Grid computing with IVOA standards and VOTech components

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Abstract. The EuroVO technology centre (‘VOTech’) is a design study for the emergent European Virtual Observatory. VOTech implements and augments the interoperability standards of the International Virtual Observatory Alliance. VOTech has a mandate to facilitate the use of compute grids in astronomy and approaches this in several ways: construction of an application grid as a common facade to regional compute grids; provision of a data grid, VOSpace, that can be made interoperable with local data grids; provision of library software, the ‘Astro Runtime’, that allows compute-grid jobs to exploit virtual-observatory services; and the formalization of EuroVO as a virtual organization with access rights to EGEE resources.

1. Introduction

The VO Technology Center (‘VOTech’) of the European Virtual Observatory (‘EuroVO’) describes itself thus:

The VOTech project is an EU FP6 funded design study which aims to complete the technical preparation for the construction of the European Virtual Observatory.

The project mandate specifies the use of grid technologies where appropriate, with particular reference to ‘offloading mass scale computational process onto the EGEE backbone’.

VOTech’s output consists in; experiments; software prototypes; technical education of potential service-providers in EuroVO; technical recommendations; papers promoting work in EuroVO; and a reference architecture. VOTech is not tasked to build or operate EuroVO, but the architectural output includes the production and distribution of software usable by service providers.

VOTech started officially in January 2005 and will complete in December 2008. The technical products of VOTech will be exploited by the EuroVO project Astronomical Infrastructure for Data Access (AIDA). To succeed, EuroVO must be integrated with the global, international virtual observatory (IVO). This means, inter alia, that EuroVO must respect and embrace the standards produced by the International Virtual Observatory Alliance (IVOA). All the science services of EuroVO should be usable by any IVO user in the world. Hence, VOTech im-

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4 http://www.ivoa.net
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VOTech implements IVOA standards; proposes new standards to IVOA; and develops European conventions to fill gaps between the VOA standards.

2. From compute grids to an application grid

In a classical compute-grid, where the grid’s commodity is simply cycles of execution, the grid standards comprise the grid middleware for submitting and monitoring jobs and the access-control arrangements. Both are traditionally chosen by grid providers and vary from region to region.

The virtual-observatory projects around the world desire to exploit separately-funded compute grids such as EGEE\(^5\) and TeraGrid\(^6\), providing a separate compute-grid for astronomy is considered redundant when multi-discipline grids are available at no charge.

Since the IVO does not run its own compute grid, and since regional grid providers do not agree on standards, it is not possible for IVOA to define a standard for access to a compute grid. VOTech could define a regional standard, by adopting EGEE’s technology and conventions, but this would not be globally interoperable.

VOTech has proposed to IVOA\(^7\) a standard for an application grid that forms a facade for compute resources. Services in the application grid have a common service-contract that (when adopted by IVOA) is interoperable throughout the IVO. Implementations of application-grid services are specialized a particular interface to compute resources. The simplest application-grid service runs jobs on the web-service host. Other implementations delegate to local compute-farms using Condor or delegate to EGEE using GLite.

By making the application grid a client of the compute grids, incompatibilities in the latter are hidden from IVO users and application-programmers. Service providers in the application grid can choose the grid middleware that best suits their needs.

In the application grid, the batch applications themselves are the commodity. Each application-grid service provides and registers a library of applications chosen by the service provider. An end user chooses an application from the IVO registry of resources and can then run it on any of a number of services, depending on the size of the job and the desired turn-around time. Registered applications are typically legacy code well-known to the astronomical community.

The registration of an application defines its input and output parameters. These metadata may be read by a desktop application and used to construct a basic user-interface to the remote, batch application. Such a desktop application automatically becomes a user interface to newly-registered batch applications.

The application-grid standards are a developed form of the Common Execution Architecture (CEA) developed by AstroGrid. The existing, operational application-grid implements version 1 of CEA, including the Common Execution Connector standard which is a standard web-service contract for application servers. CEA version 1 is a local, European standard.

Work is in progress to evolve the application grid to use CEA version 2, the latter being proposed to IVOA as a global standard\(^8\). The transition from local to global standards allows the details of CEA metadata to be refined. CEA version 2 replaces the CEC with the (draft) Universal Worker Service (UWS)\(^9\) standard of IVOA as the service contract.

VOTech intends to deliver a complete reference implementation of the application-grid software by the end of 2008. Pilot implementations, using earlier earlier versions of the standards, are already in service in EuroVO. Among them are the following applications.

- Meudon PDR model\(^{10}\)
- VONeural: neural-network tools for data mining\(^{11}\)

\(^7\) [http://www.ivoa.net/cgi-bin/twiki/bin/view/IVOA/IvoaGridAndWebServices](http://www.ivoa.net/cgi-bin/twiki/bin/view/IVOA/IvoaGridAndWebServices)
3. VOSpace: a data grid for the IVO

Compute grids work better when supported by data grids: the ability easily to access data is important to efficient use. IVOA, and hence VOTech, have the same problem with data grid as with compute grids: too many competing, incompatible sets of middleware. The solution here is the same: introduce a facade such that IVO users and desktop applications see a consistent interface to the data grid.

IVOA’s standard interface for data grids is VOSpace. It defines a minimal, but uniform, service contract for an access point to a data grid. Access is by reading an writing whole files; VOSpace does not allow a client to open a remote file and to seek within that file. VOSpace stores files in a hierarchy that resembles a distributed file-system.

VOSpace defines the service contract for a data-grid-access service but not the scope or semantics of the storage system. VOSpace is implemented both for storage local to the web-service host running the access service, and as a portal to iRODS.

IVOA has several versions of the VOSpace standard. VOSpace 1.0 (Graham et al. 2008a) defines a file space without a directory hierarchy. VOSpace 1.1 (Graham et al. 2008b) adds a directory hierarchy and the ability to embed links between spaces. VOSpace 2 is intended to replace the SOAP interface of VOSpace 1 with a REST interface while keeping the semantics of the system unchanged. At the time of writing, VOSpace 1.0 is an adopted Recommendation of IVOA and VOSpace 1.1 is a working draft.

Most data-grid software is focused on manipulating simple files: e.g. SRB, iRODS. Globus replica-location service. The data grid does not manage the contents of the file. VOSpace uses this simple approach as a basis, but allows particular nodes — ‘files’ or ‘directories’ — to have extra semantics that can be discovered from the service interface.

The additional semantics of special nodes in VOSpace concern the way that the data are stored and the availability of extra views on the data. As an example of special storage, consider a data table uploaded to VOSpace from a file. A basic VOSpace node will store and reproduce that file as a bit pattern. An advanced node might ingest it into a RDBM and provide an interface to query the table using SQL. As an example of a VOSpace view, consider a directory of files in VOSpace. An advanced directory-node might provide a view of itself that is a zip file containing the files in that directory.

4. IVO facilities for compute-grid users

EuroVO’s application grid is a way for astronomers to get benefit from a compute grid without learning to use grid middleware. Astronomers who already use a compute grid directly might wish to use VO facilities from their compute-grid jobs. VOTech supports two ways of doing this, known as ‘command coupled’ and ‘data coupled’.

In the command-coupled mode, the code on the grid element makes explicit calls to IVO services. I.e., the grid-aware program finds appropriate IVO web-services from the IVO registry of resources (which is itself a web service) and then exchanges data with those services. Grid users may code this directly if they wish; but the web-service contracts are moderately complex. VOTech provides a higher-level interface-library, the ‘Astro Runtime’ (AR) that simplifies access to IVO services. The AR is usable from any language that supports XML-RPC.

In the proposed data-coupled mode, we require the forthcoming implementation of VOSpace on iRODS and assume that the compute grid provides iRODS service to its compute elements. There is then one compute grid visible to both the IVO and the compute grid with interfaces natural to each. Therefore, a computational experiment may be run as an
IVO part and a separate grid part communicating through the shared data-grid. Typically, data will be selected from an archive on the IVO and the data extract stored in the data-grid. Processing can then be invoked on the computer grid and the results put back into the data grid for possible comparison with other IVO results.

Command coupling is simpler conceptually and more direct, but requires special applications to be developed for the grid that include the IVO interfaces. Data coupling is looser and can be used with legacy applications that already use data grids.

Command coupling of the compute grid and the IVO is possible now, using existing IVO service and the VOTech AR. Data coupling should be possible towards the end of 2008, as new implementations of VOSpace are deployed.

5. EGEE access for EuroVO users

Access to EGEE resources is granted to virtual organizations rather than to individual resources. Each such virtual organization informs EGEE sites of its membership by running an instance of the Virtual Organization Management Service (VOMS).

Some astronomical missions, e.g. Planck, are already virtual organizations with EGEE access, but many users of EuroVO are not covered by these arrangements. Therefore, EuroVO itself is to become a virtual organization with resource allocation on EGEE. The prototype VOMS instance for EuroVO is initially run by the Italian Institute of Astrophysics in Trieste. When the arrangements are completed, membership of EuroVO will allow automatic access to EGEE.

References

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