Job Management Enterprise Application

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Abstract. This paper describes the development of a Job Management Enterprise Application (JMEA) which was developed by the DEISA material science and plasma physics joint research activities. It is capable of submitting jobs to a UNICORE server infrastructure and managing them. Since it is a Java EE application, it can be used by multiple users concurrently. Furthermore, it prefetches and caches request results in order to able of responding as quick as possible to client requests. In addition to normal user credentials it also supports the use of proxy credentials and explicit trust delegation.

1 Introduction

The Distributed European Infrastructure for Supercomputing Applications (DEISA) [1] is a consortium of leading national supercomputing centers that currently deploys and operates a persistent, production quality, distributed supercomputing environment with continental scope. The purpose of this FP6 funded research infrastructure is to enable scientific discovery across a broad spectrum of science and technology, by enhancing and reinforcing European capabilities in the area of high performance computing. This becomes possible through a deep integration of existing national high-end platforms, tightly coupled by a dedicated network and supported by innovative system and grid software.

The DEISA supercomputing grid is a European research infrastructure resulting from the integration of national High Performance Computing (HPC) infrastructures. This integration of national resources – using modern grid technologies such as UNICORE [6] – is expected to contribute to a significant enhancement of HPC capability and capacity in Europe.

DEISA is structured as a layer on top of the national supercomputing services, and coexists with them. This infrastructure addresses the computational challenges that require the coordinated action of the different national supercomputing environments and services for both efficiency and performance. DEISA provides scientific users with transparent access to a European pool of computing resources. The coordinated operation of this environment is tailored to enable new, ground breaking applications in computational sciences.

Eleven partners contribute currently to the DEISA infrastructure with their top level supercomputers: BSC, Spain; CINECA, Italy; CSC, Finland; ECMWF, UK; EPCC, UK; HLRS, Germany, IDRIS, France; FZJ, Germany, LRZ, Germany;
RZG, Germany; SARA, Netherlands This heterogeneous grid of super-computers includes the most recent systems from leading vendors (IBM – PowerPC970, Power 4, 4+, 5, SGI – ALTIX, NEC – SX8).

Science Gateways, Portals and Web Service interfaces, are crucial for enhancing the user’s adoption of sophisticated supercomputing infrastructures, by hiding from them the complexities of the computational environment. This extends up to the point that users make in their view direct use of an application. The choice of resource utilization is completely left to the infrastructure providing access to this application. So the portal solutions play the role of an application service provider (ASP).

The DEISA joint research activities in material sciences and plasma physics were faced with the development of comfortable means of access to the DEISA resources for standard applications in their fields like CPMD [2] and CP2K [3] for material sciences, and TORB [4] for plasma physics, a so-called science gateway.

Within DEISA several options for job submission across Cluster boundaries exist, e.g., the Multi Cluster Load Leveler (MC-LL) allows submitting jobs from the command line to any of the connected Load Leveler clusters (but naturally not to non MC-LL sites). The middle ware service activity within the DEISA project chose to employ the UNICORE suite as the default job submission interface to all heterogeneous compute resources within DEISA. Hence any DEISA job submission portal solution should be able to interface the UNICORE infrastructure deployed in DEISA in order to submit jobs in behalf of its users.

The UNICORE suite consists essentially of three components and one local batch scheduling system interface implementation establishing the connection to resource management systems like MC-LL and others. On the server side the central component is the Network Job Scheduler (NJS). It takes care of job submission, job management as well as file transfers and work flow execution. A gateway is the central entry point from the client perspective and several NJSs can be connected to it. A grid infrastructure relying on UNICORE can have more than one gateway e.g. for an increased fault tolerance. A user typically employs a rich client application (the UNICORE Client) to connect to several NJSs via a single gateway (see Fig. 1).

In the case of a portal application the job submission and management part needs to be implemented by an appropriate interface component. This components has to be able to carry out all tasks usually performed by the UNICORE client. Ideally, this interface is as general as possible in order to be able to deal with resource management systems besides UNICORE. The next section describes the requirements for such general job submission and management interface component.

The UNICORE suite offers a client library, the Arcon library, implementing an API which offers most of the desired functionality in dealing with the UNICORE server side. Unfortunately, this client library suffers from some minor deficiencies which mainly affect its use in a multi user multi threaded environment. This will be discussed in section 3.1.