Chemomentum - UNICORE 6 Based Infrastructure for Complex Applications in Science and Technology

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Abstract. Chemomentum, Grid Services based Environment to enable Innovative Research, is an end-user focused approach to exploit Grid computing for diverse application domains. Building on top of UNICORE 6, we are designing and implementing a flexible, user-friendly Grid system focussing on high-performance processing of complex application workflows and management of data, metadata and knowledge. This paper outlines Chemomentum vision, application scenarios, technical challenges, software architecture and design of the system.

1 Introduction

The European Chemomentum [1] project[1] joins today partners from nine institutions, developing an environment for workflow-oriented scientific as well as industrial applications. A wide range of end-users in science and technology with varying IT and Grid computing expertise is targeted. The Chemomentum system is designed to be generic and thus usable in a wide range of application domains. In the applications we are targeting, data management is of crucial importance. Secure access to stored data, metadata-based lookup, global identifiers and location management comprise a few of the many challenges in this area of research and development.

Within the project, a chemical application domain in the natural and life sciences and material science, is targeted. Domain-specific additions are provided

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that will enable the building of complex workflows for predictive modelling tasks in risk assessment, biotechnology, material and drug design. Our aim is to test-drive the system together with the installed applications in the context of the European REACH legislation [2], offering *in silico* tools that may prove crucial in reducing costs and the number of animal tests. The Chemomentum extends the experience of partners gained in the OpenMolGRID [3,4], EUROGRID [5], Gemstone [6], and DEMETRA [7] projects.

At the forefront of our efforts is high usability. Therefore, we follow a user-centric approach that allows for seamless and interactive usage of software by domain experts. A flexible client architecture, based on the Eclipse platform, will enable us and the domain experts to deliver focused end-user interfaces that combine ease of use with detailed access to the system's features. For special use cases, web based access will be provided. Furthermore, a client library will allow the Chemomentum system to be coupled to any type of domain-specific user interface.

To realise such a system, we selected UNICORE 6 [8] as Grid middleware, providing basic Grid services such as security, job execution and file transfer. Furthermore, it allows to write and deploy additional services, such as a high-level workflow processing system and data management services.

The remainder of the paper is organised as follows: In section 2, we describe the characteristics of the different application domains and scenarios that the Chemomentum software is targeted towards, from which requirements can be extracted. Section 3 explains in detail the architecture of the Chemomentum system. Section 4 provides an overview of the actual testbed infrastructure that can be used to test-drive the Chemomentum framework. Finally, section 5, concludes the publication and discusses the status and plans.

2 Application Scenarios

The main application drivers for Chemomentum originate from the chemical and biochemical application domains, in particular drug and material design, predictive modelling, and toxicological and environmental risk assessment of chemicals. In this application domain, a wide array of different technologies is used for computer based modelling. As a second, complementary application scenario supply chain planning will be used to verify the generality of the Chemomentum approach.

The Chemomentum project aims to implement generic interfaces for the following application families from biochemistry and chemistry:

- Linear and non-linear predictive model building;
- 3D coordinate generation for molecules from their connectivity information;
- Chemical conformational space analysis;
- Semi-empirical and *ab initio* quantum chemical calculations;
- Molecular descriptor calculation;
- Prediction of chemical property and activity values;

- Data filtering and preprocessing: clustering and artificial intelligence for rational chemical data pre-treatment;
- Molecular docking;
- Homology modelling of proteins.

A significant challenge in Chemomentum is the integration of such diverse application families in a way that enables the user to be creative and explorative, so that innovative ways of using existing tools for a variety of application scenarios are possible. This is achieved through the Chemomentum workflow engine (see section 3.1). In the following, details about the use of these applications in certain application scenarios are described.

Quantitative structure-activity relationship. (QSAR) methods are key technologies behind computer based modelling of chemicals, including chemical and physical properties and biological activities. The QSAR methodology assumes that the activity of chemicals is determined by their molecular structures and that there exists a mathematical relationship, $P = f(s)$, between them, where P is the modelled activity and s is the numerical representation (i.e. molecular descriptors) of the molecular structure. Molecular descriptors in this context are used to calibrate various chemical properties or biological activities among a grouping of chemicals. QSAR is a complex application scenario. The process starts with the design of data sets for the model development and predictions which may require access to a variety of heterogeneous data sources. This is followed by the geometry optimisation of molecular structures (see paragraph on Quantum Chemistry) and the calculation of molecular descriptors. Both of these steps are data parallel and therefore ideal candidates for Grid computing. Once the experimental values and molecular descriptors are available, statistical methods are applied for the development of the actual mathematical model. Finally the developed QSAR models can be used for predicting activity values of chemicals from their molecular descriptor values. Our previous examples of the use of Grid technology in QSAR are the modelling of aqueous solubility [9], HIV-1 protease inhibitors [10], and acute toxicity [11].

Quantum chemistry. (QC) represents a collection of theoretical and computational methods that employ approximate solutions to the Schroedinger equation $\hat{H}\Psi = E\Psi$ to characterise the structure, properties and mechanism of reaction of molecular systems. The utilisation of QC approaches is of particular importance for addressing questions involving chemical reactions where bonds are broken or formed, and to obtain results with very high accuracy. Prominent application areas in both academia and industry include the elucidation of reaction mechanisms, the prediction of molecule properties (e.g., as part of QSAR procedures), and the computation of, for example, the effects of solvation or spectroscopic information. Unfortunately, depending on the level of their theoretical foundation, QC methods can be quite complex and computationally intensive. This means that such calculations are typically not carried out without significant intervention of the user, and in many cases require knowledge in

the field in order to properly set up and carry through computations to address questions of structure and reactivity in molecules. QC approaches are also often combined with approaches from classical mechanics, to enable the treatment of larger (e.g., biological or material) systems. Together with high-throughput investigations involving many molecules, these are the main application areas where QC can benefit from Grid computing, data, and workflow processing (see, e.g., Refs. [12,13,14] for earlier approaches). A major challenge for Grid computing in QC is that many of the highly used computer programs are legacy, and that each has their own input and output formats. However, there are now European efforts under way to agree on standardised data-exchange formats [15]. The quantum chemical program packages that will initially be tackled within the Chemomentum project include MOPAC [16] and GAMESS [17].

Molecular docking. describes the procedure of finding optimal structural fits of one component molecule within another, typically a ligand in a protein pocket. Most importantly, docking is used in the early stages of the pharmaceutical drug design pipeline, and has thus gained considerable interest from academia as well as industry. Typically one begins with a previously determined 3D structure of a protein with a certain biological function, and investigates possibilities for modification of that function. This could involve a functional modification of a ligand already embedded in the protein, or, the 'docking' of a small molecule (i.e., a potential drug candidate). The idea is to use computation to search for an optimal orientation of the two molecules (i.e., usually a binding of the ligand at the natural activity site of the protein). In this procedure, each calculation step involves computation of the free energy of the complex formation, to be determined by an empirical function. Such calculations are usually embarrassingly parallel, and therefore highly suited for high throughput-oriented Grid computing. A clear demonstration of this is the Docking@Home [18] project. Often, a number of preparation and analysis steps is necessary, for example, to apply more accurate energy functions to score the ligands, after an initial set of complexes has been identified. As such, molecular docking also profits from workflow approaches. A typical representative for a widely-distributed docking program package is AutoDock [19]. However, molecular docking methods are still topic of intensive research, in particular to obtain better scoring functions. At the University of Zurich for instance, we are currently developing a Grid-enabled docking procedure based on quantum chemistry and biomolecular continuum electrostatics [20].

Homology modelling. is a fundamental and widely used tool in molecular biology. Using such tools, biologists are able to compare DNA or protein sequences from the same or different organism. In this way, evolutionary relationships between organisms can be explored, and biological functions of new sequences can be predicted. The main task is to find statistically significant local similarities between pairs: a user-defined (protein or DNA) sequence and sequences from databases.

All of these types of application scenarios are used in many aspects of chemistry and life science related fields. Prominent examples include:

The European REACH policy. (Registration and evaluation of chemicals). Substances have to be carefully evaluated and assessed for possible risks to human health and the environment prior to marketing and distribution. This requires massive efforts in terms of time, money and animal testing. The Chemomentum system has the potential to reduce the need for animal testing as such by providing a wide variety of solutions for the computational, *in silico*, testing of chemicals. QSAR has been selected as one of the key predictive modelling techniques for REACH.

Research and development in the pharmaceutics. Computational solutions are more and more used to virtually screen large databases of compounds in order to identify potential leads concerning a given biological activity. The size of the databases requires extensive computing solutions that can be achieved via efficient use of Grid technologies. In particular, emphasis should be given to the high level of security while working with the data with significant intellectual property risk.

Research and development in biotechnology. The biotechnology sector is using the largest databases for screening and determining technologically relevant new substances. This determines their need for the extensive computational solutions to reduce the time to product and also the costs.

The scope of Chemomentum system is not limited to scientific applications. The overall architecture is generic and will be also tested on completely unrelated applications in the retail sector, such as demand prediction in supply chain management.

Supply chain planning. The purpose of this application is to apply the capabilities offered by Chemomentum to a complex scenario where different and heterogeneous applications need to work together in a common environment. The scenario is based on the tools offered by TXT e-Solutions (TXTPERFORM suite [24]), but it has a sufficiently generic degree of validity. The focus involves three different phases: 1. Demand and merchandise forecasting; 2. Assortment and allocation plan; 3. Replenishment planning. These phases are usually connected together to form a complex workflow that involves the usage of different applications. This scenario is posing some major challenges: First, in the solution that is currently deployed, maintenance costs are high due to usage of different applications requiring heterogeneous environments. A Grid based integration solution can be expected to reduce costs by providing seamless and unified access to these heterogeneous enviromnents. Second, the control of the entire workflow needs to be human driven, which is the only possible way to have full control on the behaviour of the applications.

The solution that Chemomentum is investigating is based on workflow automation, where applications are located behind an infrastructure that allows a common access to their functionalities and resources.

3 Architecture of the Chemomentum System

This section provides a birds-eye view on the Chemomentum architecture, and the primary associated functional systems. These functional systems will be explored in more detail in the subsequent sections.

As Figure 1 shows, Chemomentum consists of five major sub-systems.

- Workflow System: Executing and managing workflows, for details see section 3.1;
- Data Management: Services for accessing data and metadata, for details see section 3.2
- Grid Management: Monitoring and managing all services making up the Chemomentum systems [2];
- UNICORE 6 Hosting Environment: Hosts fabric services (such as job execution) provided by the UNICORE Grid middleware. The additional Chemomentum services will make use of the UNICORE 6 hosting environment, to benefit from its features and integrate with the UNICORE 6 security, see section 3.3;
- Client Layer: graphical interfaces for end-users and administrators for accessing and managing Chemomentum services, for details see section 3.4.

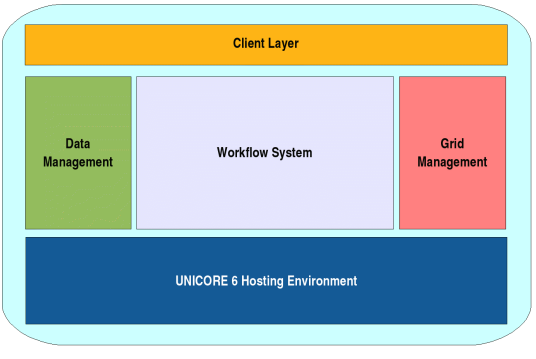

Fig. 1. Overview of the Chemomentum Architecture

3.1 Workflow Processing

Workflow processing is at the core of the Chemomentum system. As Figure 2 shows, the Workflow System is subdivided into two layers of abstraction: the Workflow Engine and Service Orchestration layers. The Workflow Engine processes a workflow on a logical level, whereas the Service Orchestrator deals with the actual execution and supervision of tasks using different services and resources on the Grid. Thus, the workflow processing logic is cleanly separated from the re-occurring invocations of low level Grid services.

[2] The Grid management components are not covered in detail in the present paper due to space constraints.

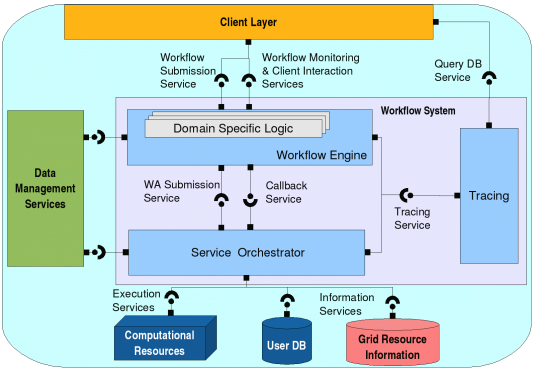

Fig. 2. Three-tier approach to workflow

In order to handle different domain specific workflow languages, the workflow engine translates incoming workflow descriptions to a generic workflow language using pluggable Domain Specific Logic (DSL) modules. Splitting and distribution of computational effort in order to maximise throughput and to make most efficient use of the available computational resources is one of the core goals of the Chemomentum system. Each activity of the translated workflow results in an atomic unit of work for the Grid, a so called "Work Assignment". Work Assignments (WAs) are abstract, in the sense that they are not bound to specific service endpoints on the Grid. They are individually submitted to the Service Orchestrator for execution. Due to dependencies and conditions in the translated workflow, WAs cannot be executed in arbitrary order. For instance, one WA may depend on the output data of another WA. The Workflow Engine keeps track of such preconditions and does not submit WAs with unmet preconditions. The Service Orchestrator transforms each incoming WA into a job, given in Job Submission Description Language (JSDL). It exchanges the logical names of input files for addresses of physical file locations. It submits the job to a computing resource, supervises job execution and informs the workflow engine of job completion or failure.

3.2 Data Management

The objectives of the Data Management System (DMS) within Chemomentum are to provide data storage and retrieval functionality and to give a global data view independent of actual data location. The DMS establishes a distributed data store that can be used to house data and, even more important, corresponding metadata that thoroughly describe the data stored. The metadata include typical descriptive information like for example the user who produced the data, the date of generation/modification or the applications that were used to produce the data. Additionally, meta information specific to a domain can be stored, e.g. the list of properties used in building a QSAR model. The set of domain specific metadata items to be stored is flexible.

A key feature of the Data Management System is the user-transparent access to external data sources of different kinds, e.g. web-based databases, flat files, etc. The data from the internal data store and the external databases is presented to the requester in data views specifically adapted to its demands. This could be, for example, a view that focuses on a specific domain or application and integrates the information gathered from external databases with data stored in the internal data store.

The DMS is accessed by the Workflow System when executing a workflow. Input data necessary for executing the workflow is retrieved, output data generated by the workflow and the metadata that describes this output data is stored. The end-user can access the data management system to browse the data in the internal data store – highly aided by the extensive metadata; access data in external databases, or manually upload interesting files to the internal data store.

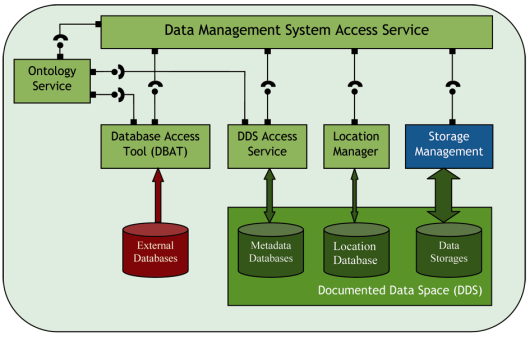

Fig. 3. Data Management System architecture

The heart of the Data Management System is the Documented Data Space (DDS), see Figure 3. It is composed of Metadata Databases, Data Storages and a Location Database. The Data Storages contain data in flat files, typically input and output data produced by Chemomentum. The Location Database acts as a global file location directory by indexing those files and assigning them globally unique logical names. The Metadata Databases contain metadata that describe the files in the data storages, referencing them by their logical names.

The central interface to the DMS is the Data Management System Access Service. It forwards service requests to the appropriate service(s), collects the results and returns them to the requester. For example, in case of a data store request containing files and metadata it
(a) instructs the Storage Management Service to stage out the files from the temporary data store to one of the Data Storages in the DDS;
(b) instructs the Location Manager Service to index the uploaded files in the Location Database and generate logical names; and
(c) instructs the DDS Access Service to insert the metadata into one of the Metadata Databases in the DDS.

The Database Access Tool (DBAT) serves as a uniform interface to external databases. It transforms a query to the data management system into the native query language used by the external database, queries the external database and transforms the result back into a format the client understands. The Ontology Service supports the DBAT in providing information, e.g. synonyms of molecular names, to broaden queries to external data sources. It provides knowledge about types and vocabulary necessary to interpret data retrieved from external sources or to store domain-specific data. The metadata vocabulary is not fixed. Given that different scientific fields and simulation environment have different needs, new domains can easily be added to the system to meet these needs and existing domains can be extended. For each domain a vocabulary is maintained, which does not only include metadata items with their respective data types, but also further properties like a human readable name or information on its range. Currently the domain vocabularies are provided as a relational database schema. Metadata and knowledge representation models like RDF[25] and Topic Maps[26] that could allow an even more expressive description of the metadata of a domain are under investigation for use in Chemomentum.

Users of the data management system do not have to know about the vocabulary of a domain beforehand. Existing domains and their vocabularies can be queried for and retrieved whenever needed. This allows to develop generic clients, e.g. a data browsing client that enables the user to browse through stored metadata regardless of the domain.

3.3 Security Considerations

The present system adopts the security infrastructure of UNICORE 6, which is based on X.509 certificates, and offers fine-grained access control to services based on user attributes stored in a user database (XUUDB). This is sufficient for simple use of UNICORE 6, for example to decide whether a given user has the permission to run a job or access a storage service.

However, Chemomentum has more complex requirements on security. For example, trust delegation mechanisms are obviously needed for Chemomentum to support the secure use of the chain of services needed to process a workflow. The Explicit Trust Delegation model of UNICORE 5 [27] is a first step, but becomes impractical for larger Grids. At the time of writing (June 2007), the final trust delegation model in UNICORE 6 was not fully defined.

Also, the Data Management System needs access to even more detailed user permission data, similar to the level of detail offered by a relational database system, in order to provide fine enough access control. Thus, the access control available in UNICORE 6 is not sufficient.

Similarly, the user management in UNICORE 6 as available in June 2007 is not sufficient for large Grids, and complex virtual organisation structures. Thus, Chemomentum aims to provide a security service offering Virtual Organisations (VO) based user management and storing extended user attributes for making access control decisions. This is intended as a drop-in replacement for the basic UNICORE 6 solution.

Irrespective of the security middleware in place, it is well known that in certain application domains data can be so sensitive that the data owners will not allow to send it over a network. Chemomentum caters for these users by allowing private data to be stored and maintained physically at a specific site, in a private instance of the DDS service discussed in 3.2.

3.4 Clients

The client layer of the Chemomentum system provides the associated interface to end-users in the different targeted application domains (see section 2) and to administrators of the infrastructure. In this way, the Chemomentum services can be easily and uniformly accessed and managed. Our main focus is on graphical user interfaces, but for certain user communities, command line interfaces might be of interest. We are developing three types of clients: (i) Eclipse [28] Rich Client Platform-based client, (ii) web portal and (iii)third-party clients.

As a common application programming interface between the clients and the server-side infrastructure, a Basic Chemomentum Client Library (BCCL) has been created. The BCCL will, in particular, enable third-party tools, for example domain-specific user interfaces such as Gemstone [6], to integrate into the Chemomentum system.

As an initial step towards building the Chemomentum graphical user interface, GridBeans [21], based directly on the underlying UNICORE environment, have been developed and already deployed in the testbed (see also the next section). GridBeans can later be included into the rich client, or used independently. A generic GridBean suitable for any type of UNICORE-deployed application has been developed and successfully tested with the quantum chemistry package GAMESS [17]. Furthermore, a GridBean for the BLAST application is available [22]. It is designed to provide a user interface organised in a similar way as the one on the NCBI-BLAST [23] website. The main purpose is to provide ease of use, particularly by scientists who are used to the NCBI website and may not want to learn about a different interface. Also, GridBeans for QSAR model development have been developed.

4 The Chemomentum Testbed

To evaluate and test the software, Chemomentum provides a special site [29], which allows the wide public to test new system capabilities. Everybody can use the test installation to evaluate the software. The site allows to request a test certificate, valid for the test site, and when certificate is issued it allows do run grid jobs on a dedicated virtual system. The testbed is intended to run quick jobs.

Setting up of a pilot installation available to a wide user community involves a security challenge. In order to minimise the risk we have used a virtualisation technique to protect the server integrity and to offer a reasonable security level. The execution system has been set up on an isolated virtual host, and be treated

as compromised all the time. A further benefit of the virtualisation technique is the possibility to share the images of the virtual systems, which allows for fast and easy replication of the pilot installation.

UNICORE provides client applications to access distributed resources. These clients offer a powerful and extensible interface to the resources, but a number of users expect web access to the Grid. This motivation, clearly expressed in the Chemomentum project, resulted in the redesign of the UNICORE Client framework to allow easy integration with portals. A client library has been created which allows for fast development of web interfaces to the Grid resources.

5 Conclusions and Outlook

Driven by application requirements, we have designed a UNICORE 6 based Grid system focussing on ease of use, high-performance processing of complex scientific and industrial workflows and elaborate data management solutions.

We have found UNICORE 6 to be an excellent basis for such a system, as its open structure makes it easy to build custom services and integrate them into the basic infrastructure. The security requirements of Chemomentum were not fully met by the beta version of UNICORE 6, but we expect marked improvements in this area with the availability of the final UNICORE 6 release.

The presented design has been validated in a number of prototype implementations. A first implementation of the full workflow processing stack is available, based on the Shark [30] XPDL workflow engine. The Data Management System in the first prototype provides storage and retrieval of data from the QSAR domain with predefined metadata. A client component allows to browse through data stored in the DDS.

The first release of the basic software framework, based on UNICORE 6 final, is targeted for August 2007, which will be available on the public testbed in October 2007.

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