An Approach to Virtual Laboratory for e-Science

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Keywords: Grid technology, Workflows, e-Science

Abstract

Grids have emerged as a global cyber-infrastructure for the next-generation of e-Science applications. Scientific communities utilize Grids to share, manage and process large data sets, workflows. Often complex scientific experiments require access to distributed resources such as computational resources, data repositories, third party applications, and scientific instruments. Grids help to virtualize infrastructure to supports data- and compute-intensive experiments, providing solutions to the scaling problem inherent to complex scientific experiments. However, they offer little to boost the sharing aspects of experiments, or to derive new findings by integrating various data sources, such as publications. The utilization of these resources requires multi-domain expertise which is beyond the common knowledge of scientists. Workflows have become a popular approach to modeling and organizing complex scientific experiments [1]. A Scientific Workflow Management System explicitly models the dependencies between the processes within an experiment and orchestrates the runtime behavior of the used resources. Scientific workflows aim also at the automation of scientific processes based on data dependencies and their control, as well as the abstraction of the usage of the needed underlying resources to help the scientist to focus on his/her own research. Over the last few years, a number of workflow management systems have been developed, e.g. Kepler [2], Taverna [3], Pegasus [4], and VLAMG [5]. The talk discuss an approach to combine Grids and workflows to build a virtual laboratory for e-science.

The Computational Science Group at the University of Amsterdam aims to be a worldwide key player in the school of thought on computational science in research and education. The group seeks to discover, through modelling and simulation, the way distributed information is being processed in complex systems. The group focuses on theory, applications and problem solving environments. It addresses issues of how physical and biological problems can be formulated in this framework and how they can be mapped onto distributed computer architectures and grid systems. The applicability of this approach is validated through the development of high-performance distributed problem solving environments for asynchronous natural processes. The group is proactive with respect to e-Science virtual laboratories. Its work has strong theoretical foundations together with tight couplings to biomedical applications. UvA has an extensive experience in (the management of) EU Framework projects, including HPCNET, CrossGrid, ACGT, Morphex, COAST, ViroLab, QosCosGrid, MeDDiCa, and MAPPER among others

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