Editorial

Special section on workflow systems and applications in e-Science

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\textbf{A R T I C L E I N F O}

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Rapid development of Internet and Grid technologies has greatly extended the number of resources which scientists can apply for research. More and more scientific advances are achieved via experiments which consist of large volumes of computing tasks and data. Scientific Workflow Management Systems (SWMS) are a key technology to integrate computing and data analysis components, and to control the execution and logical sequences among them. By hiding the complexity in an underlying infrastructure, SWMSs allow scientists to design complex scientific experiments, access geographically distributed data files, and execute the experiments using computing resources at multiple organizations. In this way, domain scientists can effectively use available resources while focusing on the logic of the experiments instead of low level technical details.

During the past few years, scientific workflow systems and applications have attracted enormous research interest. Fig. 1 shows an increasing number of workflow related publications in the journal of Future Generation Computer Systems (FGCS). A number of research foci can be found in recent publications. Running legacy applications on the Grid is essential for the domain scientists to extend execution scenarios of their experiments. Wrapping components in a scientific workflow using a standardized architecture, such as services, improves the reusability of the components and also makes the integration easy. McGough et al. [1] present a service architecture named GridSAM to manage the job submission onto Grid and to manage different abstractions of tasks at runtime. Glatard et al. [2] demonstrate how services can be dynamically grouped and optimized in the workflow enactment and scheduling at runtime. Interoperability between different workflows is essential to realizing cooperation between different scientific experiments. Describing distributed Grid resources using semantic web technologies promotes high-level sharing of components and workflows [3]. The scientific workflow has proven to be a key technology to enhance many research disciplines to manage the experiment processes and automate computation; one of the examples is the data mining application [4].

Several workshops and special issues have been organized to extensively discuss research topics covering the lifecycle of scientific experiments, i.e., the experiment design, execution, data process and publication. These fora not only cover a wide spectrum of interests in the SWMS development and application, as shown in Fig. 1 but also have different foci, e.g., WSES\textsuperscript{1} addresses the main challenges in system development, SWF\textsuperscript{2} highlights the service oriented architecture in scientific workflows, SWBES\textsuperscript{3} foci on using industrial workflow standards in e-Science, and WORKS\textsuperscript{4} has clear interests in workflows in data intensive applications. As a follow up of these workshops, several special issues on scientific workflows have been published in the journals of Scientific Programming [5], and Concurrency and Computation: Practice and Experience [6]. The book workflows for e-Science [7] is a good collection of publications about this subject.

Moreover, scientific workflows have also been the main objective of several projects: the Dutch Virtual Laboratory for e-Science (VL-e),\textsuperscript{5} the EU funded Knowledge Workflow Grid (K-WGrid)\textsuperscript{6} and the Virolab projects.\textsuperscript{7} The Dutch VL-e project aims at sharing and transferring knowledge in the form of mature experiments encoded using workflow descriptions from

\textsuperscript{4} The workshop on Workflows in Support of Large-Scale Science, http://www.isi.edu/works07/.
\textsuperscript{5} http://www.vl-e.nl.
\textsuperscript{6} http://www.kwfgrid.net/.
\textsuperscript{7} http://virolab.org.
Modeling and composing a workflow is a basic functionality provided by workflow systems. McPhillips et al. [9] argue, from the usability point of view, that a workflow system should have several important properties, such as declarativity, well-formedness, predictability and recordability and they propose an assembly line based on a workflow representation metaphor called COMAD. The workflow system adds variations and realizes languages to describe the control and data flows in applications in a specific set of domains. Many workflow systems provide a text or graphical interface for computing workflows. However, manual composition is not always practical and it is difficult to graphically render large scale and complex workflows. Using semantic technologies for (semi)automatic generation of workflows is an important trend. Mapping an abstract workflow description onto concrete computing and data storage resources, and orchestrating the runtime behavior of workflow processes comprise the basic execution procedures of a scientific workflow.

Decoupling the model of computation from the implementation of the workflow engine allows composing workflows that include multiple models of computations; however, it also requires user knowledge in understanding different combinations of the model of computation. Goderis et al. [10] discuss the characteristics of different workflow execution models and analyze compatibility between computational semantics of different execution models provided by the Ptolemy system. It is an important step towards providing high-level workflow composition support. Most of the SWMS are historically driven by applications in specific domains, e.g., bioinformatics, high energy physics and astronomical observations.

E-Science applications require the investigation of the common characteristics of domain-specific systems and their implementation as part of a generic framework. A number of research projects such MyExperiment8 and VL-e aim at developing a Grid-enabled generic framework where scientists from different domains can share their knowledge and resources to perform domain specific research. Sharing knowledge and resources requires more interoperability among the major workflow management systems. As more sophisticated solutions are needed to achieve a seamless integration of workflows, approaches such as the workflow bus [11] developed in the context of VL-e present a potential solution to the interoperability problem. Different requirements for supporting domain specific applications are an important driving force for the development of workflow systems. De Roure et al. [12] present a social web based cooperative virtual research environment, called myExperiment, for sharing workflows and experiments. A user can publish workflow descriptions, search for interesting workflows from the other community members, and execute a workflow online. In addition to the Taverna engine, the myExperiment environment also attempts to integrate several other workflow engines. Executing a workflow using multiple workflow engines is becoming steadily more feasible since the emergence of Service Oriented Architecture (SOA) as a potential architectural model to implement new generations of SWMS. A number of workflow research projects worldwide have started to move towards SOA, the monolithic implementation of SWMS is being replaced by two separate entities: the workflow composer used at the design time and the workflow engine responsible for the run time execution. Implementing the workflow engine as a standalone component and using standard technology to invoke it, such as Web services, is a potential approach to distribute a workflow among multiple workflow engines [13].

Recording the interactions and data evolution in a complex experiment, which is called data provenance, is crucial to trace the history of the experiment processes and to reproduce the

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8 http://www.virolab.org/.

experiment results. The provenance service is becoming an important part of several workflow systems and attracting much interest in the research community. Data storage and semantic technologies based annotation and queries are playing a key role. Wang et al. [14] explore how to provide provenance to the transactions of workflow activities. Shao et al. [15] discuss the discovery of critical workflows from provenance data.

This special section also includes a workflow application in Earth Systems simulation using Microsoft Workflow Foundation (WF) technology. The WF technology provides a rich set of features to support the authoring and execution of workflows, tracking services that enable the monitoring of a running workflow, and state persistence services that allow workflows to be recovered and resumed upon failure. Fairman et al. [16] discuss how Microsoft Visual Studio IDE and the Windows Presentation Foundation which delivers a browser based client interface are used to design and manage a GENIE workflow.

In development of a workflow management system, one faces two important challenges. On one hand, domain specific experiments require customized solutions in workflows for particular problems; on the other hand, to enable knowledge transfer and information sharing between different domains, a generic workflow solution is also required. A successful workflow system should not only have a mature conceptual design and engineering but, more importantly, it should effectively enhance real life applications. The usability of a workflow system is essential to make it useful in the day-to-day activity of application domain scientists: not only suitable interface for composing and executing workflow, but also a set of user oriented tools for viewing, moving and processing data and for the provenance of the workflow and reproducing the results. Sharing the knowledge in meaningful workflows is becoming an important requirement for e-Science frameworks. It is necessary to integrate different technologies, e.g., semantic annotation and searching, and collaborative working facilities, with a scientific workflow system. We can enumerate a number of foci for the future development of workflow systems: workflow sharing and discovery, provenance, human in the loop workflow execution, and workflow interoperability. These extend the list of requirements formulated recently in [17].

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References


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