Scientific workflow design: theoretical and practical issues
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Chapter 1

Introduction

Over the last few years grid computing has emerged as a concept for exploiting massive distributed computing power and managing massive distributed data. Closely related is the concept of enhanced Science or e-Science which aims to support scientific experiments through the use of grid computing and associated tools. The research presented in this thesis was conducted within the Virtual Laboratory for e-Science project (VL-e)\cite{VL-e} which states as its aim:
The aim of the “Virtual Laboratory for e-Science” project is to bridge the gap between the technology push of the high performance networking and the Grid and the application pull of a wide range of scientific experimental applications. It will provide generic functionalities that support a wide class of specific e-Science application environments and set up an experimental infrastructure for the evaluation of the ideas.

The introduction will give a brief explanation of the grid, what functionalities and tools constitute a virtual laboratory, and go into the basics of workflow tools and workflow design, the focus of this thesis.

1.0.1 Grid

In 1997 the most widely used basis for grid computing, the Globus Toolkit \cite{Globus}, started out as a way of linking parallel computing clusters as well as high speed research networks into one virtual system. It is thus no surprise that the first e-Science applications originated in projects which consume a lot of supercomputer power such as the Large Hadron Collider at CERN\footnote{http://lhc.web.cern.ch/lhc/}. Over the last few years both e-Science and grid computing have evolved to deal with ever more heterogeneous resources and to solve problems other than massive data and large scale computations.
One of the early benefits of grid computing was sharing computational, data storage and experiment related resources. Currently the list has expanded it now includes:

- computational resources, cluster computers or idle time on desktop pc's
- storage resources, raid disk arrays or harddisks in a desktop
- software resources, any software which can run on the grid in some way.
- data, that has relevance to many people, for instance genome data
- measuring equipment, such as microscopes and telescopes
- human experts, who offer a service via grid infrastructure

These resources are available for sharing through grid middleware. People with grid access can schedule jobs including shared software resources onto computational resources. Shared data can be stored in a transparent distributed fashion on storage resources. Measurement equipment can be remotely controlled as well as store its output data on storage resources through the use of grid middleware. In exceptional cases where analysis or other tasks can only be done by human experts, interaction with these experts can be offered through grid infrastructure.

This expansion of the types of shared resources was enabled by the current trend of moving to a Service Oriented Architecture (SOA), where resources are shared using web or grid services. Most notably the Open Grid Services Architecture (OGSA) [64] builds on the Globus Toolkit to allow the implementation of a Service Oriented Architecture on top of the grid.

Grid computing and e-Science have now been adopted by many more and diverse fields of science and are still growing. Grid computing has also started to branch out into the commercial domain with companies such as IBM\(^2\), SUN\(^3\), HP\(^4\) and Microsoft\(^5\) actively supporting e-Science projects. Their aim is not only to support science but to pave the way for large scale commercial use of grid computing and associated concepts. What attracts them is the concept of virtual organizations, defined in grid context as “flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources” [65]. However until issues such as security, protection of intellectual property, accounting and access are fully developed commercial adoption will be limited. Within the scientific

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\(^2\)http://www-1.ibm.com/grid/
\(^3\)http://www.network.com/
\(^4\)http://www.hp.com/go/grid
\(^5\)http://research.microsoft.com/ur/us/escience/
community that is adopting e-Science, these issues are less important. The scientific community is thus at the forefront of development for tools supporting virtual organizations. This can be seen in the amount of scientific projects around the world which have similar aims to the VL-e project. The EU has funded [2, 9, 6, 5] and continues to fund many projects building on grid technology [8, 11]. At the national level the UK e-Science programme [20] has lead the way but many other national programmes including the VL-e exist [21, 12, 14, 1, 7, 93, 15]. There are in fact so many projects that it is beyond the scope of this introduction to give an exhaustive overview. Within these many projects workflows have emerged as a key component for instance in projects such as the EU funded K-Wf Grid project [17] and in the UK funded MyGrid project [18]. Next is an explanation of what a virtual laboratory is and how workflow fits within the VL-e project.

1.1 Virtual Laboratory

In the VL-e project a virtual laboratory consists of

- Storage and computational resources that are grid enabled, that means accessible through grid middleware.
- Programming tools for creating (high performance distributed) applications that run on the grid
- Problem solving environments for running existing application specific (legacy) code on the grid
- Visualization and virtual reality interfaces
- Information management tools for dealing with distributed data
- Scientific Workflow Management Systems (SWMS) enabling sharing of (software) resources and cooperation

The VL-e aims to be generic, thus e-Science applications from diverse research areas are supported. The VL-e is of interest to these diverse research areas because it offers a sharing of the burden to gain access to the computational power and storage capacity of the grid. As an additional benefit scientific (software) resources and the knowledge on how to use them can more easily shared when this is done in a uniform environment. In this thesis we are interested in Workflow design and the way it can help the sharing of resources, so we will now introduce the concepts of workflow and SWMS.
1.2 Workflow and Scientific Workflow Management Systems

Resources in e-Science are never used on their own. Experiments in e-Science are therefore often performed with the help of Scientific Workflow Management Systems (SWMS), where workflows are used to define all connections and parameters of resources involved. While for the first e-Science applications workflows often took the form of batch jobs manually programmed in the users favorite text editor, currently most use a graphical workflow representation. The user defines a diagram with blocks representing resources and arrows indicating connections in a manner similar to programming in a visual programming language such as visual basic. A SWMS represents resources as workflow components, the links between workflow components represent data connections, the combination of workflow components and connections is called a workflow topology. A workflow engine takes care of the execution of the workflow which can be divided in two tasks. First, there is the orchestration of the workflow, which components are allowed to execute and which links transmit data at any particular time. Second, there is scheduling, that schedules each execution task onto available computational (grid) resources. Although SWMS can share measuring equipment, data and human experts, the main focus is on sharing software resources. Grid technology such as the globus toolkit takes care of sharing computational and storage resources. The place of resources in SWMS and the grid is illustrated in Figure 1.1.

When sharing knowledge on how to use a resource, workflows offer an opportunity to include knowledge on the context in which resources are used. This type of knowledge is commonly referred to as Provenance, which
can be divided into multiple types. Data Provenance is a record of the transformation and aggregation of data by workflow components which is stored as meta-data. Similarly the provenance of workflow components is stored in the collection of workflows in which it occurs.

1.3 Sharing Resources

The usability of workflows and the ability to express knowledge about an experiment through workflows is very important for e-Science. Workflows enable e-Science and grid computing to fully exploit the possibilities of sharing resources as well as offering greater usability in general.

This sharing of resources can lead to a major shift in how science is conducted, if indeed it becomes as useable as envisioned by its proponents[81]. The first step in this thesis will therefore be to explore the differences between e-Science and science in general and learn whether e-Science is or can become a paradigm shift for the way science is conducted. This look at e-Science will be concluded with a scenario of what a future scientist would do in a fully developed virtual laboratory for e-Science. This scenario will form a reference to which we can compare currently available tools and methods for sharing resources. In this way we can determine to what extent these tools and methods are already sufficient, and what still needs to happen to achieve this future scenario. Workflows are a central tool to enable the sharing of resources, thus we concentrate on a methodology for designing workflow components that can be shared.

In workflow design many issues exist relating to both the control of processes and data flow, that have long been present in parallel computing. Yet the formal approach to software design that has existed for a long time for parallel computation has not been adopted for workflow. Workflow is different in nature from parallel computing in general in that development of workflows happens at multiple levels of abstraction, there is a strict separation between the individual workflow components and the coordination that happens through the connections of these components. As the large majority of resources shared in SWMS are workflow components representing software resources, this leads us to an important question:

What is a proper design methodology for both workflow components and workflow topologies that supports the sharing of software resources?

There are several stages to finding a proper answer to this question and it incorporates both a practical and a theoretical side.

The first side is studied in two different uses of one type of software resource; data assimilation tools. Data assimilation is a technique for mini-
mizing errors both in observations as well as in the model involved in doing predictions. It finds its origins in climatological and geographical research such as weather prediction and oceanography. This type of error minimization occurs frequently in scientific experiments therefore data assimilation tools have great potential for reuse in areas other than weather prediction and oceanography. In the two cases which are studied in this thesis it is used for the prediction of bird migration and the long term prediction of road traffic. This look at the practical side will try to answer the following questions, what data assimilation tools are currently available and to what extent do they support incorporation in a virtual laboratory right now? Through employing data assimilation in two unrelated fields, what are the areas where a workflow design methodology for data assimilation can support the construction of an experiment?

The theoretical side is approached by looking at the theoretical limits of what constitutes a workflow design space and which formalisms are most suitable to reason about workflows inside of this design space. Design space and design methodologies have been the subject in many related fields such as embedded systems design[107, 108] as well as parallel computing[55]. While formal approaches to workflows exist they focus mainly on the expressiveness of workflow design[24] or the automatic construction of workflows[71]. A design methodology for going from initial experiment hypothesis to concrete executable workflow has not yet been documented. The theoretical side will try to answer the following questions: How does the methodology for e-Science relate to scientific methodology in general and what is the importance and place of a design methodology for workflows and workflow components within the e-Science methodology in general? What is the workflow design space and what are its limits; what can and cannot be achieved in workflow design? What is a suitable formalism to reason about workflows in such a design space?

On the basis of a careful study of both these practical and theoretical issues, a method for sharing data assimilation resources is proposed. The conclusion of this thesis will try to answer the following:

- To what extent a methodology for sharing data assimilation as a software resource can provide answers to the main research question, the proper design methodology for shared software resources in general?
- Do current tools lend themselves to sharing resources, and what are the areas that need improvement to realize the full potential of e-Science.

The thesis starts with describing how e-Science methodology relates to general scientific methodology and what future use of a fully developed virtual laboratory could look like in chapter 2. In the following chapters the theoretical issues are addressed, both workflow design space in chapter 3 and suitable workflow formalisms in chapter 4. The practical part starts
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with an overview of what existing Scientific Workflow Management Systems have to offer in chapter 5, followed in chapter 6 by an introduction into data assimilation. The details of both bird migration and traffic prediction case studies are presented in chapter 7. Lessons learned from the investigation into both the practical and theoretical issues are applied in chapter 8 with a method for sharing data assimilation resources in a workflow environment. This method is presented as an ideal workflow for data assimilation. Finally other issues encountered during research are discussed and conclusions are reached in the final chapter.