GRDI2020 WG contribution

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Virtual Research Environment

Virtual Research Environments (VREs) have been conceived as a framework enabling secure, cost-effective and on-demand *resource sharing* across organisation boundaries. A resource is here intended as a generic entity, *physical* (e.g. storage and computing resources) or *digital* (e.g. software, processes, data), that can be shared and interact with other resources to synergistically provide functions serving its clients, either human or inanimate. A VRE does not only act as a "*mediator*" in a market of resources originally born to accommodate the needs of resource providers and consumers. Rather it has to provide facilities for communication, collaboration and any kind of interaction among scientists and researchers.

Relevance to the overall theme of a Global Research Data Infrastructure

By its definition a VRE constitutes the necessary facilitator of the Global Research Data Infrastructure (GRDI). GRDI cannot be envisaged as a single market of resources where heterogeneous communities operate on. Storage, computing, data, software and applications resources have to be aggregated and disaggregated continuously according to the needs of the diverse communities flowing into GRDI. Those needs change along the time and GRDI should evolve with them seamlessly by incessantly offering a costless solution for their satisfaction.

Issues and challenges

To operate in a market of heterogeneous resources dynamically added to a common and on-demand created virtual environment poses a number of issues that have to be properly addressed.

- Heterogeneous resources are provided by parties operating in decentralised data centres. Despite the collective business model usually characterising the newly created environment and the social value for consumers and providers generated by the sharing of resources, security is pervasive and security enforcement is a pre-requisite of any successful VRE realization.
- Resources are added and removed according to the needs of resource providers. Resources live in a wide and disperse area network with different characteristics in terms of quality of service. Robustness, resilience, fault tolerance, latency tolerance, and inactiveness discovery are key constituents of any VRE realization.
- Resources have to be described and published in order to be discovered. Resource profiling is a major issue in absence of widely-accepted standards.

Current practices

Today research activities require collaborations among parties that are widely dispersed and autonomous. Each party operates in a well-defined and usually secure administrative domain pre-existing to the collaboration needs. Moreover, collaborations are often cross-discipline and require innovative environment to seamlessly integrate data, computer and storage resources and exploit intensive workflows to produce new knowledge able to stimulate further research.

e-Infrastructures give support to: (*i*) *resource providers*, in “selling” their resources through it; (*ii*) *resource consumers*, in “buying” and orchestrating such resources to build their applications. Further, they provide organizations with logistic and technical aids for application building, maintenance, and monitoring. A well-known instance of such an e-Infrastructure is represented by the Grid, where a service-based paradigm is adopted to share and reuse low-level physical resources. Application-specific e-Infrastructures are in their turn inspired by the generic e-Infrastructure framework and bring this vision into specific application domains by enriching the infrastructural *resource model* with specific *service* resources, i.e. software units that deliver functionality or content by exploiting available physical resources.

Communities operating in Grid empowered e-Infrastructure are named Virtual Organizations (VOs). A VO specifies how a set of users can access a set of resources. In particular it specifies what is shares, who is allowed to share and the conditions under which sharing can occur.

The realization of the VO mechanism is usually not adequate to represent a growing aggregation of resources tailored to satisfy the evolving needs of the user communities. Data needs to be assessed before to make it publically exploitable by the VO members. Restricted set of users have to collaborate to refine processes and implement show cases. Products generated through elaboration of data or simulation have to be validated by expert users. To manage those cases the VRE approach allowing aggregation of subset of VOs resources and their assignment to a subset of VO users seems more adequate. gCube[1] is a first example of a VRE management system where the aggregation and the assignment of resources to VO users for a limited timeframe and at little or no cost for the providers of the e-Infrastructure is performed via interfaces.

Proposed approach

gCube system has been partially funded in the context of three large European projects in the last seven years, namely Diligent (2004-2007), D4Science (2008-2009), and D4Science-II (2009-2011).

gCube lifts the Grid computing paradigm to the application-level. gCube allows to deploy e-Infrastructures falling in the category of Service Oriented Infrastructures, i.e. the application of the Service Orientation principles in realizing an infrastructure. This results in facilities for the reusability and dynamic allocation of the resources forming the

[1] gCube system: http://www.gcube-system.org

infrastructure itself. In addition, gCube supports a very flexible and agile application development model based on the notion of Software as a Service (SaaS) in which components may be bound instantly, just at the time they are needed and then the binding may be discarded. Moreover the gCube infrastructure model is compatible with Infrastructure as Service (IaaS) models being based on federation of private clouds providing computing and storage resources elastically assigned to users.

Such development and deployment model materialises in the support for Virtual Research Environments representing a distinguishing feature of gCube.

In particular, gCube relies on a set of e-Infrastructure enabling services. This pool of services specifically conceived to support a Grid-based approach to autonomic, extensible, and maintainable resources sharing provides facilities for resource registration, discovery, assignment, and management. Thanks to these enabling services, each community (VO) registers its own resources under its domain, registers and authorises its users, assigning to some of them special administrative roles. An indefinite number of VREs can then be defined, deployed in the e-Infrastructure and made accessible to groups of users. Each user logins to the VO's personalised portal and access to the VREs she has been authorised to. From there, the user will search, elaborate and store shared and personal information. Later on the community administrators will dynamically add or remove resources and users from their domain. Similarly, each VRE will be modified by the VRE administrators during its lifetime to adapt to the changing requirements. The correct operation of the infrastructure is constantly monitored by means of the infrastructure support tools and ensured by the autonomic behaviour provided by its services.

Recommendations

- Data generated in a VRE must be equipped with provenance information. Provenance data adds the necessary information to assess the generated data and evaluate their quality. Standards to describe provenance data are needed;
- Guidelines and procedures for data and metadata protection (security, privacy, confidentiality) have to be defined to sustain data exchange and interoperation;
- Resources profile are a key element in a dynamically federation of resources. If the profiling of computing resources is addressed by de-facto standards, the profiling of raw data and collections are still application specific; the profiling of services and applications is only partially covered by technology-specific specifications.

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