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WEBALLTED: INTERDISCIPLINARY MODELING IN GRID AND CLOUD

Abstract *This paper presents a multi-layered architecture of computer simulation software capable of utilizing grid and cloud resources, characterized in that the functionality of the system is distributed according to a service-oriented approach, and the system supports the execution of custom user-defined computing scenarios in grid or in cloud (by web services orchestration with an adherence to existing standards) but hides the complexity of direct web services management from the user with the help of the abstract workflow model and a web-accessible problem solving environment with a graphical workflow editor.*

Keywords simulation, grid computing, cloud computing, SOA, Web services

1. Introduction

The wide range of today's demands for simulation software can be categorized into the following groups of requirements:

- Functionality: multiple physical domains support (electronics, mechanics, hydraulics etc.), interoperability with existing modeling tools.
- Usability: customizable models and computing scenarios, rich toolkits for analysis and visualization, support for collective work, graphical user-friendly interface.
- Performance: harnessing the power of computing clusters, heterogeneous grid and cloud resources to overcome the limitations of local computing resources.
- Availability: Internet access to the system allowing remote work sessions.

There is an urgent need in scientific and engineering simulation tools that can benefit from web, grid and cloud technologies to satisfy these requirements. Today there are many existing tools that provide some particular functionalities from that list. They include: web portals for information resource sharing, experience exchange and collective work, grid portals and rich clients providing user interface for grid applications, workflow tools enabling user-defined computing scenarios composition and automatic execution [9] etc. But unfortunately there is no single *comprehensive solution* that sufficiently meets all of these requirements to simulation software with respect to the engineering community.

2. Interdisciplinary simulation complex

To meet previously mentioned demands from the engineering community a new service-oriented [11] infrastructure was implemented on top of existing computing grid and cloud infrastructure. This solution has the following features.

- Web-accessible problem solving environment supporting grid authentication, user workspace personalization, project artifacts sharing, collective work, specialized graph editors to work with models of objects of different domains, data visualizers.
- Workflow editor allowing to define a custom computing scenario built up of computer aided design and engineering procedures and submit workflow description for automatic execution in grid or cloud.
- Workflow management system responsible for the execution of user-defined scenarios represented as web and grid service orchestration scenarios complying with existing standards like WSDL and WS-BPEL [5].
- A set of web and grid services allowing us to access the functionality of computer aided design and engineering tools (operations with large-scale mathematical models, steady state, transient and frequency domain analysis, parametric optimization etc.) and supporting procedures (cross-domain mathematical model description translation, software-specific data formats translation etc.).

- Service registration and discovery tools for easy integration of new functionality to the system exposed as a web service and for automated service selection according to the user's goals.

These features together form the list of capabilities of the grid-aware Interdisciplinary engineering Complex of Optimal design and Mathematical Modeling (ICOMM) WebALLTED. It is based on innovative numeric methods which functionality being distributed as a set of web and grid services capable of being orchestrated for execution of simulation workflows.

3. High-Level architecture overview

The implementation of ICOMM WebALLTED relies on a distributed multi-layered software architecture with minimal interdependencies between layers. The functional responsibilities are distributed between these layers to make the overall system more flexible, customizable and scalable.

Access layer forms a specialized grid portal providing user-friendly graphical interface, a set of various object model editors, resource browsers, data visualizers and a workflow editor with a browser of available building blocks for user workflows. The workflow editor is also responsible for user-defined workflow validation before execution, automated selection of necessary workflow items, preparing workflow description for execution with specific workflow management system, controlling the overall execution progress, retrieving and saving workflow results. User interface is accessible with an ordinary web browser.

Execution layer is responsible for the execution of abstract workflows described in simplified XML-based format as the composition of web service invocations. It exposes a web service interface for the interaction of clients (user access layer) with execution layer's logic and consists of two main units: concrete workflow management system (WfMS) for automatic workflow execution and workflow manager responsible for correct translation of abstract workflow description to concrete input language of the specific WfMS (e.g. WS-BPEL for web service orchestration engines) and launching its execution.

Service layer consists of a set of distributed SOAP web services that provide both general-purpose and domain-specific functionality and can be invoked by the workflow management system during workflow execution. This layer also contains grid and cloud services. Grid services are referred to here as entities having web service interface on one hand and providing access to grid resources (e.g. enabling grid execution of some compute-intensive tasks) on the other hand. In a similar way cloud services are referred here as web services that either are dynamically deployed in the cloud or used to control cloud computations internally.

Resource layer represents resources available for web and grid services (single machines, computing clusters, grid infrastructures, computing clouds with the necessary applications and middleware preinstalled and preconfigured).

Minimal interdependencies between layers enable the various configurations of the problem-solving environments build on top of this service-oriented infrastructure: alternative user environments consuming the same workflow execution layer functionality, alternative concrete WfMS, alternative web service implementations etc. (see Fig. 1).

For example, different user environments for various user communities (engineers, scientists, students) can be developed to interact with the same execution layer. The execution layer itself can leverage different service orchestration tools: from standard business process management engines to some non-standard but popular solutions like Taverna WfMS. Grid services can interoperate with different grid middleware (ARC, gLite, Unicore etc.) to access different grid infrastructures and so on. This briefly illustrates the extensibility options of ICOMM WebALLTED architecture.

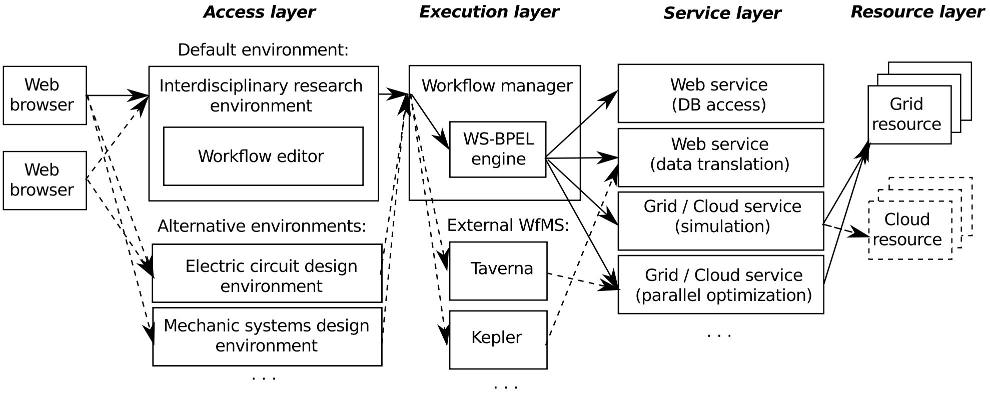

Figure 1. ICOMM WebALLTED architecture layers with possible interconnections of components.

4. Mathematical modeling capabilities

Interdisciplinary complex of optimal mathematical modeling in grid and cloud environment (ICOMM WebALLTED), which architecture is based on the proposed approach offers the following features.

- Automatic development of mathematical model (MM) of an object (or a process) based on description of its structure and component properties as algebraic-differential or differential equations (represented in the intermediate data format which other subsystems of complex can operate with). The reduction of the dimensions of the formed MM by modifying object structure (a triangle to a star transformation) is supported as well as object macro model obtaining.
- 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 matrix and other specific approaches to deal with MM.

- Steady-state analysis of an object based on MM using various methods: Newton-Raphson, method of continuation of solving with a changeable parameter, the search for the curve of decision and others.
- Time domain analysis of an object based on MM by the use of implicit methods of variable order (1st–6th) and variable step, and also the automatic determination of the corresponding design parameters (delay time, rise and fall times etc.).
- Analysis of sensitivities of design parameters of an object based on MM in time or frequency domains to changes in the parameters of the internal components.
- Parametric optimization of characteristics of an object based on MM in time or frequency domains by using the novel method of variable order (1st–4th), which covers the gradient methods of 1st order and the Quasi-Newton methods of variable metric of 2nd order as particular cases.
- Statistical analysis of parameters and characteristics of an object based on MM in time or frequency domains by the Monte-Carlo method with possibility to optimize the coefficient of output (yields).
- Visualization of calculation results in a graphic form, demo with the examples of solving applied tasks from energy, electronics, mechanics, ecology and other fields, and an educational system for teaching the necessary routes of mathematical experiments stowage and other supporting functionality.

The ICOMM WebALLTED is based on the experience of its successful predecessors such as ALLTED multi-domain simulation and design software (supporting design of nonlinear dynamic systems composed of electronic, hydraulic, pneumatic, mechanical, electromagnetic and other types of elements) and its further evolution ALLTED Studio and NetALLTED. It is worth noting that most algorithms of the ICOMM's core are original [12, 13]. Among them it is possible to mention the method of diagonal modification for the solving ill-conditioned linear tasks, the method of searching a curve of solution for the reliable solving non-linear tasks, the implicit method of variable order and step for the solving hard differential non-linear equations, the method of optimization of variable order which exceeds the possibilities of existing methods; the method of maximization of yield coefficient and many others. New methods are also developed for calculations management, which differs from existing ones in strategies of choice of Q-point and criteria of current step acceptance which provide minimum influence of instrumental and methodical errors on the quality and efficiency of the dynamic analysis tasks solution for complex objects or processes.

Let's consider some examples of methods and algorithms being used in ICOMM WebALLTED.

4.1. Macromodel generation

One of the examples of interdisciplinary tasks that are possible to solve with ICOMM WebALLTED is the simulation of mechanical components with circuit design software tools and their methods which can be used, for example, for MEMS design. This requires us to obtain the models of non-electric objects as equivalent electric circuits according to electric-mechanical analogies.

For the objects with complex geometry and a lot of degrees of freedom their finite-element models can contain hundreds of thousands equations. In this case the equivalent circuit can contain millions and more elements. That is why such interdisciplinary simulation scenarios can benefit from algorithms of reduction of circuit dimension on the basis of Y-Δ transformation [8].

The essence of the methods based on the Y-Δ transformation can be briefly described as follows. Let's consider the i-th node with its k connected neighbours (cf. Fig. 2).

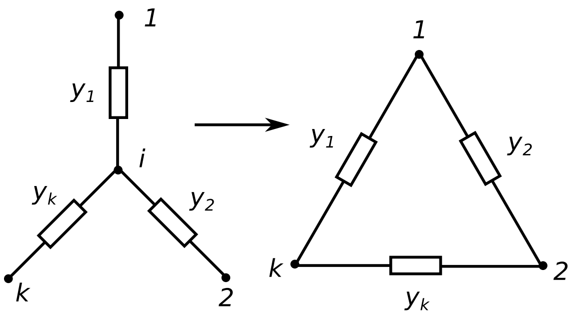

Figure 2. A work node of RLC circuit.

Then, the component equation of i-th row looks like:

$$Y_i V_i - y_1 V_1 - y_2 V_2 - \cdots - y_n V_n = 0 \tag{1}$$

where conductance $Y_i = \sum_{j=1}^{k} y_j$. To exclude V_i from (1), that is equivalent to excluding i-th node, let's define V_i as:

$$V_i = \frac{1}{Y_i} \left(\sum_{j=1}^{k} y_j V_j \right) \tag{2}$$

and replace V_i with (2) in k equations where it is present. Then, the equation for the first node next to i-th is like:

$$\left(\overline{Y}_1 + y_1 - y_1^2/Y_i\right) V_1 - \frac{1}{Y_i} \sum_{j=2}^{k} y_1 y_j V_j - \sum_{r=1, r\neq i}^{k1} y_r V_r = 0 \tag{3}$$

where $\overline{Y}_1 = \sum_{r=1,r\neq i}^{k1} y_r$ is a sum of all conductances of the first node, $k1$ is a number of nodes connected to the first node. Then (3) can be simplified (that is equal to adding $k-1$ new elements between the first node and the $k-1$ former neighbours of

i-th node):

$$\left(\overline{Y}_1 + \frac{1}{Y_i}\sum_{j=2}^{k} y_1 y_j\right) V_1 - \frac{1}{Y_i}\sum_{j=2}^{k} y_1 y_j V_j - \sum_{r=1, r\neq i}^{k1} y_r V_r = 0 \tag{4}$$

For any two nodes next to i-th (let's refer to them as a and b) excluding of the i-th node leads to adding a new element between these nodes. Conductance of this element will be equal to:

$$y_{ab} = \frac{y_a y_b}{Y_i} \tag{5}$$

By repeating this process for all k neighbors of the i-th node we can finally remove this node.

For each node in the circuit, there are two time constants defined: $\tau_{RCi} = C_i/G_i$ and $\tau_{LCi} = \sqrt{C_i/B_i}$, where $C_i = \sum_{j=1}^{k} c_j$ is a sum of all capacitances, $B_i = \sum_{j=1}^{k} b_j$ is a sum of all reactive conductances (reverse to inductances) and $G_i = \sum_{j=1}^{k} g_j$ is a sum of all conductances connected to i-th node. Then:

$$\tau_i = \max(\tau_{RCi}, \tau_{LCi}) \tag{6}$$

the i-th node is considered as fast when:

$$\tau_i < \tau_{min} = \frac{2\pi}{\omega_{\max}} \tag{7}$$

where τ_{min} is user-defined time constant depending on the maximal frequency of the circuit ω_{max}. If the i-th node is a fast one it can be removed. In practice a compromise between accuracy and dimension of received models can be reached by the variation of τ_{min}. Often, it is preferable to obtain macro models just with the defined size limit because it is difficult to estimate a priori τ_{min}.

The diagram of operations for mechanical component simulation in ICOMM WebALLTED is presented in Figure 3.

4.2. Optimization method of variable order

The method of variable order (MVO) [12] is one example from the pack of efficient original methods being utilized by ICOMM WebALLTED. It is used for obtaining such values of the variable parameters $x = [x_1, x_2, \ldots, x_n]^T$ that turn the gradient of the objective function into zero which means to solve non-linear operator equation $\Phi'(x) = 0$ in n-dimensional space. The MVO uses derivatives of the objective function of orders up to 4th. The general iteration formula of the MVO can be expressed as:

$$x^{(k+1)} = x^{(k)} - h_s(\lambda) \tag{8}$$

where $h_s(\lambda)$ – vector polynomial of scalar parameter λ, s – constant equal to the highest order of the objective function's derivatives being used in calculations.

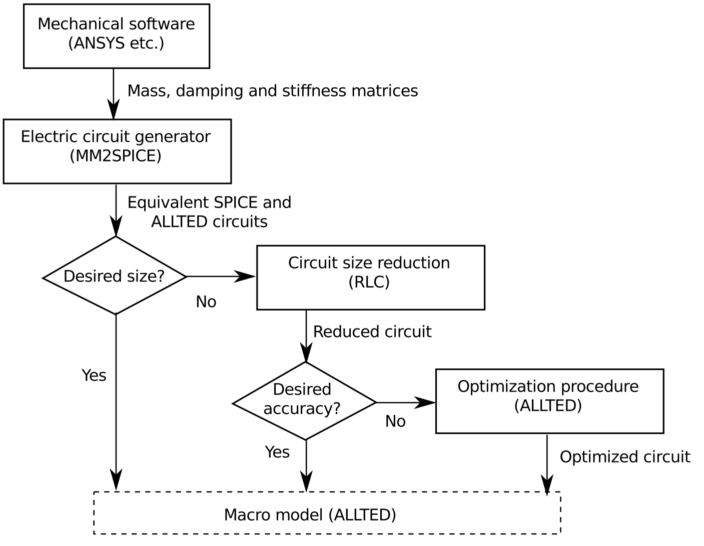

Figure 3. Process of obtaining a circuit model for mechanical components.

The concrete form of the polynomial depends on s:

- s=2: $h_2(\lambda) = \lambda d_2^{(k)}$, $d_2^{(k)} = [\Phi''(x^{(x+1)})]^{-1}\Phi'(x^{(k)})$
- s=3:

$$h_3(\lambda) = \lambda d_2^{(k)} \frac{3}{2} + \left(d_3^{(k)} - \frac{1}{2} d_2^{(k)}\right) \lambda^2 \tag{9}$$

$$d_3^{(k)} = \frac{1}{2} \left[\Phi''(x^{(x)})\right]^{-1} \Phi''' \left(x^{(k)}\right) d_2^{(k)} d_2^{(k)} \tag{10}$$

- s=4:

$$h_4(\lambda) = \frac{11}{6} d_2^{(k)} \lambda + \left(2d_3^{(k)} - d_2^{(k)}\right) \lambda^2 + \left(d_4^{(k)} + \frac{1}{6} d_2^{(k)} - d_3^{(k)}\right) \lambda^3 \tag{11}$$

$$d_4^{(k)} = \left[\Phi''(x^{(x)})\right]^{-1} \left[\Phi'''(x^{(k)}) d_2^{(k)} d_3^{(k)} - \frac{1}{6} \Phi^{IV}\left(x^{(k)}\right) d_2^{(k)} d_2^{(k)} d_2^{(k)}\right] \tag{12}$$

To estimate inverse Hessian $[\Phi''(x^{(k)})]^{-1}$ in practical implementations the matrix $\eta^{(k)}$ is used which is calculated according to one of Quasi-Newton formulas.

In most real cases the objective function's derivatives of 3rd and 4th orders are impracticable to calculate. To eliminate this shortcoming the following relation is used for vectors $d_3^{(k)}$ and $d_4^{(k)}$ calculation:

$$d_s^{(k)} = \eta^{(k)} \Phi'(x^{(k)} - \sum_{i=2}^{s-1} d_i^{(k)}),\ s = 3, 4 \tag{13}$$

It is possible to show that if matrix $\eta^{(k)}$ is equal to $[\Phi''(x^{(k)})]^{-1}$ then calculation error for $d_3^{(k)}$ and $d_4^{(k)}$ according to (13) is defined by $\left(||d_2^{(k)}||\right)^{s+1}$.

The concrete form of the polynomial $h_s(\lambda)$ being used on each step of optimum search can be defined according to the analysis of the objective function and its derivatives behavior in the neighborhood of the operating point $x^{(k)}$ with the special procedure. This results in the possibility of a dynamic change of the method's order during the calculation process and choosing its optimal value.

5. Implementation

The access layer of ICOMM WebALLTED is implemented as a web portal with specialized pages: workflow editor, circuit editor, plot visualizer etc. Most layer's logic connected with users, projects, workflows management is implemented in PHP programming language. The web interface implemented is accessible from any web browser with only JavaScript enabled but no heavyweight extensions preinstalled (even Flash, Java, Tcl/Tk etc.).

Figure 4 shows the example of the workflow designed with the workflow editor: it consists from AC (frequency domain) and TR (transient) basic analyses to be executed independently. They preceded by DC (steady-state) analysis. Basic analysis steps are then followed by optimization procedure (OPTIM) as well as by a sensitivities analysis (SA) and a worst case design analysis (WCD). Figure 5 shows the possibilities of calculation parameters adjusting for a specific workflow item (DC analysis).

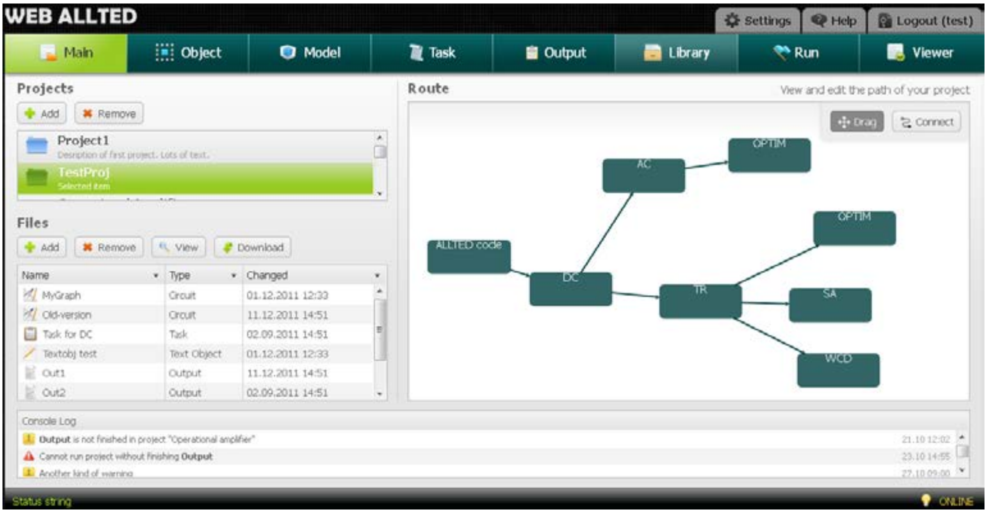

Figure 4. Example of analysis workflow.

The execution layer of ICOMM WebALLTED is based on WS-BPEL 2.0 compatible orchestration engine. At this layer the initial XML-based description of an

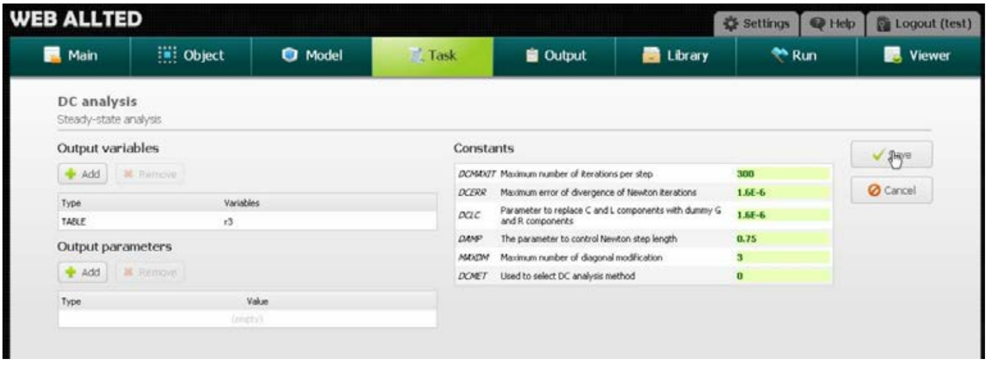

Figure 5. Adjusting calculation parameters for DC analysis workflow item.

abstract workflow of simulation procedures and their parameters (prepared by the user with the help of the workflow editor) is translated to the WS-BPEL (Business Process Execution Language). script of invocations of web services from service layer. One of the goals of this architectural decision is to provide the ability to integrate both grid and cloud services (each having its own strengths) into a single complex thus forming a "grid-cloud bridge" [14, 7, 2, 10].

The orchestration engine invokes web services passing the necessary task description and parameters to each service. Every grid or cloud web service which is capable of launching long-term computations has the pre-set of operations to start and cancel jobs, monitor their status, retrieve the results etc. Grid services use Nordugrid ARC middleware to launch and control grid computations. The deployment base for the test prototype of this system is located at the High-Performance Computing Center of the National Technical University of Ukraine "KPI".

As for modeling tools, the closest competitor of ICOMM WebALLTED is Grid-Modelica [1] and pAlecsis [6] but they lack workflow capabilities and have weaker mathematical background. The closest analog of a service-oriented workflow management system is Taverna Workbench [4] but it is not primarily designed for remote web access, has its own (non-standard) orchestration language and is not tailored for engineering simulation.

6. Conclusion

In this paper the multi-layered architecture of the grid-enabled computer simulation software ICOMM WebALLTED based on web services was presented. This architecture differs from the traditional monolithic approach in that the functional blocks of the system are implemented as web/grid services, and computational scenarios in such a system are executed as web service orchestration scenarios. The system described has the following main advantages:

- compute-intensive tasks can be submitted to remote resources with the help of grid and cloud technologies;
- computing scenarios can be constructed and customized directly by users and not by programmers;
- new functionality as well as an access to unique hardware or software resources can be easily added in the form of web services.

This project can be beneficial for engineers requiring flexible and functional grid tools to solve complex cross-domain problems and design optimal solutions. But, the general architecture described here is not restricted to engineering tasks exclusively.

There are several directions planned of further research and development that can enhance the the proposed architecture and enrich the functionality of the complex:

- further extending the set of available web and grid services to add new application areas and enhance possibilities for interdisciplinary research;
- integration with existing popular workflow management systems like Taverna Workbench, Kepler, Unicore workflows etc;
- semantically-powered service discovery and automatic composition of service workflows;
- further study of cloud-specific standards such as topology and orchestration specification for cloud applications (TOSCA) [3, 15].

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