Chapter XL

Networked Experiments in Global E–Science

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ABSTRACT

In current economic and scientific scenarios, interactions and organization models tend to be more and more oriented to flexibility of relationships, heterogeneity of elements, and collaboration among divisions. A possible approach, which is a technical solution and an organizing paradigm at the same time, is based on the concept of Virtual Organization. This paper, starting from the Virtual Organization paradigm and from workflows, shows an approach to the definition and execution of distributed scientific experiments as set of services executed on distributed collaborating sites at different heterogeneous organizations. The focus is on flexibility, reuse, orchestration, collaboration, and interoperability of services within a cooperation process. The workflow of the experiment can be specified by actors with low information technology but high domain knowledge. The context of the work is e-Science, in particular, bioinformatics, but the presented concepts can be easily generalized and extended to other classes of business interaction.

INTRODUCTION

Science nowadays is more and more a question of a critical mass of skilled people, often with complementary background, becoming a unique global organism in pursuit of a substantial common goal: this is the most interesting form of collaboration in science. For this purpose, traditionally in physics, specialized workforces have historically been concentrated in unique sites with special instruments like great particle accelerators. On the contrary, many of the faced problems in the present renaissance of biology do not need a unique big site, while other disciplines, like geol-
ogy, are intrinsically distributed as for obtaining significant data. The availability of information and communication technologies thus enables a full network to be built linking remote sites when only information gained from experiment possible at almost any site need to be shared. It becomes thus of interest to resort to a possible network of experimenters, physically not necessarily together, but logically co-present in the framework of the same cooperative big experiment involving all their complementary competences. In the paradigmatic bioinformatics application domain dealt with in this paper within the framework of e-Science, collaboration among different actors possibly with complementary background and expertise, may be even more needed than in other areas such as financial transactions (although any technologically assisted business interaction could be described in the same way). A proper virtual organisation is thus required in order to manage the flow of information over a given network. A networked organisation such as this may be logically defined through workflows acting over Web services, possibly exploiting a grid context. The technology addressed in this chapter would thus allow the most competent scientist to design the workflow even if he is not at a very high level of competence in information and communication technologies (which are, in a sense, logically embedded), as is common in application contexts like the bioinformatics one faced here, as well as in other application domains, where the proposed tools can also be applied. A framework is in fact proposed that creates, uses, and communicates information, whose organizational dynamics allows to perform a distributed cooperative enterprise also in public environments, even over open source systems. The approach assumes the Web services as the enacting paradigm, possibly over a grid, to formalize interactions as cooperative services on various computational nodes of a network. The responsibility of e-nodes in offering services are defined, as well as the set of rules under which each service can be accessed by e-nodes through service invocation. By discussing the bioinformatics case study, the chapter will detail how specific classes of interactions can be mapped into a service-oriented model whose implementation will be carried out in a prototypical public environment. Thus, problems linked to both virtualization of resources and orchestration of services in the heterogeneous and distributed context of e-Science (De Roure, Gil, & Hendler, 2004) are faced in this chapter: in this sense, approaches like the proposed one could provide a tremendous impact in globalisation, both by improving the capability to easily recruit a higher portion of the human capital not yet fully involved in global scientific research, fostering the diffusion of science and participation for local scientists in the developing world where labs might not be easily available, as well as by helping to overcome the subtle form of digital divide affecting people much more skilled in their own field than in instrumental information and communication technologies.

BACKGROUND

The concept of virtual organization has been developed in the recent few years also thanks to the grid computing paradigm (Foster & Kesselman, 2004; Foster, Kesselman, Nick, & Tuecke, 2002) as a general conceptual model, abstracted from specific technical solutions. Such virtual organization is a set of individuals and institutions having direct access to services, knowledge, tools, data, software, computers, and possible other resources in an heterogeneous dynamic way, aiming to achieve a common goal through collaboration. The basis of virtual organization is the virtualization of resources, consisting in creating and associating to resources a generic interface to allow services to be used through remote control, possibly by ensuring a given quality of service.