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Integration of the Laboratory Instruments with e-Infrastructure

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Abstract: A combination of networks, computational, storage infrastructure and the scientific instrumentation (equipped with sensor networks) composes a new kind of e-Infrastructure. The integration of scientific instruments into e-Infrastructure empowers possibilities in conducting experiments. The development of technologies that allow remote and shared access to laboratory instruments opens up new opportunities for researchers. This paper presents an approach to integrate the laboratory instruments with e-Infrastructure, focusing on the results of the EU FP7 DORII project.

Key words: instrumentation, sensors, instruments, Grid, e-Infrastructure, virtual laboratory, scientific workflows, middleware

I. INTRODUCTION

Integration of scientific instruments into e-Infrastructure empowers possibilities in conducting experiments. Access to equipment infrastructures is very often a precondition for successful research in many scientific disciplines. The necessity of using unique and expensive equipment, which is often locally unavailable, is the key issue for the success of a number of experiments. Thus the development and spreading of remote instrumentation techniques and technologies that allow remote and shared access to laboratory instruments opens up new opportunities for researchers. The term instrumentation covers a wide range of laboratory equipment that is necessary for experimental sciences, such as biochemistry, physics and astronomy. Remote instrumentation is the method of providing data acquisition and/or control of scientific instruments from remote locations. Integration with the computational infrastructures (Grid, HPC) is used to integrate operations on instruments with computing farms where complex models and computations coming from instruments could run and store a large amount of data. The Grid handles issues related to authorization, resource management, data transfer and storing. The network infrastructure is used with the available mechanism for QoS handling.

There are several solutions that aim at realizing complete systems to integrate instruments with e-Infrastructure and build virtual laboratories. While mentioning the most relevant of such systems in the state of the art section, the paper is focusing on the outcome of the EU-funded FP7th project – Deployment of the Remote Instrumentation Infrastructure (DORII). The goal of DORII was to deploy e-Infrastructure for new scientific communities specifically for experimental equipment and instrumentation that are not or only partially integrated with the e-Infrastructure. The paper is organized as follows. In Section II, worldwide state of the art is presented. In Section III general requirements and challenges for integrating instruments are illustrated with an example of the DORII project. Next sections give an overview of the proposed solution and middleware framework. Section V presents on the example use case how the middleware is used. Section VI presents standardisation efforts. Finally, the future possible activities are discussed.

II. STATE OF THE ART

Various international projects have already tried to target some of the aspects involved in the integration of instrumentation in e-Infrastructure. Worldwide efforts can be grouped thematically into the following domains: conceptual work, complete general system solutions and user specific domain systems.

Some projects provided conceptual work, performing an analysis of current systems' states and user requirements. The final outcome of these projects is usually the proposition of a general architecture and mechanisms for building instrumentation systems. For example, in the Common Instrument Middleware Architecture (CIMA) [12] project, semantic descriptions of instruments were investigated. They are consumed by interested peers to generate dynamic clients and invoke their functionality according to those descriptions. The CIMA project was supported by the NSF Middleware Initiative to integrate instruments and sensors as real-time data sources into grid computing environments through a Service Oriented Architecture. The RINGrid [14] project was focused on systematic identification of instruments and corresponding user communities, a definition of their requirements, as well as a careful analysis of the remote instrumentation synergy with nextgeneration high-speed communications networks and the Grid infrastructure.

There are also several solutions that aim at realizing complete general purpose systems to integrate instruments and build virtual laboratories. The idea of such a system is to be easily adaptable for new use cases. The example from the USA, the CIMA project, has already been mentioned. The goal of another project called GRIDCC [13] was to build a geographically distributed system that is able to remotely control and monitor complex instrumentation, ranging over a large number of diverse environments. The goal of GRIDCC was to exploit grid opportunities for the secure and collaborative work of distributed teams in order to remotely operate and monitor scientific equipment using the grid's massive memory and computing resources for storing and processing data generated by this kind of equipment. The Virtual Laboratory [16] project develops a universal system architecture capable of handling a wide variety of different laboratory equipment. Additionally, an attempt was made to generalize the concepts of task and resource in the Grid environment, where laboratory equipment can be seen as a resource, while research experiments can be considered as system tasks. The Observatory Middleware Framework project has built a working prototype of an observatory framework designed and implemented to scale to a national or international level and interoperate with other large environmental observatories. It provides a new framework and techniques to access and process both raw and derived data streams from multiple observatories independent of their specific technological implementation. Another example of such project is the DORII project, described in details later in this article, that continues efforts started in the GRIDCC and Virtual Laboratory project, and which is based on experience from the RINGrid project.

In the scientific domains like astronomy, earth science and microscopy, it is common to build sophisticated field specific systems. For example, AugerAccess [17] (Integrating Auger Observatory and European Research Institutions into a worldwide Grid) is a project dedicated to improving the access capabilities of European research groups working on the Pierre Auger Observatory (Argentina). It is designed and developed with the aim of implementing a system of remote monitoring and control of the data from the Auger Observatory. Another project - Gemini Observatory [18] - is an initiative that uses Internet2 to allow remote users to manipulate their twin telescopes. The OpenTel [10] - An Open Network for Robotic Telescopes Project - provides the means for interconnecting single robotic telescopes to a global network for sharing observation time, programs and data. The NanoManipulator [7] project uses Internet2 to allow remote control and visualization of images from their scanning probe microscopes. SpectroGrid [15] – a software system based on open-source technologies was implemented to provide secure access to remote Nuclear Magnetic Resonance (NMR) spectroscopy instruments.

III. REQUIREMENTS FOR INSTRUMENTATION INFRASTRUCTURE

The DORII project with its applications and user communities can be considered as a good representative instrumentation infrastructure because of the number of user communities coming from different areas of science and a wide spectrum of the considered instruments.

In terms of the DORII project, the main focus was on supporting the following selected scientific user communities and applications:

- earthquake community (with various sensor networks): earthquake early warning system design and simulation, network-centric seismic simulations
- environmental science community: oceanographic and coastal observation and modelling, inland waters and reservoirs monitoring
- experimental science community: on-line data analysis in experimental science coming from increased efficiency of the light sources (synchrotron and free electron lasers) and of the detectors with higher resolution and faster readouts.



Fig. 1. Experimental instrumentation

DORII e-Infrastructure includes a wide spectrum of the hardware devices used by applications:

- Actuators: Actuators are devices applying forces to the specimen, while a sensor network is used to monitor the specimen's reaction
- Seismic sensors
- Float: Lagrangian (passively following the ocean current) instrument
- Glider: Autonomous gliding Underwater Vehicle (AUV)
- Digital Cameras
- Pressure sensors
- Temperature sensors
- CTD (Conductivity-Temperature-Depth), optical sensors [21]
- SAXS: Small Angle X-ray Scattering [20]

- XRD: BeamLine [20]
- SYRMEP: SYnchrotron Radiation for MEdical Physics
- LEGO Mindstorm
- Digital Camera.

Since the description of requirements of each of the mentioned application/instruments could be longer than the limit of this paper, general requirements are presented (basing on the analysis presented in DORII deliverables [3, 9]).

Taking into account the variety of the applications, different aspects have to be considered. Basic requirements are related to accessing the remote instrumentation distributed in a wide geographical area; it concerns applications like floats, the glider or monitoring through images. This has to be done in a standardised and unified way mostly in real time. It is worth mentioning that the collaborative behaviour is of great importance to users: this refers to the possibility of sharing the experiment, sharing the input data, sharing the output data, and exchanging the ideas. Some of the applications are expecting to use the virtual laboratory environment in order to remotely access the sometimes expensive equipment located in a real laboratory - this concerns mostly applications like the earthquake networked simulations. Most of the DORII communities would also like to profit from the Grid infrastructures in order to improve their work by reducing the computation time and increasing the storage possibilities (storage requirements can grow up to the order of Petabytes). Some of the applications are also challenging in terms of the network requirements, for example, in case of on-line processing applications data set of gigabytes should be transferred in real time, processed and visualized to the user. There are also requirements related to visualization, scientific workflows (automation of work), interactive behaviour, security and implementation of different authorisation policies.



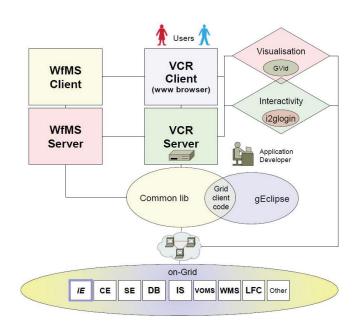
Fig. 2. Synchotron in ELETTRA, Trieste

IV. PROPOSED FRAMEWORK

The presented framework aims at fulfilling the user communities (and their applications) requirements on the Remote Instrumentation Services integrated with the Grid environment. As mentioned in the previous section, applications require the integration of scientific instruments with computational and storage resources to facilitate data acquisition, storage and processing. To fulfil the requirements, the DORII project utilizes the capabilities of Grid infrastructures. The main principle is the use of existing e-Infrastructures in Europe adding the necessary components and services to facilitate remote instrumentation. The DORII e-Infrastructure is mainly based on the EGEE (Enabling Grids for E-sciencE) [1] infrastructure and its middleware of choice gLite [2]. DORII extends the EGEE architecture adding the services and middleware on the level of the infrastructure (Instrument Element), access layer (g-Eclipse and common library), scientific gateway layer (VCR: Virtual Control Room and Wf-Man System: Workflow Management System). The overall picture of the architecture is presented in Figure 3. In this paper we will focus rather on the extensions than the gLite infrastructure itself. As presented in Figure 3, graphical collaborative clients (VCR, Wf-Man System) are using the common access layer libraries to interact with all kind of the infrastructure services, like Workload Management System, Computing Element, Storage Element or Instrument Element. For the applications that require advanced visualisation capabilities DORII provides a set of remote visualisation techniques by means of GVid. GVid is a Gridenabling video streaming service intended for grid-based visualizations in scientific applications. GVid allows visualization applications to render remotely, in combination with gLogin(ssh over grid) also using grid authentication. The visualisation application on the remote site renders the graphics output in background and transfers the output image in a MPEG-4 encoded video stream to the client. The client application displays this video stream and allows to user to interact with the visualisation. The user interaction event is sent to the server where it is passed to the visualisation application which can react on the user input.

The key middleware services and components dealing with the management of remote instrumentation are:

- Instrument Element (IE) presented in Fig. 4 is used for the interaction with instruments. The IE was initially developed by the GRIDCC project [13]. It is an abstraction of the instrument (or group of instruments) into a standard interface. The term instrument is used in this context to define a piece of equipment that needs to be initialized, configured, operated (start, stop, standby, resume, application specific commands), monitored or reset. The DORII extension of the Instrument Element is a set of WS-I compliant web services virtualizing the concept of instrument and sensor and presenting it as a grid component that works conjoined with the EGEE gLite software [2].
- VCR (Virtual Control Room) [8] is a kind of a scientific gateway which allows registered users to interactively



IE - instrument element CE - computing element SE - storage element WMS - workload management system (CE broker) LFC - location file catalog (SE broker) DB - database element IS - information system VOMS - VO management system OtherS - other services (e.g. OGC) VCR - virtual control rooom G-Eclipse - developer workbench Wf-Editor - workflow editor Wf monitor - workflow monitor Wf-Man System - workflow management system Script Man - script manager Apps Man - application manager

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Fig. 3. DORII Architecture

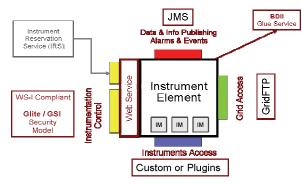


Fig. 4. Instrument Element architecture

access all the computational, storage and instrument resources, providing them with additional collaboration services. VCR supports applications with workflows through an external workflow management system (Wf-Man System), a native client application launcher and also with a tunneling technology which can be used to integrate the application components and to support interactivity. VCR is using Instrument Element services to interact with the instruments.

- The Workflow Management System (Wf-Man System) [5] supports users in the definition, management and monitoring of scientific workflow. The Wf-Man System facilitates the measurement process from the preparation stage through experimental and computational processes, to results analysis. It allows for execution of complex instrumental and computational scenarios with just one-click. Low time-to-Grid and user-entrance thresholds are provided thanks to predefined scenarios, a user-friendly monitoring interface and e-Infrastructure resources browsing facilities.
- g-elipse is used to prepare common interfaces and is the development platform for DORII. The g-Eclipse framework, initially developed within the g-Eclipse project [4], provides a set of tools for accessing e-Infrastructure, including tracing and debugging tools for parallel applications. The DORII extensions of the framework concern mainly handling of the Instrument Element and instrumentation services.

The middleware architecture proposed by DORII aims at setting up a highly configurable, user-centric and open source user and development environment. The proposed solution is generic, and it can be easily used for fast prototyping and further deployments.

V. EXAMPLE USE CASE

One of the example use case concerns the environmental application. It was introduced by Ecohydros S.L that has deployed a mobile autonomous sensor platform in the Cuerda del Pozo water reservoir, located in Soria, Spain. The purpose of this sensor platform is to continously monitor typical water quality markers and register nutrient concentrations in order to better understand, detect, and predict cyanophiceae algae blooms, which cause the water to be unsuitable for human consumption, and which have historically appeared in the reservoir watershed. The platform hosts an heterogeneous set of sensors located on its surface (meteorological sensors, GPS, radiometers) as well as below water level, and the set of power elements required for the platform to be autonomous during long periods of time (batteries, solar panels, a wind turbine ...).

In this specific application the DORII infrastructure provides the user the required interface for remotely monitor and operate the set of sensors deployed in the platform; and to exploit the acquired data in specific simulations.

The typical use cases can be considered for monitoring the data acquisition process and for launching simulations to the grid infrastructure:

- 1. Login to Virtual Control Room (VCR)
- 2. Upload user certificates
- 3. Obtain valid user credentials
- 4. Choose Instrument Element, set-up parameters
- Start Instrument. Automatically the latest data acquired from the sensors show up in the monitoring section in VCR
- Select the range of outputs. After executing the input files for the desired simulation are created in the user local folder in the VCR
- 8. Select a Computing Element and send computation job to WMS/CE services
- 9. Get results

This is one of the possible simple example that shows how different components introduced by DORII are being used.

VI. STANDARDISATION INITIATIVES

Standards are of key importance to achieve sustainable solutions adequate for a wide range of use cases. DORII has the leading role in this field, and project partners have established a research group inside the standardization body named the Open Grid Forum [6], i.e. RISGE – Remote Instrumentation Services in a Grid Environment. The main goals of the group as well as the scope have been defined within the OGF charter [11]: "RISGE-RG explores issues related to the exploitation of Grid technologies for conducting and monitoring measurement tasks and experiments on complex remote scientific equipment. The main purpose of this research group is to bring together various existing approaches in defining remote access interfaces to sophisticated laboratory equipment, and to come up with use cases that can dictate the requirements for integrating scientific instruments with the Grid. As such, it mostly concerns the steering and monitoring of instrument resources, although more typical problems such as user access and authorization are also in scope". The activity of this group is focused on providing an overview of existing solutions as well as on indicating some requirements and future directions of e-Infrastructure functionality development to facilitate access to instruments. This group gathers people that are involved in the field of remote instrumentation and Grid, in order to document experiences, present best practices and document different use cases. The group has identified possible standardisation activities in the field: accessing instruments in a standard way/unique interface, data handling - getting data out of the instruments, monitoring instruments, accounting for instruments, scheduling of the instruments. Basing on the result of research of the group towards existing standards, the group tries to establish new working groups to standardize the relevant capabilities. One of such new initiatives is the ARI group (Access to Remote Instrumentation in a distributed environment) that will focus its efforts on providing a Shared Information Model (SIM) and defining concrete interfaces for accessing remote instruments.

VII. FUTURE WORK

Virtualisation technologies combined with next generation networks open new possibilities in the area of facilitating access to instruments. It concerns, for example, dynamic creation of the whole virtual environment including the instrument resources. Such approach would require development of the services aiming to create a dynamic and temporarily isolated environment which allows the user to proceed with the experiment. One of the aspects necessary to provide such an environment is the development of techniques allowing for automatic reservation of the instruments.

New requirements would come from emerging large research infrastructures in the following years. In Europe, this corresponds to the ESFRI (European Strategy Forum on Research Infrastructures) [19] installations. Most of these infrastructures have thousands of different kinds of instruments and sensors that would have to be integrated in e-Infrastructure. Taking into account new user communities and a number of possible new deployments and developments in the area, it is obvious that the standardisation effort has to be continued (for example, in terms of the OGF). As already mentioned, standards are of key importance to achieve sustainable solutions. It is important to work out standards, especially the one which defines the access interface to the instruments.

VII. CONCLUDING REMARKS

A combination of the network, computational and storage infrastructure and the scientific instrumentation (equipped with sensor networks) composes a new kind of e-Infrastructure. Remote control of scientific facilities has the potential of revolutionizing the mode of operation and the degree of exploitation of scientific instruments. This paper presents an approach to the integration of laboratory instruments with e-Infrastructure, focusing on the results of the EU FP7 DORII project. It presents the requirements of the applications and instruments and describes the proposed framework. The infrastructure that is set up by the DORII project offers a promising vision how the modern grid computing technology can support and enhance the level of managing, maintaining and exploiting heterogeneous instruments and acquisition devices for the e-Science. As the proposed solution is generalized, it can be used for further deployment in a reasonable time, including appropriate performance, scalability and reliability not only in the mentioned scientific areas.

In the context of emerging new large research infrastructures (like ESFRI in Europe) as well as next generation networks, the intensive usage of instrumentation will be common, and solutions like DORII would constitute a base platform for scientists.

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