Instrumentation for eScience

Preface

The global dimension of science and its grand challenges would not be possible without integrating research processes with information and communication technologies. This integration defines the e-Science approach which requires common availability of research infrastructure including networks and grids, i.e. e-Infrastructure in Europe or Cyberinfrastructure in USA. The network infrastructure in Europe is built by the pan-European network GEANT 2/3 and national research networks (NREN), e.g. PIONIER in Poland, GARR in Italy, GRNET in Greece or DFN in Germany. The Grid is a fully distributed, dynamically reconfigurable, scalable, and autonomous infrastructure to provide location-independent, pervasive, reliable, secure, and efficient access to a coordinated set of services encapsulating and virtualizing resources (computing power, storage, data, instruments, etc.) in order to generate knowledge (a definition by the Network of Excellence CoreGRID, http://www.coregrid.net). Several examples of the Grid infrastructure built in Europe (EGEE, BalticGrid, int.eu.grid) and the U.S. (TeraGrid) as well as activities towards establishing a sustainable Grid infrastructure (European Grid Initiative, http://web.eu-egi.eu/) can be shown.

Two special issue numbers of The Computational Method in Science and Technology (CMST, http://www.man.poznan.pl/cmst) gave attention to the e-Infrastructure challenges:

- *The World of Pervasive Networking* (Volume 11, 2005),
- *Grid Applications – New Challenges for Computational Methods* (Volume 12, 2006).

This number of CMST is devoted to one of the important topics concerning instrumentation, being a part of the worldwide e-Infrastructure.

Instrumentation is widely used for laboratory equipment which is necessary for daily use in experimental sciences, e.g. chemistry, biochemistry, physics, and astronomy, but also by industry solutions. Instrumentation is, however, not only limited to laboratory equipment but may also cover various sensors, which can be remotely controlled and monitored. Implementing remote instrumentation services allows us to operate instrumentation remotely independently of the location of the end user and the equipment. The necessity of using interactively advanced, unique, and expensive equipment infrastructure, which is often locally unavailable, as well as the advantages of broad international cooperation, are the key issues for the success of a great number of scientific disciplines. Remote assisted use of scientific equipment will substantially reduce the human and financial cost, as it provides the possibility of sharing the results in real time with other researchers at different geographic locations, making a better use of senior researchers' time.

Thus, the development and spreading of remote instrumentation techniques and technologies that allow virtualized, remote, and shared access to such infrastructure opens up new opportunities for scientific communities.

Grid technologies facilitate the sharing of these resources across a distributed computing environment, and its integration as part of the e-Infrastructure. In particular, the Grid handles issues of authentication, authorization, resource description and location, data transfer and resource accounting. Moreover, Grid technologies can be used to integrate operations with computing resources where complex models of the experimental facility can be executed.

Efforts in this direction were made worldwide, e.g. in Australia, Europe and the U.S. As examples, we can mention such projects as CIMA (Common Instrument Middleware Architecture) from the U.S. with significant effort made in Australia, the former GRIDCC (Grid-Enabled Remote Instrumentation with Distributed Control and Computation) and RINGrid (Remote Instrumentation in Next Generation Grids) projects and the currently funded DORII project (Deployment of Remote Instrumentation Infrastructure, http://www.dorii.eu).

This issue is structured in two parts: Applications in e-Science and Middleware for Instrumentation. Both parts contain a number of chapters. Part I, Applications in e-Science, describes best practices from experimental sciences.

The first paper in part I considers an off-line three-dimensional coupled eco-hydrodynamic simulation model used for biogeochemical and ecosystem-level predictions with results of research activities devoted to the adaptation of the parallel OPATM-BFM application for an efficient usage in modern Grid-based e-Infrastructures. The second article addresses integration of experimental stations like synchrotrons and free electron lasers in the Grid for on-line and off-line processing based on the DORII infrastructure. The third chapter deals with genomics experiments supported by the virtual laboratory system approach. Chapter four discusses how remote instrumentation services can be fruitfully employed even with smaller and relatively widespread measurement instrumentation adopted in engineering applications. In this context, this chapter considers the case of telecommunication measurements, and of their execution within the eInfrastructure, by using a subset of the service capabilities. Chapter five proposes some modifications and advanced services for observations provided by oceanographic remote instruments which are essential to the purposes of the operational oceanography. Management of a network of instruments deployed in the Mediterranean Sea is a complex task that may be greatly supported by the Grid technology. The last applications' chapter describes the Development of Biological Warfare Sensors Using SGI High Performance Computers.

Part II is divided into six chapters. The first chapter aims at setting up an advanced Grid-based e-Infrastructure specifically oriented to the support of remote instrumentation devices on the Grid extending the level of scientific instruments' exploitation. This chapter highlights the main application areas and usage scenarios, key tasks of the Remote Instrumentation Infrastructure's deployment, and presents the joint research architecture for DORII in terms of advanced middleware solutions addressing the main tasks of identified applications. The second chapter describes VIRA, a CIMA-based system for the operation of remote scientific instruments. The common Instrument Middleware Architecture (CIMA) has been adopted and is being further developed as part of a project that includes the use of virtual instruments in a Web browser driven system for remote access to scientific instruments. Enhancements include distinct separation of concern for the modular components that make up the system, and a flexible message parcel schema. The next section of the book explores the role of the Real World Web as a paradigm for sharing instruments, sensors and other real-time data sources in e-Research collaboration as experiences from the U.S. Chapter four describes the design of the integration of radio-astronomical VLBI experiments with the workflow management technology which facilitates the daily procedures of managing large worldwide experiments (based on the EXPReS project). The next section evaluates the already existing remote control software packages to be used in data processing projects, explains the demands for developing a high throughput data acquisition system with the introduced requirements, shows the advantages of using Grid technologies, and proposes an architecture for developing such a system. The last chapter is a white paper on remote instrumentation which was the final outcome of the RINGrid EU project. The white paper provides recommendations concerning the usage of scientific instrumentation in a Grid environment, and makes it available to the e-Infrastructure by introducing remote instrumentation services.

We would like to thank all the authors for their contributions to this CMST journal. We hope the effort we have made is valuable and will move us closer to a reliable distributed e-Infrastructure.

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