Resource Provisioning for e-Science Environments

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ABSTRACT

Recent works have proposed a number of models and tools to address the growing needs and expectations in the field of e-Science. At the same time, the availability and models of use of networked computing resources needed by e-Science are rapidly changing and see the coexistence of many disparate paradigms: high performance computing, grid and recently cloud, which brings very promising expectations due to its high flexibility. In this paper we suggest a model to promote the convergence and the integration of different computing paradigms and infrastructures for the dynamic on-demand provisioning of the resources needed by e-Science environments, leveraging the Service-Oriented Architecture model. In addition, its design aims at endorsing a flexible, modular, workflow-based collaborative environment for e-Science. A working implementation used to validate the proposed approach is described together with some performance tests.

Keywords: *Business Process Execution Language (BPEL), Cloud, e-Science, Grid, High Performance Computing (HPC), Resource Provisioning, Service Oriented Architectures, Web Services, Workflows*

INTRODUCTION

Recent works (Akram, 2006; Deelman, 2009; Elmroth, 2010; McPhillips, 2009) have proposed a number of models and tools to address the growing needs and expectations in the field of e-Science. In particular, Akram (2006) and Bosin (2011a) have shown the advantages and the feasibility, but also the problems, of modeling e-Science environments and infrastructures according to the Service-Oriented Architecture (SOA) and its enabling technologies such as Web Services (WS). Among the main advantages of such approach we find: interoperability, open standards, modularity, dynamic publish-find-bind, and programmatic access.

At the same time, the availability and models of use of networked computing resources needed by e-Science are rapidly changing and see the coexistence of many disparate paradigms, featuring their own characteristics, advantages and limitations. Among the main paradigms we find High Performance (HPC), Grid and Cloud Computing. In all cases, the objective is to best provide hardware and software resources to user applications with the help of schedulers, reservation systems, control interfaces, authentication mechanisms and so

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on. A detailed comparison of the characteristics of HPC, grid and cloud paradigms is presented by Mateescu (2011), which observes that none of these paradigms is the ultimate solution, and a convergence of HPC, grid and cloud resources should be pursued. Such a convergence must take into account a number of differences between both resources and provisioning systems, which can be intrinsic but may also depend on the different user requirements:

- Hardware capabilities,
- Network connectivity,
- Operating systems,
- Middleware,
- Software and libraries,
- Application programming interface (API),
- Authentication models, and
- Usage models.

It is important to underline that such differences are essential in allowing the execution of applications with very different requirements, even if they may constitute an obstacle in the quest for the perfect computing paradigm. According to our experience, an important point in the usability of computing infrastructures available to e-Science is then to guarantee user access to the widest spectrum of resources in a technology agnostic way.

In this paper we suggest a model to promote the convergence and the integration of different computing paradigms and infrastructures for the dynamic on-demand provisioning of the resources needed by e-Science environments, leveraging the SOA model. At the same time, the design aims at endorsing a flexible, modular, workflow-based collaborative environment for e-Science. The latter sees the integration and inter-operation of a number of software components, such as:

- Workflows, to define and coordinate complex scientific application or experiments;
- Service interfaces, to expose the business logic of scientific applications; and
- Components, to implement business rules and perform business tasks related to a specific scientific domain.

At the implementation level, the choice of SOA as the enabling technology for a common integration and inter-operation framework sounds realistic due to

- Availability of SOA standards for workflow systems;
- Availability of web service libraries to build new applications and to wrap existing ones;
- Existence of SOA standards covering areas like data access, security, reliability, etc.; and
- Access to a number of computing infrastructures (e.g. grid) is, at least partially, SOA-aware.

Our model is not meant to replace existing HPC, grid and cloud paradigms, rather it is an attempt aimed at complementing, integrating and building on them by playing the role of a dynamic resource aggregator exposing a technology agnostic abstraction layer.

Our proposal borrows many SOA concepts and standards from the business domain, including the adoption of the Business Process Execution Language (BPEL) for workflow design and execution. A motivation of our approach is almost evident: the SOA paradigm, and in particular web services and BPEL, are based on widely accepted standards and supported by many software tools, both open source and commercial. In addition, an important feature of BPEL, essential in highly dynamic environments, is the capability of setting at run-time the network endpoint of the services to be invoked. This allows BPEL to work with services which may be brought into existence even after the workflow has started (e.g. by the workflow itself) and disposed before the workflow has ended (e.g. again by the workflow). However, SOA and WS do not preclude the use of other technologies and tools: the point is not whether they can be adopted by e-Science environments,

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