

Scientific and Administrative Report

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1 Summary

This is the report of my stay at Budapest (Hungary) as a CoreGRID PostDoc since April to August 2008.

The work I have performed during these five months in Budapest has been focused on Goals 3 and 4 of the initial research plan. These goals are related with the obtainment of a good knowledge about existing solutions to support the dynamic composition and execution of workflows, and the development of proposals based on HOCL that contribute to enhance the support of the identified issues, respectively. Eventually, these goals have been focused specifically in the support of dynamicity in scientific workflows.

In relation with the activities and outcomes proposed I have performed the fourth and partially the fifth one. Activity 4 involved the development of a workflow management model based on HOCL that supports the management of dynamic composition and execution workflow issues. This model supports the execution of (scientific) workflows including typical workflow operators (AND, OR, XOR, LOOP, SubProcess), specific data oriented operators (one-to-one, all-to-all, data-loop), and dynamic changes in the processes during their execution.

Activity 5 is about the evaluation of the proposed workflow management model in relation with existing solutions. A initial validation and evaluation of the proposal has been performed through the development of an application in CLIPS (a expert systems development tool <http://clipsrules.sourceforge.net/>). This application has enabled us to perform an initial validation of the proposed workflow model. Nevertheless, this is just an initial evaluation. Tests about dynamicity need to be carried. In addition, it would be needed to develop a prototype of the workflow management model in a way closer to the chemical computation model.

2 Publications

During this period I have produced a report describing the the workflow management model based on HOCL. In addition, I have been working in a report about workflow systems based on events, but it is not complete. Currently, I am working in some papers to publish the proposals in some workshops and conferences.

The report is entitled as “*The Chemical Workflow Engine and the Support of Dynamicity*”.

Abstract

This document describes the proposal of a Chemical Workflow Engine (CWE) to support the enactment of scientific workflows. Scientific workflows can be described as processes involving the coordination of tasks and data related to scientific experiments and applications. During the last years, numerous research areas have adopted the use of these workflows to enhance their results: astronomy, genetics, physics, chemistry, etc. In conjunction, scientific workflows share some common features, such as the use of large data volumes and computational resources, and needs, such as the support of dynamicity. The CWE introduced in this report is based on the foundations of classical workflow formalisms (e.g., Petri Nets and Event-driven Process Chains), but it is realized through a completely new computational model: the chemical computation. The result is a fully cooperative and concurrent system, where a large number of processors can be actively involved in the workflow coordination. In addition, the performance of changes to support dynamicity is taken into account through a well-defined separation among the enactment elements and states. The main goal of this document is to describe the CWE and to evaluate its validity to support scientific workflows and their dynamicity needs.

3 Travels

I have performed one travel during my stay in Budapest:

1. To Trondheim, Norway (13/05/2008 to 16/05/2008). I attended to the Mynisimposia “Workflow Abstractions for Parallel and Distributed Computing in e-Science” in the PARA 2008 conference (<http://para08.idi.ntnu.no/index.php?page=minisymposia#Workflow-eScience>) to present the paper entitled *A Proposal to Support the Execution of Scientific Workflows based on a Higher Order Chemical Language*.