Distributed Modelling and Simulation for collaborative E-science in Grid Infrastructure

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Abstract: - E-science is collaborative science that is made possible by the sharing across the Internet of resources that is often very compute intensive, often very data intensive and crosses organizational and administrative boundaries. The semantic grid annotates the grid with metadata describing the resources it makes available. Semantic grid aims to incorporate the advantages of the grid, semantic web and web services. The aim of VVT information portal is to provide information about possibilities to use high performance computing available for the research and scientific workers of Slovak academy of sciences.

Key-Words: - Distributed computing, Grid infrastructure, Services, e-Science, Knowledge, Semantics, Ontology, Web portal

1 Introduction

The grid is an emerging infrastructure that aims at integrating distributed, heterogeneous, and dynamic computing resources. The main thrust comes from e-science, a term that designates large-scale scientific research carried out through distributed global collaborations enabled by the Internet. Such scientific enterprises typically require very large processing power, of the order of Tera instructions per second, and access to very large, Petabyte-scale, data collections.

Grids are tools for data intensive science that facilitate remote access to vary large amounts of data that is managed in remote storage resources and analysed by remote compute resources, all of which are integrated into the scientist's software environment. Grids are persistent environments and tools to facilitate large-scale collaboration among global collaborators.

There are three main issues that characterise computational and data grids:

- Heterogeneity: a grid involves a multiplicity of resources that are heterogeneous.
- Scalability: a grid might grow from few resources to millions.
- Adaptability: in a grid, a resource failure is the rule, not the exception.

1.1 Distributed computing and large scale simulation

Distribution introduces notions of concurrency and locality [10]. The traditional view of a computation involves the data, program and computational state (memory, processor registers) coinciding at one processing node. There are many techniques for achieving this in a distributed system: Remote procedure calls, Services, Distributed object systems, Database queries, Client-side scripting, Message passing, Peer-to-peer, Web-based computing.

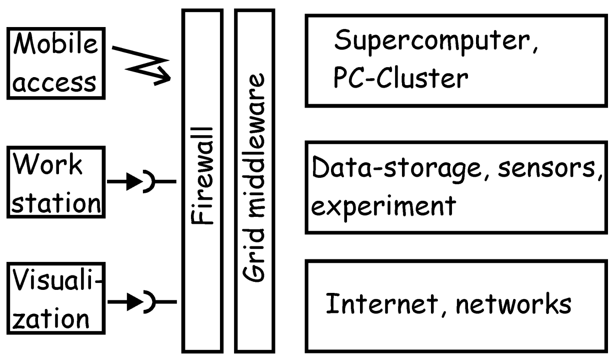

Fig. 1 Grid vision

Technology and architecture of grids involve several types of middleware (see Fig. 1) that sits between science portals and application, and the underlying resources (compute, data, and instrument).

Large-scale science and research engineering are done through the interaction of people, heterogeneous computing resources, information systems, and instruments all of which are geographically and organizationally dispersed.

Large-scale science and engineering problems [14] require integrating applications and data that are developed and/or maintained by different teams of researchers or obtained from different instruments.

Further, these activities almost always involve large data volumes and high data transfer rates to and from the instruments and data archives and between computing systems.

1.2 Motivation for Science Grids

Multi-disciplinary simulations (e.g. multi-component aircraft simulations) are an example of a class of applications that require aggregation and coordinated use of many widely distributed computing, data, and intellectual resources [4]. These system simulations require coupling codes and data across many compute and data systems located at multiple organizations.

Real-time operation of scientific instrument-based experiments [8] is a vision in high-speed distributed systems, which led directly to the grid. Real-time data analysis should allow experimenters to be able to interact directly with the subject of the experiment rather than running the experiment "blind" and reconstructing after the fact what happened. One goal of grids is to facilitate direct coupling of scientific experiments to large-scale computing systems for real-time data analysis and/or computation simulations of the subject phenomenon.

E-science is collaborative science [1] that is made possible by the sharing across the Internet of resources (data, instruments, computation, people's expertise...). Typically a feature of such collaborative scientific enterprises is that they will require access to very large data collections, very large scale computing resources and high performance visualization back to the individual scientists.

Scientific workflows allow scientists to automate repetitive data management, analysis, and visualization tasks, and to document the provenance of analysis results [11, 13]. A workflow can be viewed as a mechanism that orchestrates and enacts a range of local and remote services. Scientific workflow systems can often benefit from both, grid and semantic web capabilities. Taken together, resource management provided by grid services and knowledge capture and management through semantic web technologies, provide essential capabilities of any general purpose, large-scale scientific workflow systems.

Grids are being adopted and developed in several scientific disciplines that have to deal with large-scale collaboration, massive distributed data, and distributed computing problems [3]:

- Astronomers can locate, retrieve and analyse together all the available data from telescopes working at many wavelengths located around the world and in space to better study a particular class of objects.
- Climate modellers can run statistically significant samples of 100 year global coupled atmosphere and ocean simulations assimilating available observational data to better understand long term climate change.
- Molecular biologists can assemble databases of molecular dynamics simulations of tens of thousands or even more of atom protein molecules to understand their structure and functional behaviour for potential use in drug design.
- Medical researchers can use the information contained in hundreds of thousands of clinical records across the country to quantify the relative effectiveness of different cancer therapies.

2 Grids are evolving to a service-oriented architecture

Users are primarily interested in services - databases, applications, text extraction, and other elements that the user uses as his basic tools, something that performs a useful function, such as a particular type of simulation, or a broker that finds the best system to run a job. Even many grid tool developers, such as those that develop application portals, are primarily interested in services – resource discovery, event management, user security credential management, etc.

We can define a service in many ways [9]. In the context of computer science and electronic services, a service can be described as an aggregation of functionality published for use, or, in computing terms, a service is simply a function that can be invoked via a well-defined remote interface or a self-contained, stateless function, which accepts a request and returns a response through a well-defined interface.

Three generations of the grid can be identified [5]:

- First generation systems involved proprietary solutions for sharing high performance computing resources.
- Second generation systems introduced middleware to cope with scale and heterogeneity, with a focus on large-scale computational power and large volumes of data.
- Third generation systems are adopting a service-oriented approach, are metadata-enabled and may exhibit autonomic features.

Basic grid services are being deployed to support uniform and secure access to computing, data, and instrument systems that are distributed across organizations, resource discovery, uniform access to geographically and organizationally dispersed computing and data resources, job management, security, including single sign-on (users authenticate once for access to all authorized resources), secure inter-process communication.

Problems of enabling knowledge discovery services on grids are discussed in [15]. Although the grid today is still mainly used for supporting high-performance computing intensive applications in science and engineering, it is going to be effectively exploited for implementing data intensive and knowledge discovery applications. To succeed in supporting this class of applications, tools and services for data mining and knowledge discovery on grids are essential.

3 The semantic grid

The semantic grid (some authors talk about a grid with semantics) annotates the grid with metadata describing the resources it makes available, just as the semantic web does with the web. Semantic grid aims to incorporate the advantages of the grid, semantic web and web services.

Different terms that seem to be related are used. The knowledge grid is only dealing with sharing knowledge, while the semantic grid is dealing with sharing resources in general, not only knowledge, where well defined meaning is added to the resources. The cognitive grid is sometimes used interchangeably with the term semantic grid and is understood as intelligent management of grid resources. It can be defined as a grid that incorporates grid services, ontologies and knowledge driven services.

The scope of e-Science, as described in [10], includes information and knowledge. It has become popular to conceptualise the computing infrastructure as consisting of three conceptual layers:

1) Data/computation: This layer deals with the way that computational resources are allocated, scheduled and executed and the way in which data is shipped between the various processing resources. It is characterised as being able to deal with large volumes of data, providing fast networks and presenting diverse resources as a single metacomputer (i.e. a single virtual computer).
2) Information: This layer deals with the way that information is represented, stored, accessed, shared and maintained. Given its key role in many scientific endeavours, the world wide web (www) is the obvious point of departure for this level.
3) Knowledge: This layer is concerned with the way that knowledge is acquired, used, retrieved, published and maintained to assist e-Scientists to achieve their particular goals and objectives.

Although we often suffer from a deluge of data and too much information (info smog), all too often what we have is still insufficient or too poorly specified to address our problems, goals and objectives. In short, we have insufficient knowledge. According to [10], the knowledge lifecycle consists of:

- Knowledge acquisition
- Knowledge modelling
- Knowledge retrieval
- Knowledge reuse
- Knowledge publishing
- Knowledge maintenance.

The architecture of the grid is classically described in terms of 4 layers, each providing a specific function. In general, the higher layers are focussed on the user, whereas the lower layers are more focussed on computers and networks. Five-layered grid architecture is proposed in [12] that implements a knowledge layer and that can be used for building semantic grid infrastructure:

- Fabric layer (network layer + resources layer)
- Core middleware layer (secure access to resources and services)
- High level middleware layer (brokering, diagnostics and monitoring)
- Knowledge layer
- Application layer (tool, application and service-ware layer).

The modules implemented in the knowledge layer use semantic web's approach of making information understandable by computers. Computer understandable information is one that is annotated with semantics, which describes the meaning of the information. The annotations themselves have to be defined so that computers can interpret and reason with them.

3.1 Semantic annotation

The role of data descriptions, i.e., metadata [10], is critical in the discovery, analysis, management, and sharing of scientific data. The web is an infrastructure for distributed applications, where information is exchanged between programs rather than being presented for a human reader.

A standard way of expressing metadata, specifically resources on the web is RDF (Resource Description Framework). It is based on triples where each triple expresses the fact that an object O has attribute A with value V, written A(O,V).

Annotation, especially semantic annotation in the context of the semantic web [9], may be referred to as meta-data associated to actual data used during computations and to the process of generating such metadata. An annotation is a formal note added to a specific part of the data, or the whole data. There are three types of annotation in the context of grid services:

- Data annotation is the association of metadata to static data sets, i.e., data that resides in some kind of repository such as file systems, relational databases, web pages, etc. This is the most common type of annotation, and has received extensive attention in the semantic web community. In the context of grid environments, however, additional issues appear and should be taken into consideration, like data distributed across different administrative domains, or huge data sets and massive data access and movements.

- Service annotation is the association of metadata to dynamic services. The annotation of semantic services is important when services are to be automatically discovered and configured.
  We distinguish between functional and non-functional properties:
  - Functional properties relate to what the service offers (i.e. capabilities).
  - Non-functional properties of the service (such as pricing, timing, availability, security, discounts, trust).
- Provenance annotation is the association of metadata to results computed in a distributed grid environment. In the context of semantic grid services, it is important to know the source of data or their reliability.

3.2 Ontology driven knowledge management

While the basic concepts and languages of the semantic web are generally appropriate for specifying and delivering services at the information layer, they lack the expressive power to be used as the basis for modelling and reasoning with knowledge. To this end, the concept of ontology is necessary. Generally speaking, ontology determines the extension of terms and the relationships between them. In the context of knowledge and web engineering, ontology is simply a published conceptualisation of an area of content. The ontology may describe objects, processes, resources, capabilities or whatever.

Computer understandable information is one that is annotated with semantics, which describes the meaning of the information. The annotations themselves have to be defined so that computers can interpret and reason with them. A collection of annotations where their meanings are described is called ontology. Ontologies are used to capture knowledge about some domain of interest. Ontology describes the concepts in the domain and also the relationships that hold between those concepts.

According to [9] the stack of ontologies needed in semantic web is composed of the following ontologies: (1) an ontology describing the upper-level concepts that define the features of a service; (2) an ontology to describe problem-solving methods and the domain in which the service will be used; (3) an ontology to define the knowledge representation entities used to model a domain ontology; and (4) an ontology to describe the data types to be used in the domain ontology.

From methodological and technological point of view, three different approaches to semantic annotation can be currently found:

Linguistic semantic annotation: Nowadays the most used are frame-based semantic annotations. The frames can be simple – small static scenes or states of affairs, simple patterns of contrast, relations between entities and the roles they serve – or quite complex event types that provide the background for words that profile one or more of their phases or participants.

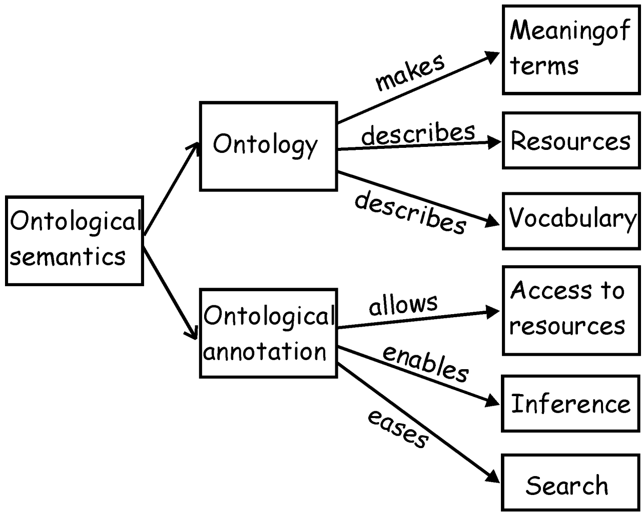

Fig. 2 Ontology and ontological annotations

Ontology-based semantic annotation: Ontological semantics (see Fig. 2) is a theory of meaning in natural language and an approach to natural language processing which uses a constructed world model – the ontology – as the central resource for extracting and representing meaning of natural language texts, for reasoning about knowledge derived from texts as well as for generating natural language texts based on representations of their meaning.

Hybrid (Linguistic and ontological) annotation: Linguistic annotation can be considered a special case of semantic annotation with regard to an ontology. Ontologies are formal specifications of a conceptualisation so that it seems straightforward to formalize annotation schemes as ontologies and make use of semantic annotation tools for the purpose of linguistic annotation. This makes this kind of annotation a hybrid one.

4 An accession to grid infrastructure

A web portal allows application scientists and researchers to access resources specific to a particular domain of interest via a web interface [10]. Unlike typical web subject portals, a grid portal may also provide access to grid resources. For example a grid portal may authenticate users, permit them to access remote resources, help them make decisions about scheduling jobs, allowing users to access and manipulate resource information obtained and stored on a remote database. Grid portal access can also be personalised by the use of profiles, which are created and stored for each portal user. These attributes, and others, make grid portals the appropriate means for e-Science users to access grid resources.

The Slovak EGEE information portal (see Fig. 3) created in the frame of the EGEE project in Slovakia [2, 7] provides grid related (especially EGEE grid related) information to users from all communities (science, education, industry, and developers).

The aim of VVT information portal of SAS [7] is to provide information about possibilities to use high performance computing available for the research and scientific workers of Slovak academy of sciences. One possibility is to use computer clusters connected in grid infrastructure, such as EGEE. Research workers of SAS can acquire access to high-performance clusters in Europe by membership in virtual organizations.

Fig. 3 Screenshot of EGEE SK portal

VVT information portal of SAS (see Fig. 4) gives comprehensive information about above- mentioned computing possibilities.

In Basic information part, one can find information about supercomputers in the neighbouring countries and an introduction to grid computing. Further, there is information about partners, activities, frequently asked questions, used acronyms, contact information and interesting links.

In Part for users, there is information about EGEE project, information about possibilities to try the grid using testing portals P-GRADE or GENIUS. Grid monitoring possibility will be also given.

The P-GRADE grid portal [6] is a workflow-oriented grid portal that enables the creation, execution and monitoring workflows in grid environments through high-level, graphical web interfaces. Components of the workflows can be sequential and parallel jobs. The P-GRADE grid portal hides the low-level details of grid access mechanisms by providing a high-level grid user interface that can be used for any grid.

P-GRADE portal is available as service for the different grid systems and also in Central European Virtual Organization (VOCE) of the EGEE grid infrastructure.

GENIUS is grid portal system giving - alongside with standard command line environment - the most simple and the most used usage mode of EGEE grid infrastructure services by gLite grid software.

For beginner users, the VVT portal provides flash animation of personal certificate requirement demonstration and flash animation of importing personal certificate into a browser in GENIUS–GILDA environment.

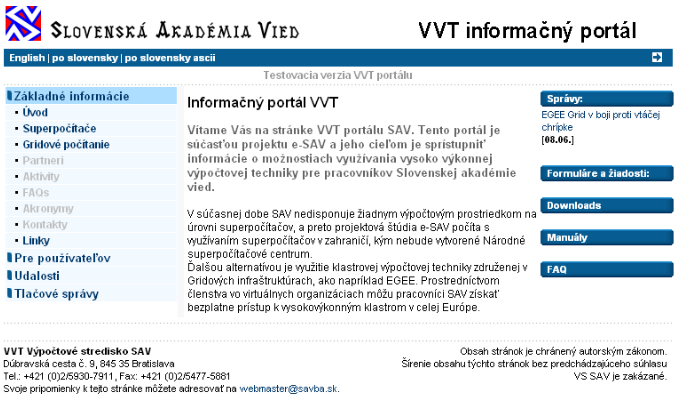

Fig. 4 Screenshot of VVT portal

VVT information portal also brings actual information about related events, e.g. conferences, workshops, seminars, courses, and news releases related to grids.

5 Conclusion

EGEE grid project aims to provide researchers in academia and industry with access to major computing resources, independent of their geographic location. The EGEE project also focuses on attracting a wide range of new users to the grid. Semantic grid aims to incorporate the advantages of the grid, semantic web and web services. The aim of VVT information portal is to provide information about possibilities to use high performance computing available for the research and scientific workers of Slovak academy of sciences.

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