WebALLTED: Interdisciplinary Simulator Based on Grid Services

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Abstract

The architecture and possibilities of the novel grid-aware simulation system which uses service-oriented approach and is based on grid services as separate independent functional units are presented. The concept of analysis workflows is covered briefly. The solution based on the orchestration of web and grid services to provide the ability to customize simulation scenarios is proposed.

1. Introduction

There are a number of challenges being faced by the developers of modern CAE/CAD software tools. Interdisciplinary research tools capable of different physical nature objects modeling are in high demand now. These interdisciplinary complexes often must combine the functionality of different tools thus facing the urgent problem of interoperability of the third-party software that can be involved in the complex scenarios of analysis. At the same time the complexity of such objects of analysis forces users to utilize the high performance computing resources to reach the desired accuracy at the reasonable time. Modern tools must provide some collaboration opportunities which lead to the virtual lab environments capable to support collective work by the groups of engineers or researchers. It worth noticing that both computing resources and their users can be (and often are) geographically distributed across multiple countries.

Such wide range of today's demands to simulation software design can be summed up in the following requirements.

Functional capabilities: multiple physical domains support, rich analysis and visualization toolkits, compatibility with existing modeling tools.

Performance: harnessing the power of computing clusters, heterogeneous grid and cloud resources.

User environment: highly customizable models and computing scenarios, collective work support, visual user-friendly interface.

Availability: internet access to the system allowing remote work sessions.

Deployment and maintenance: cross-platform, distributed solutions, easy to extend and to upgrade and so on.

2. Service-oriented approach

In order to cope with requirements specified above the architecture of modern simulation tools must be flexible and extensible, which can be hardly reached by traditional all-in-one standalone applications. The solution proposed relies on the service-oriented approach [1] and web services technology. Besides common reasons of using web services in computer simulation tools architecture (modularity, composability etc.) there are some specific ones.

First, WS-standards are also accepted within the grid community (e.g. OGSA, WSRF specifications concerning the concept of grid service). This simplifies the utilization of grid computing resources for compute-intense analysis.

Second, service orchestration mechanism can be leveraged to organize the execution of customizable scenarios of computations in the form of *web service workflows*.

3. Workflows for analysis

Currently, the project named "Interdisciplinary complex of optimal mathematical modeling in grid environment with the automatic composition and solving of equations of corresponding mathematical models" is implemented by the National Technical University of Ukraine "Kyiv Polytechnic Institute". The basic goal of the project is to satisfy the requirements of domestic users of Ukrainian grid for scientific and applied research tools supporting networked collective design and analysis of complex objects.

The basic idea of the proposed solution is the dynamic composition of both web and grid services for the execution of custom simulation scenarios in the form of a workflow: a set of activities arranged to be executed in the specific order. This idea is also shared by the so-called scientific workflow systems [2] (e.g. Kepler, web services-capable Taverna [3], grid-aware Askalon), but they are mostly general frameworks and are not specially tailored for engineering tasks being solved by CAE tools.

The main difference between web service orchestration tools like Taverna and the proposed approach is that the latter has an extra abstraction layer (abstract workflow named “task”). This means that user does not compose the workflow from web services directly but connects abstract activities being later mapped to concrete web service invocation scenario automatically by the system. This implies that the web service registry should be also supplemented with activities library and mapper logic.

Such additional overhead from the architectural point of view reduces the overhead from the user’s point of view. First, user does not need to deal with all web service metadata and concrete orchestration specifics like invocation details or XML message handling. Second, non-trivial mapping becomes possible when single activity can be mapped to a several communicating web services as well as when several activities can be mapped to a single web service invocation. In other words, such abstract workflow concept allows orchestrating details separation from user scenarios increasing overall flexibility of the system.

4. General architecture

The proposed architecture of the grid-enabled service-oriented simulation platform consists of the several layers (see Figure 1).

User access is organized via the web interface in the form of web/grid portal accessible through the ordinary web-browser. As soon as the current web technologies and tools like JavaScript, AJAX or RIA (Rich Internet Application) frameworks allow the creation of user friendly but sophisticated and powerful enough graphical user interface this approach can reveal many benefits. It needs no specific client software preinstalled but the web browser (thus enabling access from wide variety of networked devices besides desktop PCs like netbooks, smart phones, tablet PCs etc.). It also simplifies the provision of the virtual collaborative lab environment.

User interface provides the following functionality: authorization, graphical workflow editing, project artefacts browsing (input and output files management, simulation results visualization etc.), task execution monitoring and others.

The server-side part of the architecture has several layers to reflect the abstract workflow concept described earlier. The first tier is the portal which organizes user environment: holds user data and preferences, controls user access, provides information support, provides user interface. Its modules are also responsible for: abstract workflow description generation according to user inputs, passing this task description to lower architecture layers for further execution, retrieving the finished task results and keeping all the project artefacts in the database.

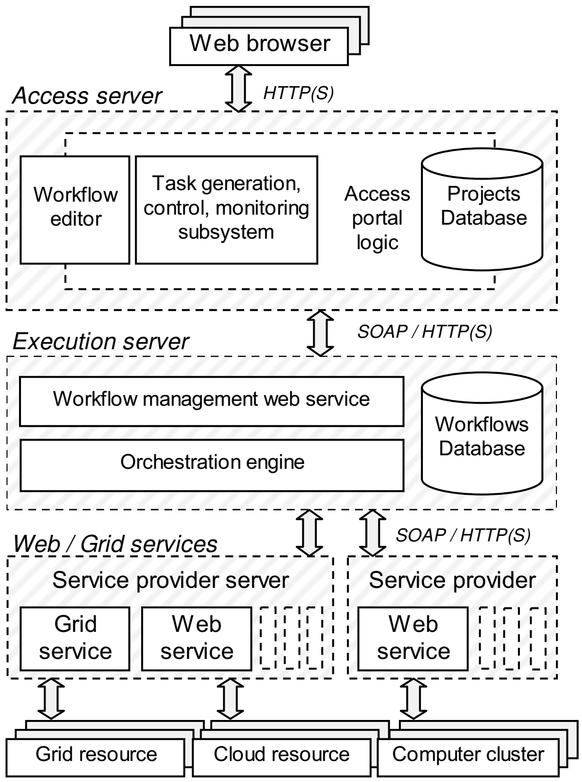

Figure 1. General architecture layers and elements of the grid-enabled simulator

The next tier is the workflow manager running on the execution server. It is responsible for mapping (with the help of service registry) the abstract workflow description to the concrete web services orchestration scenario expressed in the orchestrator-specific input language (like WS-BPEL for BPEL engines or t2flow for Taverna [3]). It also initiates the execution of the concrete workflow with the help of the external orchestrator, monitors its state and fetches the results.

Concrete workflow operates with functional SOAP web services representing the basic building blocks of system functionality for data preparation and adaptation, simulation, optimization, results processing etc. Compute-intensive steps are implemented as grid services interacting with grid resources to run computations as grid jobs. Introduction of the new functionality to the system is accomplished through the registration of the new web or grid services.

5. Functional grid services

Interdisciplinary complex of optimal mathematical modeling in grid environment WebALLTED (ALL Technologies Designer) offers the following:

- automatic forming of mathematical model of an object (or a process) from the description of its structure and component properties as algebraic-differential or differential equations provided in the format which other subsystems of the complex can work with;
- the dimension reduction of the formed mathematical model of an object (or a process) by transformation of the object structure and developing the macromodel of an object;
- steady-state analysis of an object (or a process) based on the automatically formed model with the use of different methods: Newton-Raphson, continuation of solving with a changeable parameter, the search for curve of decision;
- application of the diagonal modification method for solving ill-conditional systems of linear equations, which excludes necessity of equations reordering in the cases of zero pilot elements of the matrix;
- frequency domain analysis of an object (or a process) based on the automatically formed model by solving the linear systems of equations with complex coefficients and automatic determination of corresponding design parameters (frequency band, resonance frequencies and values etc.);
- dynamic analysis of an object (or a process) in time domain based on the automatically formed model by the use of implicit methods of variable order (1-6) and variable step, as well as the automatic determination of corresponding design parameters (delay time, rise and fall times, etc.);
- analysis of sensitivities of design parameters to changes of parameters of internal components of an object (or a process) based on its automatically formed model in time or frequency domains;
- parametric optimization of parameters and characteristics of an object (or a process) based on its automatically formed model in time or frequency domains by using the newest method of variable order (1th-4th), which covers the gradient methods of 1th order and the quasi-Newton methods of variable metric of 2th order as particular cases;
- statistical analysis of parameters and characteristics of an object (or a process) based on its model in time or frequency domains by the Monte-Carlo method with possibility to optimize the coefficient of output (yield).

It is important to remark, that most algorithms on which this Interdisciplinary complex of optimal mathematical modeling is built are original [4, 5].

All this functionality is exposed via the web service interface. Each web service capable to launch grid computations (so it is actually a grid service), has a set of operations to start and cancel grid jobs, monitor their status, retrieve the results etc. Typical functional grid service unit consists of the two parts: interface part and functional part. Interface part is deployed at the web server and is responsible for service input data pre-processing, job description generation, security checks etc. Actually it generates grid job description expressed via the middleware-specific language (like xRSL) according to the parameters provided by service client (e.g. WebALLTED task descripltion) and then submits such grid job for execution. Functional part is pre-installed and configured at the grid resources and is launched by the grid middleware when the grid job submitted by the interface part is scheduled for execution.

Server-side concrete workflow management is based on the standard web service orchestration description language WS-BPEL 2.0 (Business Process Execution Language) [6]. Simulation grid services rely on the functionality of the WebALLTED simulation software and compatible with computing resources accessible through Nordugrid ARC [7] grid middleware. In case of the WebALLTED-aware services the input data transformation is organized as follows. The initial XML-based description of the abstract workflow containing WebALLTED task description parameters (prepared by user with the help of the visual editor) is transformed to the WS-BPEL description. Then the orchestration engine invokes functional grid services which wrap WebALLTED task description into the xRSL job description prepared for grid execution. The test prototype of this system was deployed at the resources of the NTUU "KPI" HPC Centre.

The possible ways of the description of an object for mathematical research are shown on fig.2 and the example of the workflow for mathematical experiment is shown on fig.3.

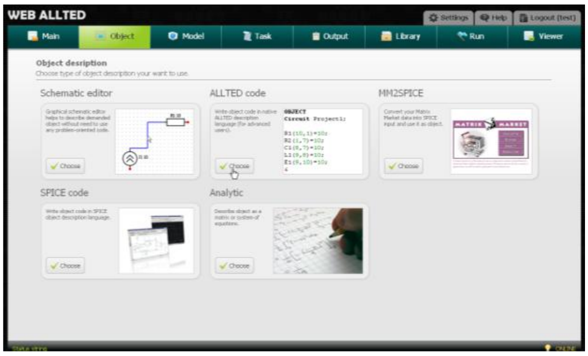

Figure 2. Object of investigation description type selection screen

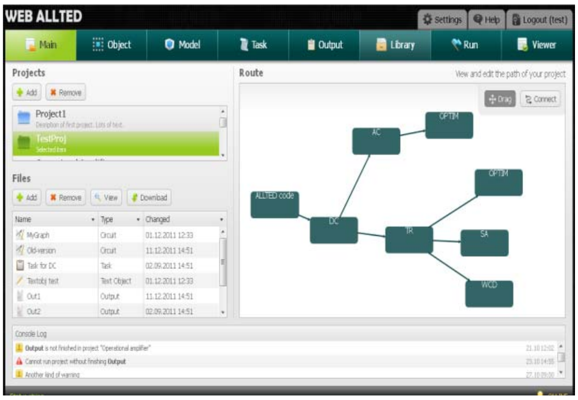

Figure 3. An example of workflow

6. Conclusion and future work

The multi-layered architecture of the grid-enabled computer simulation software was presented. This architecture characterized in that: it is web-accessible, its functionality is distributed across the ecosystem of both web services and grid services (enabling utilization of grid computing resources); it is compatible with adopted standards and protocols; it supports custom user analysis scenario development and execution; it hides the complexity of web-service interaction from the user with abstract workflow concept and graphical workflow editor.

The prototype of WebALLTED developed according to this architecture has proven the working ability of the proposed solution. Currently, WebALLTED has no complete analogs [8]. Thus it is comparable with only few programs such as GridModelica [9] or pAlecsis [10] with substantially weaker possibilities and characteristics.

We believe that this work can be of interest not only for Ukrainian engineers but for European members of engineering community as well. Our further research in this direction will be concerned with the semantic technologies for automatic workflow synthesis and analysis.

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