulation during the measurements are automatic.

Atomic Absorption Spectrophotometer

This instrument provides accurate quantitative analyses for metals in water, sediments, soils or rocks. It can be used also for analyses of trace quantities of metals in foods, natural and industrial probes, medical and pharmaceutical specimens. Samples are analyzed in solution form, so solid samples must be leached or dissolved prior to analysis. Typically, the technique uses a flame to atomize the sample, but other atomizers such as a graphite furnace are also used. Three steps are involved in turning a liquid sample into an atomic gas:

- Desolvation – the liquid solvent is evaporated, and the dry sample remains
- Vaporization – the solid sample vaporizes to a gas
- Volatilization – the compounds making up the sample are broken into free atoms.

It is pointed out that the instrument can not be used in configuration with other equipment situated in different location.

Measurement /observation procedure – Prior to be placed in the instrument samples need specific preparation. The material is prepared depending on its origin. This can be done from the remote user or in the laboratory immediately before the analysis. Besides, there is a range of calibration procedures and parameter setting before running the experiment. If the experiment requires reference parameters, they must be executed prior to receiving the resulting graphs and to obtain the required data.

The measurement process, sample preparation and sample mounting (insertion and ejection) are made by specialized personal. Ones the sample is mounted in sample holder, the process of the analysis is automotive. It is no possibility to install a multiple sample holders and to perform more than one experiment in sample at time. The analytical results can be represented as numerical data and graphic (as image). No video is necessary.

Remote access ability – The equipment has a computer connected to the network through an interface fast Ethernet. Measurements can be accessed from the remote location only offline – no possibilities for data and video streaming are checked. The instrument can be indirectly controlled by the remote user, but not to be operated directly. The obtained row data must be filtered before sending to the remote site.

Service and infrastructure requirements: The requirements for realization of remote usage of the Atomic Absorption Spectrograph are:

- Memory –512 Mb;
- Processing - 100 Mb;
- Storage requirements –10Gb;
- Requirements for streaming media (audio and video) are not pointed out;
- One user at time can access streaming media produced by observations;
- No requirements are pointed out having an opinion on the interactive access to the instrument.
- Streaming requirements - Although access in real time to the measurements cannot be held, the results can be obtained offline. It is suggested that the equipment that will be

used for the media flow, counts on the corresponding suitable reproducer: audio and video.

10 users are expected to access streaming media produced by the observation. Requirements of software for the remote display and execution of the remote programs client are VNS and LabVIEW. Visualization can be realized online and offline. Network bandwidth, at which rate data need to be transmitted to remote users, is 1 Mbits/second.

No requirements for prioritized message transmissions, supporting critical remote control, operations or alarms are set.

The obtained results do not need any offline data processing. For storage of data 10 GB space is necessary. To prevent data loss the results from the observation must be always kept in digital format. If the file is lost, the user has to repeat the experiment, with the corresponding cost of the samples that were used. No additional computational needs are pointed out.

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 millimetre square up to intact four-inch wafers. The radiation used is Cu Kα with a wavelength of 1.5418 Å. 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 Θ (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. Regarding restrictions about access to the observed data in the academic and research use the investigator has the exclusive right of use of the collected data. 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. The instrument can not be used in configuration with other equipment situated in different location.

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 analysed. Moreover, some specific sample preparation is necessary prior the measurement process. For the analysis a minimum amount of 1 to 2 grams of sample is required, free of humidity and with inferior granularity to 65 μm. There are also two techniques for mounting samples. Centimetre-sized pieces are usually mounted on clay in a plastic sample holder available in 406 Cory Hall for a nominal charge. Whole wafers and large pieces of wafers are more conveniently held in a three-jawed clamp. Clay mounting is carried out placing a small ball of clay in the well of the sample holder, centre your sample on top and press the sample into the clay using a flat, clean surface. The goal is to make the top surface of your sample perfectly even with the top surface of the sample holder. Ideally the clay should be completely hidden by the sample. It pays to be fussy about mounting; tilt in the sample that's too small to see can easily shift peaks enough to make them very hard to find.

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 1 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 analysed 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. No video is needed in this case. A remote user can directly operate the apparatus, but the user can not indirectly control the remote instrument. Before sending the results to the remote user, obtained row data need filtering.

Service and infrastructure requirements – The necessary computational requirements are:

- Memory –512Mb;
- Processing - 1 Gb;
- Storage requirements – 20 Gb;

- There are no requirements for streaming media (audio and video) Web cam is also not necessary;
- No visualization is necessary during the measurement process;
- Network bandwidth, at which rate data need to be transmitted to remote users is 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. Very often spreadsheet programs are used to prepare graphics for use in publications. The export format is called "Universal" and is essentially ASCII text. Header information contains plain-text information on machine parameters (tube voltage/current, starting angle, step size, number of steps, etc.) followed by a list of numbers representing count rates at each step.

The needed storage space is 40 GB.

After data acquisition is performed on the sample, then if a data file is lost, it can be quite critical and the measurement must be repeated. No additional computational needs are pointed out.

Brazilian Synchrotron Light Laboratory (LNLS)

- Brazilian Synchrotron Light Laboratory (LNLS) is equipped with 11 beamline stations:

- D03B - MX1 Protein Crystallography beamline.
- D06A - DXAS Beamline dispersive X-ray absorption spectroscopy.
- D11A – SAXS small angle X-ray scattering
- D08A - SGM spherical grating monochromator beamline VUV and soft X-ray spectroscopy
- D04A – SXS soft X-ray spectroscopy beamline
- D05A - TGM Toroidal grating monochromator beamline for vacuum ultraviolet (VUV) Spectroscopy
- D04B - X-ray absorption spectroscopy beamline
- D12A - XRD1 X – ray diffraction beamline

- D10A-XRD2 high resolution X-ray diffraction beamline
- D10B-XPD Polycrystals X-ray diffraction beamline
- D09B - XRFX-ray fluorescence beamline

Although for all 11 stations 1 summary Instrument Information Form is filled in, many of the users have an intention to use namely some of the Synchrotron Radiation Stations in their research. Therefore, we include briefly description of the beamlines of the LNLS with the comments and requirements of potential and actual users of this equipment. Another reason to include LNLS in our analysis is that at some stations remote access is already implemented and may be used as a model.

The beamlines of LNLS collectively span the photon spectrum from 10 eV to more then 10 eV. Each beamline has a particular purpose and the correspondent set of scientific instruments to cover its fields. The set of computer-managed instruments consists of motors, devices and detectors.

Owner access polices description – As an important restriction regarding instrument operation on the end stations, the owners of LNLS point out the need of training/assistance of each visiting researcher by the physicist responsible for each beamline. No restrictions are set regarding access to the obtained data –LNLS grants to the researcher exclusive rights of the acquired data and the results will be realized to scientific publications.

Measurement/observation procedure – There is a wide range of procedures of calibration and installation, according to the specific purpose of the beamline and the particular experiment performed. Samples are prepared for experiment in a specific way depending on the material, which will be studied, and the particular goal of the investigation. The obtained results are presented as a numerical data and as images and video. Prior to the experiment all visitors must have received safety training and must wear an individual dosimeter badge. At all end station beamline a specialized personal is needed for mounting and measurement of the samples. During the measurement sample manipulation is automatic. Most of the sample holders are motorized. The Synchrotron equipment is a good example for capability for performing more than one sample per time.

Remote access ability – Remote access is realized through Ethernet 10/100. However, the measurements can be accessed from a remote location in real time – by data- and video streaming, as well as offline. The instruments at the LNLS facility are not disposed for indirect control for the users, but it is pointed out that the instrument could be directly operated by a remote user.

Service and infrastructure requirements are as follow:

- Memory –512 Mb;
- Processing -~ 1Gb;
- Storage requirements –40Gb;
- Requirements for streaming media (audio and video) - video streaming may not be necessary. Collaborative tools like VNS could be enough.
- One user at time can access streaming media produced by observations;
- No requirements are pointed out having an opinion on the interactive access to the instrument.
- Network bandwidth, at which rate data need to be transmitted to remote users is 10 Mbits/second

The obtained by the experiments results are in plain text, images and binary CCD files. They need additionally offline data processing. 40 Gb is the space pointed as a storage space.

Data set loss can be quite critical. Multiple acquisitions are usually performed on the same sample, to improve statistics. If a data file is lost, that could not represent a serious loss. In other cases loosing just one file could damage whole series of data, for example a micro-tomography experiment.

3.2. Assessment of the specifications and requirements of instrument owners and end users for the Engineering domain

The technical analysis of information from Users and Owners from Engineering group according IIFs and UIFs received in this field of application can be summarized as follow:

- demand for use of a common browser to remotely access an application
- request for an adaptive system not using sophisticated hardware, or using wide commercial versions of DAS and DSPs
- request for an adaptive system not using sophisticated software, or using wide commercial versions of PC-instrument communication software (e.g. TCP/IP + CGI)
- if possible, parallel access to multitask communication facilities, permitting e.g. to beginners to be tutored by more experienced ones.
- if possible, accept of adaptable virtual instruments in order to operate the instrumentation program, remotely control the selected hardware, analyse data, directly overtake already displayed models or results

- other individual requests: possibility of concurrently work in the same project/task, platform independence, extensibility and scalability, to keep track on the interactions and results
- environment availability not to require high-end workstations, making the remote access affordable for small universities, training centres, independent specialists, NGOs, SMEs, or for centres operating in developing countries.

The system features high performance dielectric, conductivity, electrochemical, impedance and gain phase measurements in the frequency domain. The system is modular and all test interfaces for impedance measurement offer in addition high general purpose performance like highest accuracy and ultra wide impedance and frequency range.

Permittivity, conductivity and impedance of nearly all materials or components including special functions can be measured broadband and over a wide temperature range without changing sample geometry or sample cells.

Broad frequency range $3 \cdot 10^{-5}$ .. $2 \cdot 10^{7}$ Hz including low frequencies for characterization of dielectric relaxations, electrochemical and high impedance effects.

Ultra wide impedance range 10^{-3} .. 10^{15} W (18 decades) covers range from conductors to best isolators.

Ultra wide capacity range 10^{-15} .. 1 F allows broadband measurement of smallest capacities down to 1 fF.

High phase $2 \cdot 10^{-3}$ ° and loss factor tan(d) absolute accuracy $3 \cdot 10^{-5}$ for low loss dielectric materials and isolators broadband characterization.

Supports a series of test interfaces for customized applications with special functionality.

Supports non linear Dielectric, Conductivity and Impedance Spectroscopy or gain phase measurements in combination with all test interfaces.

Supports high speed measurements rates up to 157 impedance - or 210 gain phase measurement points per second via the GPIB port for online monitoring of time variant processes in the 5 ms range by mainframe option F.

New test interface concept with adaptive system functionality and single port operation by high level GPIB commands for easy and straightforward implementation in own programs or existing measurement set-ups.

Automatic self calibration and diagnosis by user cancels out long term internal drift and verifies functionality.

Precision digital frequency response analyzer up to 40 MHz for two channel gain phase measurements with 0.001° phase - and 10^{-5} in amplitude resolution included. Operates like a broadband locking amplifier with two channels, extended accuracy and frequency range.

Control software for turnkey calibration, operation, data evaluation, 2- and 3- dimensional graphical representation including non linear spectroscopy.

The additional temperature controller has four circuits controlling the sample temperature, the gas temperature, the temperature of the liquid nitrogen in the dewar and the pressure in the dewar. In addition the vacuum pressure is measured. It allows a very fast, precise and save operation, which is required for automatically driven systems. Even if sensors would fail or the liquid nitrogen dewar becomes empty, the system will automatically shut down in order to protect itself and the sample. Features:

High precision turn key temperature control system

Temperature range -160 ... 400 °C

Temperature ramps from 0.01 .. 30 °C/min

0.01 °C temperature stability

Low nitrogen consumption typically 1 l/hr at T> -100 °C

Temperature overshooting after setpoint step typically < 0.2 °C

Stabilization times typically < 8 minutes (for 0.1 °C stability)

Automatic adaptation of controller parameters (self tune)

4 loop microprocessor with ***16 bit ADC and GPIB communication port***

Vacuum isolated cryostat and nitrogen line

Equivalent circuit analysis / modelling tries to describe the impedance measured at a system under test by an equivalent circuit made up of electronic components. The components are often resistors, capacitors and inductors. For a given circuit, the task is to find the optimal value for each circuit component, so that the equivalent circuit impedance function matches the measured impedance is as accurate as possible. With the equivalent circuit analysis function, arbitrary models can be defined and the best set of values (parameters) is automatically detected. In addition, arbitrary components described by any complex impedance function can be defined.

4. Preliminary determination of WP6 test groups

According to the TA of RINGrid project, a determination of test group of instruments and user concerning preparation of work prototype of remote access model has to be done. Based on the analysis that includes all the received in WP2 information till now, two domains of instruments and user communities are most suitable for this purpose. The first one is the instruments and users in the Material Sciences domain. The IIF and UIF data analysis show that it is the largest group of users and expensive instruments. Furthermore, some practical experience connected with the remote access of instruments is reported from the electron-microscopy lab in Campinas, Brazil (our CLARA /REUNA-RNP partner). Another experience is reported by the electron microscopy lab in Physical Institute from UNAM, Mexico. Training activities defined from USERS and OWNERS as important part of remote access procedures concerning user introduction to the instrument access protocols are also available (i.e. UCRAV project of REUNA). The shearing of this experience in the field of remote access usage with European researchers could be a good advantage for the RINGrid project purposes as well as for the next integration initiatives concerning EC and Latin America.

The second domain of instruments (i.e. optical and radio telescopes) and users suitable for such kind of prototype tests are Astronomy and Astrophysics. Telescopes, together with the synchrotron light sources are large-scale facilities. They were specified as the most expensive and rare equipment defined in the Global group of instruments according our classification described in the D2.1 report (p.15-16). Some experience in remote access usage of this kind of equipment is also reported from both instrument owners and user communities in this domain. In the field of Engineering, particularly in food engineering, there are reported interest and preliminary tests with remote access on the grid environment with instruments for freezing process at the Multidisciplinary Experimental Laboratory at UNAM, Mexico that can share experience with the European researches particularly from TUI. Unfortunately, there is a lack of IIFs and UIFs received from Astronomy and Astrophysics community till now that could fix the model test preparation in this field.

The diversity of instruments and speciality field of the user communities show that the cooperation with other projects can be improved. In the EELA project there are an application in the field of remote instrumentation on the Grid environment and the users communities can collaborate like tests groups for WP6.

5. Summary

The completed D2.3 task concerning formal specification of requirements defined by potential end users and instrumentation owners gives the basic systematization and analysing of information regarding the new opportunities for implementation of remote accessed instruments in the next generation grids. It also uses the information and activities from D2.1 and D2.2 task. The DB tool proposed as interface between OWNER and USER groups concerning their activities in planning and searching of instruments available for remote access is used in the analyze of the information. The database can be also implemented as analytical tool in the next RINGrid project activities. This product could be used also as prototype of the future large-scale databases that should be used on the Remote Access Information Gates / Gateways (RAIG).

The information used in this report has been collected mainly through IIF and UIF questionnaires, which was completed by a significant number of instrument owners and users, members of different communities. The analysis has been carried out on the basis of more than 30 completed IIFs and about 60 UIFs received from both European and non-European countries separated into the following combined domains: material science, astronomy and astrophysics, computer science, earth and environmental science, engineering and biomedical science. Additional information was received through the work contacts of all RINGrid project partners. The preliminary WP6 group’s determination for prototype tests of remote access model, based on all the received till now information in WP2 was done.

Definitions, abbreviations, acronyms

IIF	–	Instrument Information Form
UIF	–	User Information Form
DB	–	Database
RAIG	–	Remote Access Information Gates
NGO	-	Non-Governmental Organisation
SME	-	Small and Medium Enterprises

References

RINGrid Technical Annex – Annex I "Description of work" – RINGrid_TA-Description_ work_Approved_v1.1.pdf

D2.1 Report – RINGRID_WP2_D2_1-2006-12-14-02-Identification_of_scientific_instruments_and_user_communities

D2.2 Report - RINGRID_WP2_D2_2-2007-01-31-Creation_of_database_with_information_collected_in_D2.1

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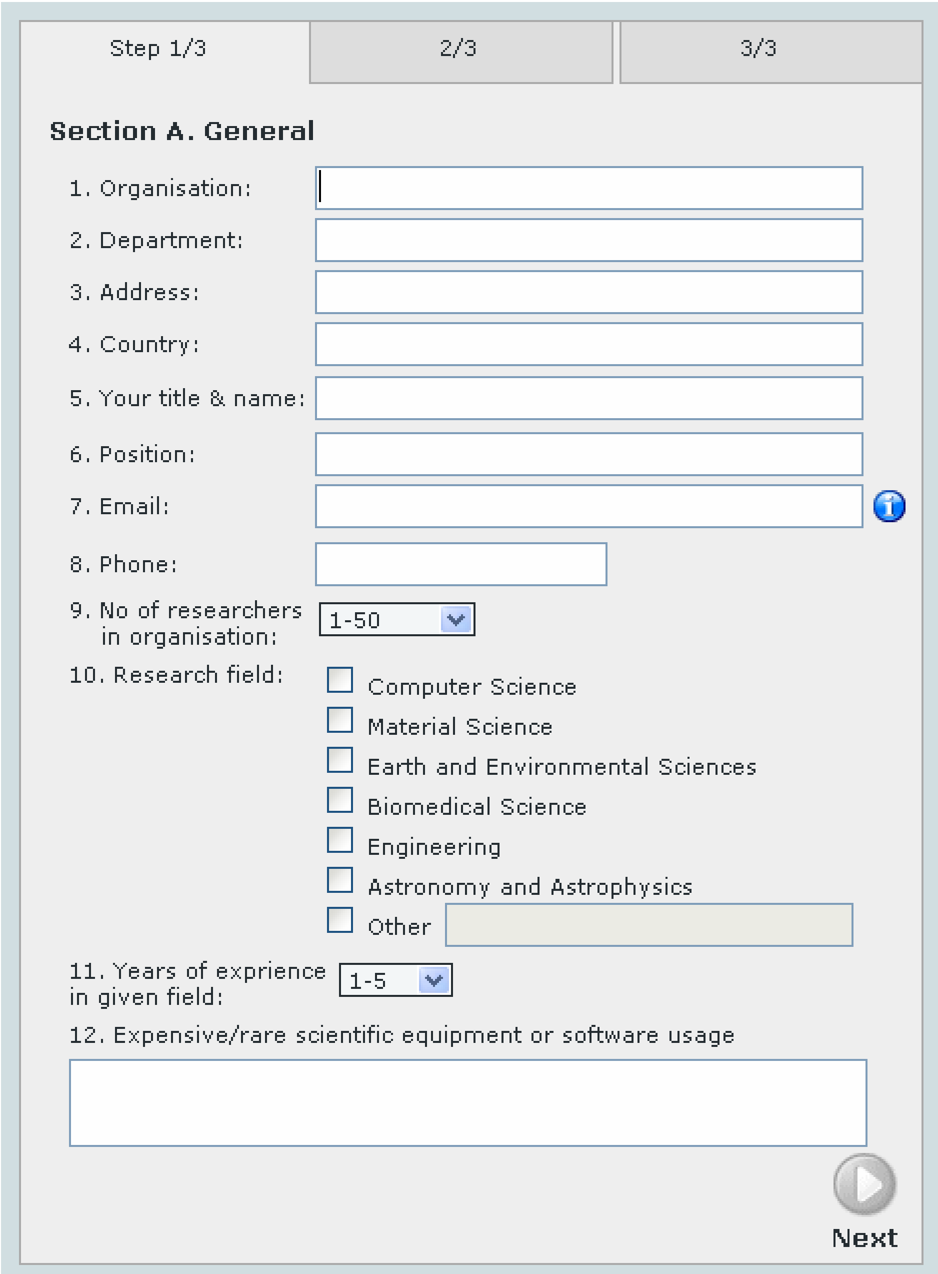
Appendix 1

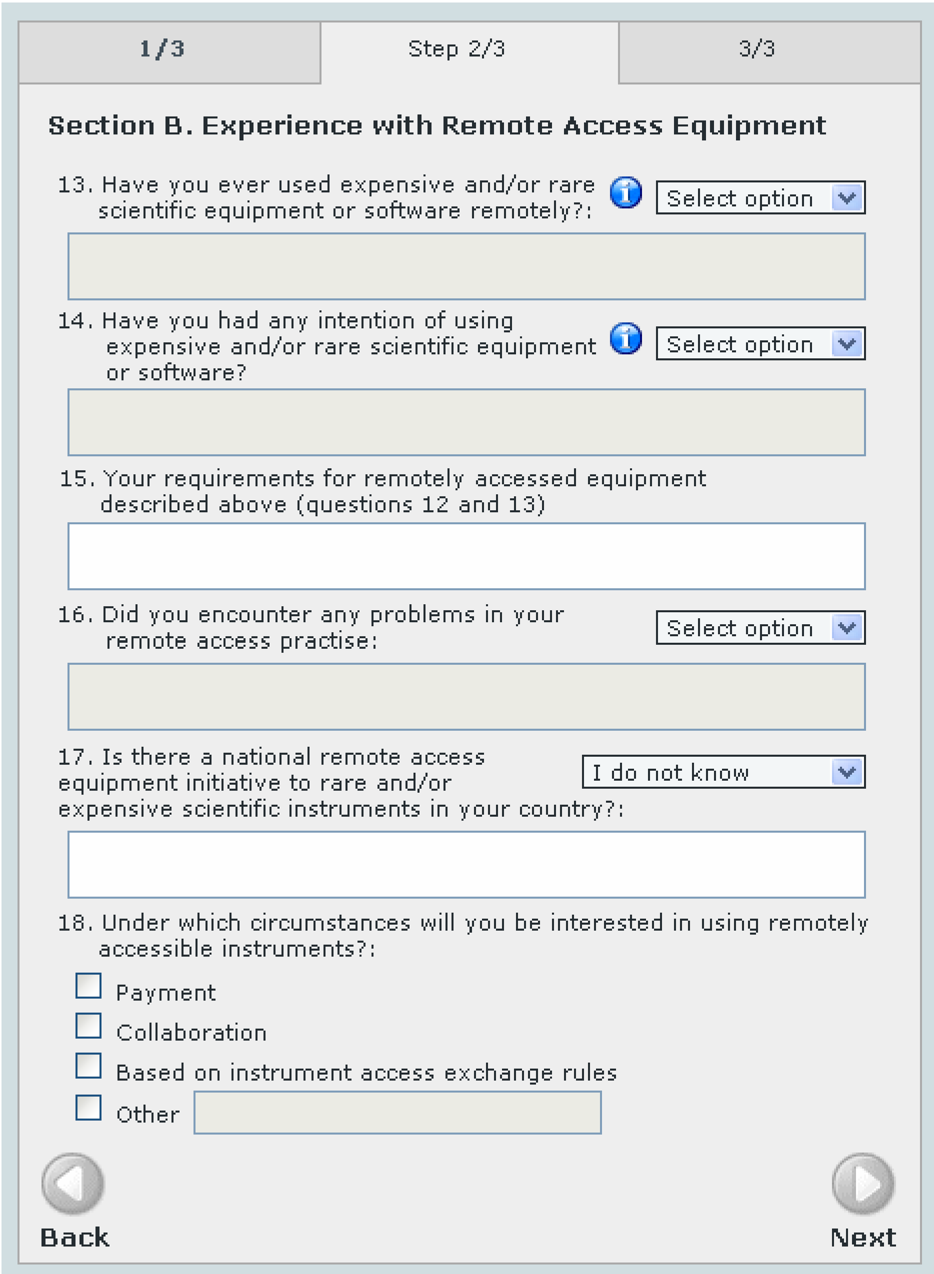


Step 1/3 | 2/3 | 3/3

Section A. General

1. Organisation:
2. Department:
3. Address:
4. Country:
5. Your title & name:
6. Position:
7. Email:
8. Phone:
9. No of researchers in organisation: 1-50
10. Research field:
    - Computer Science
    - Material Science
    - Earth and Environmental Sciences
    - Biomedical Science
    - Engineering
    - Astronomy and Astrophysics
    - Other
11. Years of exprience in given field: 1-5
12. Expensive/rare scientific equipment or software usage

Next


1/3 | Step 2/3 | 3/3

Section B. Experience with Remote Access Equipment

13. Have you ever used expensive and/or rare scientific equipment or software remotely?: [Select option]

14. Have you had any intention of using expensive and/or rare scientific equipment or software? [Select option]

15. Your requirements for remotely accessed equipment described above (questions 12 and 13)

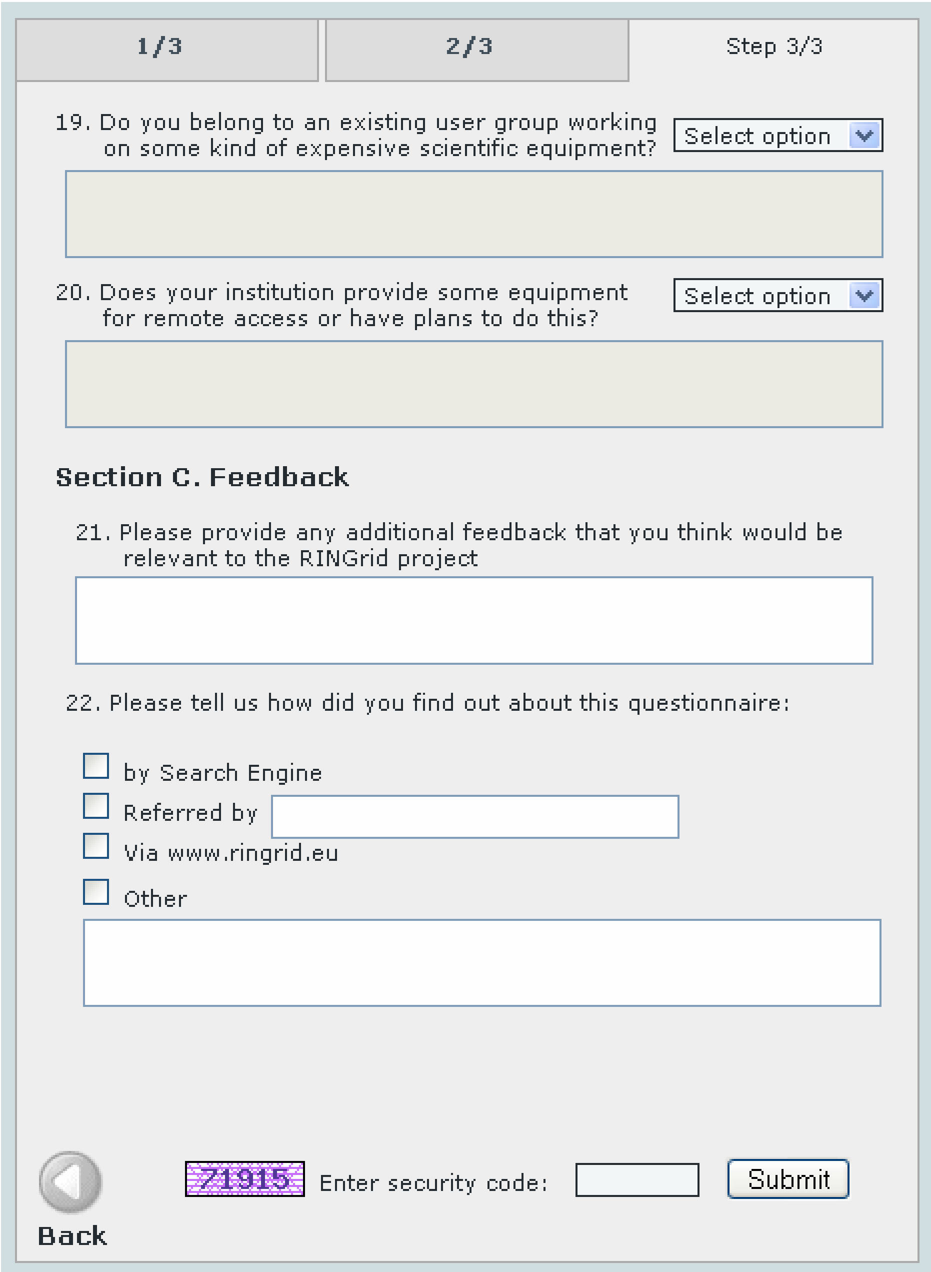
16. Did you encounter any problems in your remote access practise: [Select option]

17. Is there a national remote access equipment initiative to rare and/or expensive scientific instruments in your country?: [I do not know]

18. Under which circumstances will you be interested in using remotely accessible instruments?:

- [ ] Payment
- [ ] Collaboration
- [ ] Based on instrument access exchange rules
- [ ] Other

Back Next



1/3 | 2/3 | Step 3/3

19. Do you belong to an existing user group working on some kind of expensive scientific equipment? Select option

20. Does your institution provide some equipment for remote access or have plans to do this? Select option

Section C. Feedback

21. Please provide any additional feedback that you think would be relevant to the RINGrid project

22. Please tell us how did you find out about this questionnaire:

- by Search Engine
- Referred by
- Via www.ringrid.eu
- Other

Back

71915 Enter security code: Submit