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QUALITY OF SERVICES IN SCIENTIFIC WORKFLOWS

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Abstract. *Scientific workflows are based on Web-, Grid- and Cloud services. Creating the workflow, the problem of services search, ranking and selection among the functionally similar ones arises, driven by the non-functional properties. In this paper the usage of Logic Scoring of Preference method for scientific workflows service ranking has been proposed.*

Keywords: *scientific workflow, service oriented architecture, quality of service, Logic Scoring of Preference.*

Introduction

Scientific workflow is the representation of the scientific research process in the form of automated sequence of several steps using computer and communication technologies. Scientific workflows are widely used in the researches on astrophysics, bioinformatics, chemistry, medicine, climatology, earthquakes and in other fields. Scientific workflows provide automation, which increases the productivity of scientists in studies conduction based on calculations [1, 2, 3]. Owing to automation and network communication technologies, scientists can flexibly apply various applications and resources around the world, e.g., unique laboratory equipment, Grid-resources, parallel computers, storages with accumulated experimental data, proven scientific workflows, Cloud-based scientific online applications, etc.

Generally, the processes of scientific research consist of the following milestones: hypothesis formulation, information search, experiments conduction, results processing and its presentation in publications. These milestones can consist of the sequence of tasks and actions, for instance, information retrieval can include the selection of information sources, filtering and relevance assessment of retrieved information, and smart storage of information in the repositories. Various technologies, applications and equipment can be used for each milestone and action. In addition, to connect the milestones and actions into a single scientific workflow, it is necessary to provide the data exchange between them, establish the correct sequence of actions execution or so-called sequence choreography and monitoring.

For the purpose of these milestones, tasks, activities and corresponding data exchanges mapping into the computer environment, the scientific workflow management systems (WMS) have been developed. These systems are based on special languages, usually the XML dialects, or standard languages (BPEL, WSBPEL, WSDL), graphical tools and notations (UML, BPMN) to describe the scenarios, simulate and execute scientific workflows.

Numerous WMSs are known, e.g., Taverna [4], Triana, Kepler, Askalon, VisTrails, Galaxy, Pegasus, Knime, e-BioFlow, Weka4WS, GWES, Karajan, DIS3GNO, Wings, etc. [1–5]. Many of these systems have been focused on performing the *in-silico* experiments across the diverse domains, e.g. Life Sciences, Geosciences, Earthquakes, Meteorology, Astronomy, Machine Learning [5].

To share and reuse the scientific workflows, the online repositories have been created, e.g., myExperiment [3], CrowdLab [5], the repositories of Kepler and Galaxy WMSs, SHIWA [6]. These repositories already comprise the thousands of workflows.

Most of the computing resources for scientific workflows are built on a service-oriented architecture (SOA) [4]. WMS may manage the processes of composition, orchestration and choreography of services during the planning, scheduling and execution of scientific workflow, as well as in the compliance estimation of existing services with a particular scientific workflow.

The selection of service, based on the non-functional parameters of services or Quality of Service (QoS) for scientific workflows, has not yet been adequately covered in the literature on WMS. The main goal of this paper is to examine one of the approaches to search and ranking of services, taking into account the user's preferences, which can be used in WMS.

1. Services for scientific workflows

In Figure 1, the example of scientific workflow that operates in WMS Taverna 2 is shown. This workflow extracts bibliographic sources from Literature Web Service of NED (the NASA/IPAC Extragalactic Database). The list of source names is supplemented by a column of the links to bibliography in the NED website. This information is formatted to XML-based format for tabular data VOTable maintained by the International Virtual Observatory Alliance. The VOTable is the output of this workflow and can be sent via SAMP (Simple Application Messaging Protocol) to TOPCAT (Tool for Operations on Catalogues And Tables). Thus, this workflow receives information from the Web service NED and can itself be a service, providing the its work results for other Web services.

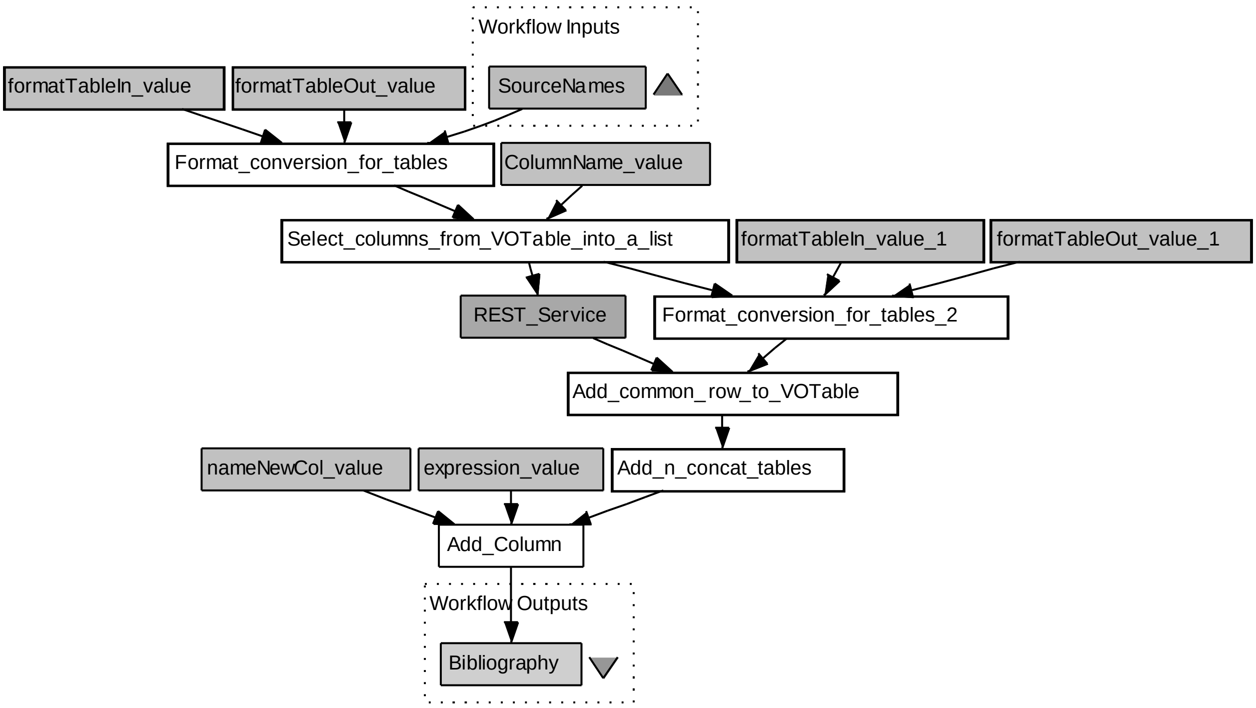

Fig. 1. Example of scientific workflow (www.myexperiment.org/workflows/3556.html)

The life cycle of the scientific research contains several milestones, from the hypothesis formulation to the results publications. It is possible to select or develop an appropriate service for each milestone. These services can be directly applied to the creation of scientific product or scientific research process providing. So, the scientific workflows can consist of a wide variety of services, e.g., Web services, Grid services and Cloud services (Fig. 2). The service-oriented architecture can be considered to become the common paradigm, ensuring the interoperability, loose coupling between these services and the independence from platforms of their implementation. This is achieved through the standardization of interaction interfaces, although these standards may be different for different domains.

Along with the services listed above, the computer applications, database management systems and the libraries, used on the daily basis, can also be involved in scientific workflows (e.g., Matlab, Scilab, Modelio, MySQL, Docear, graphics and text editors, LaTeX, IDEs, MPI, OpenMP, etc.). To this end, conventional computer applications must be provided with suitable interfaces or wrappers and have appropriate meta-descriptions in WSDL in the SOA style.

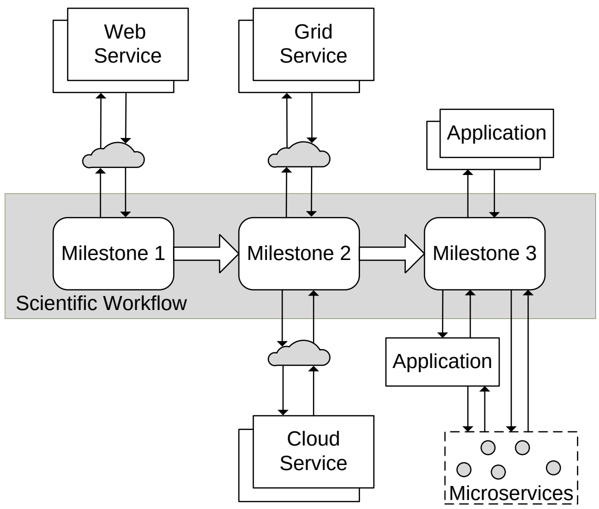

Fig. 2. Diversity of services in scientific workflows

Moreover, if user applications are designed in accordance with the architectural style of the microservices [7], certain microservices can also be the constituent parts of scientific workflows. For this purpose, the microservices should have appropriate interfaces and data exchange protocols that are independent from the platform and implementation language and represent small scientific capability.

2. QoS-based service selection

There is a plethora of different Web-, Grid- and Cloud services on the Internet. When searching for a specific service, many services with the same functionality can be detected though. One approach to discovering and matching of functionally similar services is to rank these services by corresponding non-functional parameters. These QoS-parameters can be specified in the requirements of service consumer or announced by the service provider or declared explicitly in Service Level Agreement (SLA) between the provider and the consumer of service.

The selection of services for the particular scientific workflow is related to the problem of suitable services choosing among the ones with similar functionality. This process can be demonstrated by the example of the formation of a concrete workflow for the Grid calculation in Fig. 3 [8], where the circles with $A_1, B_1, \ldots$ letters denote services of the first type with the same functionality, $A_2, B_2, \ldots$ denote services of second type with the same functionality, etc.

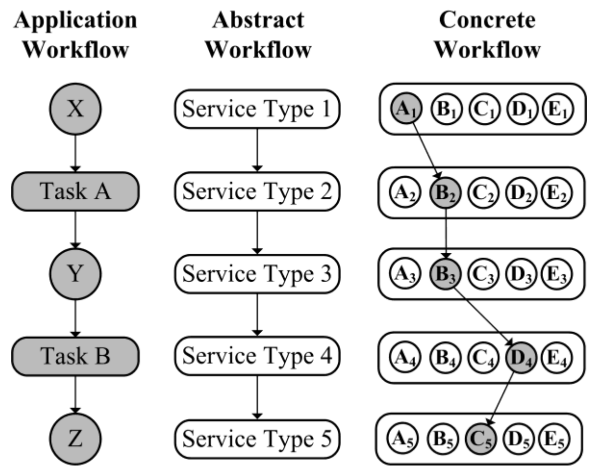

Fig. 3. Application, Abstract and Concrete Workflows (adopted from [8])

Wide variety of QoS-parameters for Web services have been presented in literature, the example of the most frequently used set of QoS-parameters is given in [9, 10]:

– **Response Time**: a characteristic of a Web service, which tells us how quickly a Web service responds to a request, i.e. the time duration between the request sending time (T_{req}) and response receiving time (T_{res}):

$$Rt = T_{res} - T_{req};$$

– **Execute Time**: the time, during which the service finishes processing of the request (execute the task);

– **Throughput**: the amount of requests N that service can during given time period T:

$$Tp = N / T;$$

– **Availability**: the ratio between the time period when the Web service is not available or ready for usage and the total measurement time:

$$Av = 1 - Td / Tm,$$

where Td is the time when Web service is not available for usage, and Tm is the total measurement time;

– **Reliability**: the ability of Web service to execute the required functions within a particular time interval;

– **Accessibility**: the probability that system is operating normally and can process requests without any delay;

– **Cost**: the cost per Web service request (e.g. cents per service request or invocation).

In addition, the tasks of the process may have different requirements for the infrastructure of computing facilities on which the services are implemented. For example, the capacity of disk and RAM, number of CPU cores, number of nodes in cluster provided for parallel computations, network traffic, etc.

In the process of searching and selection on the basis of QoS-parameters, it is necessary to take into consideration the requirements of service consumer and the service provider's offer [11]. Today, there is no generally accepted way of QoS-service values documenting, so these values can be obtained by way of measuring and evaluation.

To rank services by QoS-characteristics, it is necessary to calculate the integral (generalized) value of the quality of each service. To do this, the aggregation function, which maps $(x_1, x_2, \ldots, x_n)$ set of measured or estimated values of QoS-parameters for each service to real number y, can be used:

$$y = F(x_1, x_2, \ldots, x_n).$$

The ranking of services is calculated by comparing the integral values of service quality.

QoS-parameters can have different significance for the customer of service and ultimately for the scientific workflow. This can be taken into account by introducing the weights $(w_1, w_2, \ldots, w_n)$ for each

QoS-parameter. Then the aggregation function will be presented as

$$y = F(w_1 x_1, w_2 x_2, \ldots, w_n x_n).$$

In addition, the customer's requirements to the quality of service may vary depending on the conditions or context, for instance, on the urgency of service or financial capacity. These aspects are taken into account in the Logic Scoring of Preference (LSP) method proposed by J. Dumović for hardware and software evaluation, comparison and selecting [12]. In this method the aggregation function is used:

$$L = \left(w_1 E_1^r + w_2 E_2^r + \ldots + w_n E_n^r\right)^{1/r}, \qquad (1)$$

where E_i – evaluation function for scoring the service on i^{th} criterion and $0 \le E_i \le 1$; w_i is the weight of i^{th} criterion and $0 \le w_i \le 1$, $\sum_{i=1}^{n} w_i = 1$; the power r is a real number selected, to achieve the desired logical relations between the criteria.

The r power depends on α parameter which is called as *orness degree* and can range from pure "and" (conjunction or simultaneity, $\alpha = 0$) to pure "or" (disjunction or replaceability, $\alpha = 1$). The commonly used values of α are 0, 1/16, 1/8, ..., 1. For this values of α the special names have been assigned: from "strong quasi-conjunction+" $(\alpha = 0{,}0625)$ to "strong quasi-disjunction+" $(\alpha = 0{,}9375)$. If the aggregation function comprises from 2 to 5 criteria, the r value can be taken from Tab. 1 [12].

Table 1

Logic Scoring of Preference

α	*r*2	*r*3	*r*4	*r*5
1,0000	+∞	+∞	+∞	+∞
0,9375	20,630	24,300	27,110	30,090
0,8750	9,521	11,095	12,270	13,235
0,8125	5,802	6,675	7,316	7,819
0,7500	3,929	4,450	4,825	5,111
0,6875	2,792	3,101	3,318	3,479
0,6250	2,018	2,187	2,302	2,384
0,6232	2,000	2,000	2,000	2,000
0,5625	1,449	1,519	1,565	1,596
0,5000	1,000	1,000	1,000	1,000
0,4375	0,619	0,573	0,546	0,526
0,3750	0,261	0,192	0,153	0,129
0,3333	0,000	0,000	0,000	0,000
0,3125	-0,148	-0,208	-0,235	-0,251
0,2500	-0,720	-0,732	-0,721	-0,707
0,2274	-1,000	-1,000	-1,000	-1,000
0,1875	-1,655	-1,550	-1,455	-1,380
0,1250	-3,510	-3,114	-2,823	-2,606
0,0625	-9,060	-7,639	-6,689	-6,013
0,0000	-∞	-∞	-∞	-∞

In the general case the following numeric approximation of r can be used [13]:

$$r = \frac{a_0 + a_1 y + a_2 y^2 + a_3 y^3 - a_4 y^4}{\alpha(1-\alpha)}, \qquad (2)$$

where $a_0 = 0{,}25$, $a_1 = 1{,}89425$, $a_2 = 1{,}7044$, $a_3 = 1{,}47532$ $a_4 = 1{,}42532$; $y = \alpha - 0{,}5$, $0 < \alpha < 1$.

The curves graphs of the dependency of the r power from *orness* parameter for different numbers of criteria are shown in Fig. 4. Simple solid curves are constructed from the Tab. 1 data. The curve marked with circles was obtained by approximating this dependency by (2).

A detailed technique for calculating the r power from the value of the *orness* parameter and the number of criteria is given in the work of J. Duimović and substantiated in his earlier work on the study of the application of continuous logic for complex criteria. Examples of the practical usage of (2) can be found in the papers [14, 15].

The aggregation function (1) allows to model the spectrum of logical relationships between the quality criteria. The dependency of relationships simultaneity and replaceability of quality criteria from *orness* parameter is shown in Fig. 5.

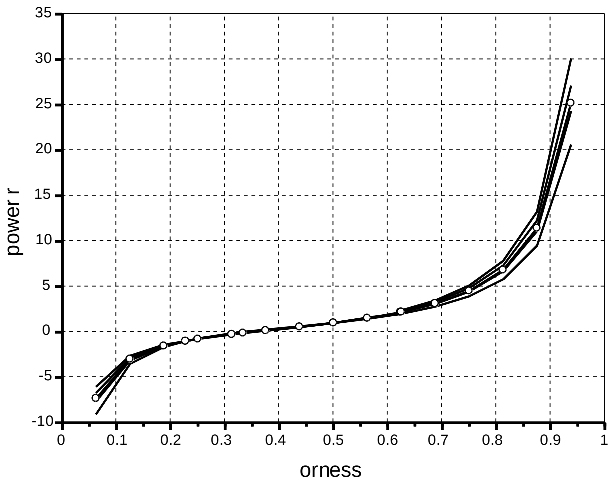

Fig. 4. Relation between r power and *orness* parameter

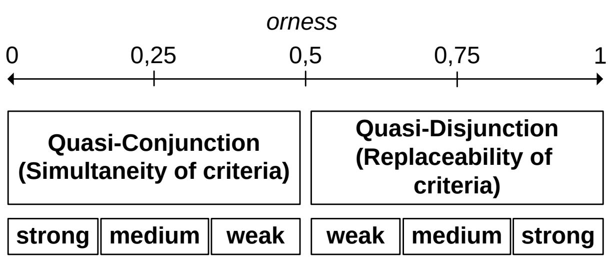

Fig. 5. Relations between parameter *orness* and simultaneity and replaceability

To compute the elementary preference, in case we want to evaluate the x parameter with increasing function, this function can be defined as follows:

$$E(x)=\begin{cases}0, & \text{if } x \le x_{\min};\\ \dfrac{x-x_{\min}}{x_{\max}-x_{\min}}, & \text{if } x_{\min} < x < x_{\max};\\ 1, & \text{if } x \ge x_{\max}.\end{cases} \quad (3)$$

For instance, let’s suppose that the measured values of throughput for the five competitive services are 3.4, 6.2, 8.5, 2.7 and 4.1. Then, according to function (3), we get the following normalized values: 0.1, 0.6, 1.0, 0.0, and 0.2, respectively.

In case we want to evaluate the x parameter by function decrease, this function can be defined as follows:

$$E(x)=\begin{cases}1, & \text{if } x \le x_{\min};\\ \dfrac{x_{\max}-x}{x_{\max}-x_{\min}}, & \text{if } x_{\min} < x < x_{\max};\\ 0, & \text{if } x \ge x_{\max}.\end{cases} \quad (4)$$

For instance, if the costs of competitive services are 2.8, 1.2, 3.4, 1.7, and 4.0, then, according to function (4) we obtain the following normalized values of these costs respectively: 0.4, 1.0, 0.2, 0.8, and 0.0.

The LSP method can be used for services ranking based on QoS-parameters when scientific workflow creation is given. Let’s consider the example, in which three services are ranked according to three QoS-parameters: **Response time** (Rt), **Throughput** (Tp) and **Cost** (C).

In Tab. 2 the values of QoS-parameters measured for three services are shown. In Tab. 3 the calculated values of these parameters according to (3) and (4), are presented.

Table 2

Measured QoS-parameters

Service	QoS-parameters		
	Rt (ms)	***Tp*** (r/min)	***C*** (c/i)
1	320	6	1,6
2	380	5	0,2
3	540	3	0,5

Table 3

Calculated QoS-parameters

Service	QoS-parameters		
	Rt (ms)	***Tp*** (r/min)	***C***(c/i)
1	1	1	0
2	0,72	0,67	1
3	0	0	0,78

The L_1, L_2 and L_3 values, given in Tab. 4, are the calculated with (1) formula as integral quality values or global preferences of services 1, 2 and 3, respectively, for different r and vector of weights $w=(0.5, 0.3, 0.2)$. In the middle column of Tab. 4 the values of L for the parameter $\alpha = 0{,}5$ are given, for which the power r is 1. In this case the (1) function gives the weighted arithmetic mean of the QoS-parameters. In the left column the results of calculations for $\alpha = 0{,}625$ ($r = 2.187$) are presented.

Table 4

Logic Scoring of Preference

r	2,187	1	0,192
L_1	**0,90**	**0,80**	0,31
L_2	0,78	0,76	**0,76**
L_3	0,38	0,16	0,0

In this case, according to the terminology of J. Dumović, the (1) function has the property of “weak quasi-disjunction”. In this property the service consumer’s certain preference, in which the consumer allows some compensation of one parameter by another and service 1 ($L_1 = 0{,}9$) as the most preferable for him, is expressed. In the right column the data is given for the case when $\alpha = 0{,}375$ ($r = 0.192$) and the (1) function has the property of “weak quasi-conjunction”. In this case, the service consumer almost does not allow mutual compensation of the parameters and the most preferable for him is the service 2.

Accumulating the scientific workflows in the repositories, the new challenges for these collections of scientific workflows management arise. These challenges include the detection of functionally equivalent workflows, their retrieval or the use of existing workflows in the design of novel workflows. The authors of [6] investigate the methods of scientific workflows search and detection on the basis of corresponding functional properties similarities. In our viewpoint, the proposed approach to Logic Scoring of Preference method usage can be applicable to the selection of scientific workflows fragments, as well to the ones as a whole.

Apparently, in this case, it will be necessary to take into account the integral QoS of the scientific workflow, based on QoS-parameters of all services involved into workflow, as well as certain parameters that are inherent in the scientific workflows. Such parameters can be the availability for resources and services, scalability, the ability to execute the workflow for a long time and in the background, the ability to change the direction of workflow by user at run time, reproducibility of experimental results, the ability to capture the data provenance. The provenance of information is decisive for determining the reliability of information, the trust in its source and the possibility of using this information in a scientific research [16, 17, 18].

3. Conclusion

In this paper we have presented some challenges and opportunities, addressed to future development of scientific workflows. Since the scientific workflows are formed from different types of services (Web services, Grid services, Cloud services) it is necessary to take into account the quality issues of these services and the improvement of service discovery and ranking methods, based on QoS-characteristics. Perhaps, the systems for managing scientific workflows will integrate Web-, Grid-, Cloud services with conventional computer applications and microservices in the future. The challenges of search and choice of the services and applications, as well as the elements of infrastructure, when creating scientific workflows with the use of QoS-characteristics will remain topical. Creating a lot of new scientific workflows and accumulating them in repositories will cause scientists to choose the relevant scientific workflows. The design of new scientific workflows may involve the use of other scientific workflows or corresponding parts. Therefore, the issues of quality criteria for scientific workflows and methods for suitable scientific workflows selection by these criteria development are also topical.

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ЯКІСТЬ СЕРВІСІВ У НАУКОВИХ ПРОЦЕСАХ

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Анотація. *Автоматизовані науково-дослідні процеси (Scientific Workflows) поліпшують продуктивність науковців при проведенні досліджень, що ґрунтуються на виконанні обчислень. Завдяки автоматизації і мережним технологіям науковці з усього світу мають змогу гнучко застосовувати різноманітні програмні системи та ресурси, наприклад, унікальне лабораторне устаткування, Grid-ресурси, паралельні обчислювальні системи, накопичені експериментальні дані, науково-дослідні онлайн-додатки на основі хмарних технологій. Більшість обчислювальних ресурсів для науково-дослідних процесів побудовано на основі сервіс-орієнтованої архітектури. Системи управління такими процесами (Workflow Management Systems, WMS) дозволяють виконувати композицію, хореографію та оркестрування сервісів упродовж як планування, так і виконання процесів, зокрема при оцінюванні придатності доступних сервісів до застосування в окремому науково-дослідному процесі. Питання вибору сервісів на основі нефункціональних характеристик (Quality of Service, QoS) для їх залучення до науково-дослідних процесів ще не було в достатній мірі висвітленим у публікаціях на зазначену тему. Запропоновано застосування методу логічного оцінювання вподобань (Logic Scoring of Preference, LSP) для ранжування сервісів-кандидатів на залучення до науково-дослідних процесів. Метод дозволяє враховувати вимоги користувача до нефункціональних характеристик сервісів, а також його вподобання, що можуть залежати від сфери застосування сервісів. Проектне рішення нового науково-дослідного процесу може включати використання вже існуючих процесів або їх складових. Тому розробка підходів до QoS-орієнтованого вибору та ранжування сервісів є актуальним питанням. На нашу думку, запропонований підхід до застосування методу логічного оцінювання вподобань може бути застосований як при виборі складових науково-дослідних процесів, так і при виборі безпосередньо процесів.*

Ключові слова: *науково-дослідні процеси, сервіс-орієнтована архітектура, якість сервісу, метод логічного оцінювання вподобань.*

КАЧЕСТВО СЕРВИСОВ В НАУЧНЫХ ПРОЦЕССАХ

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Аннотация. *Автоматизированные научно-исследовательские процессы (Scientific Workflows) базируются на Web-, Grid- и облачных сервисах. При формировании научно-исследовательского процесса возникает проблема поиска, ранжирования и выбора среди множества функционально схожих сервисов тех, которые наиболее подходят по их нефункциональным свойствам. Для этой цели в статье предложено использовать метод логической оценки предпочтений (Logic Scoring of Preference).*

Ключевые слова: *научно-исследовательские процессы, сервис-ориентированная архитектура, качество сервиса, метод логической оценки предпочтений.*

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