Dear Editor,

I believe that our paper “On the enhancing of GriF a Workflow-oriented Grid Framework combining High-level services” has been improperly dealt by the Editor of the “Journal of Grid Computing”. In fact, while some objections of the enclosed reports of the referees are well acceptable for a revision of the paper (and actually improve it) in our opinion rejection is not sufficiently motivated (as we detail below). Therefore I would be happy if you can place the present contribution in the SCIENCE REJECT Section of your e-magazine Virt&L-Comm and allow me to emphasize that:

A – The editor evaluation does not reflect the opinion of 4 out of 5 referees which do not suggest rejection but only improvements;

B – The order of the listed referees, with our surprise, does not follow the numbering sequence and puts in the first place the third, and the most critical, one.

With anticipated thanks.

Carlo Manuali

> From: "Journal of Grid Computing" <jubilyn.hilario@springer.com>
> Date: March 24, 2012 14:39:04 PM GMT+01:00
> To: "Carlo Manuali" <carlo@unipg.it>
> Subject: Your Submission GRID593
>
> Dear Dr. Carlo Manuali,
>
> We have received the reports from our advisors on your manuscript GRID593 "On the Enhancing of GriF a Workflow-oriented Grid Framework combining High-level Services".

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>
> With regret, I must inform you that, based on the advice received, the Editors have decided that your manuscript cannot be accepted for publication in Journal of Grid Computing.
>
> Below, please find the comments for your perusal.
>
> You are kindly requested to also check the website for possible reviewer attachments.
>
> I would like to thank you very much for forwarding your manuscript to us for consideration and wish you every success in finding an alternative place of publication.
>
> With kind regards,
> Journals Editorial Office
> Springer
>
> Comments for the Author:
>
> Reviewer #3: The paper fails to meet the basic criteria of scientific publications and is recommended for rejection. The problems at a high level are:
> - the paper does not articulate what the goal of the research was
> - the paper does not include a description of the state of the art
> - the paper does not describe what its contribution was beyond this state of the art
> - the structure of the paper is disjoint, it lacks of a thread that leads the read through the performed research
> Before these problems are fixed the paper cannot be considered and reviewed as a scientific publication.
>
> Detailed comments:
> - The title is misleading. Does it mean that the framework was enhanced by high level services, or does it mean that the framework itself is the high level services?
> - The abstract consist of too long sentences and does not tell what the scientific contribution of the paper is to the field.
> - Several sentences are too long. Break them into shorter ones. (e.g.

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GriF is a workflow-oriented Grid Framework designed within...)
> - The Introduction section does not provide an introduction to the paper. It does not describe the topic of research, the particular problem that was solved (or tried to be solved) and provide insight into the solution.
> - According to the last section of Section 2 the reader can assume, that the new contributions of the paper are: (1) Better efficiency of execution with GriF than with P-GRADE; (2) Better modality in UI than before. Are these the new contributions? Neither of them is not elaborated in later; The terms efficiency and modularity are not defined for this context; The improvements are not quantified.
> - Step 6 is missing from Fig 2.
> - Fig 2 is a standard SOA architecture, where YR is the service registry, YP is a job/task execution service. There are several similar solutions in the literature built on various middleware (Java, Jini, Globus, GLite; ARC; GEMLCA; AHE, etc.) None of these are mentioned.
> - Based on Section 3.2 the authors developed a chemistry-oriented GUI on top of a gLite parameter study service. This is not new, there are several examples, most notably from the EGEE and EGI communities. None of these are mentioned.
> - Using the reference [37] to backup the term "Science Gateway" is meaningless.
> - Using the reference [38] to refer to task distribution models is meaningless. Find better references and explain which models do you talk about.
> - The paper calls the grid as the HPC platform. To HTC platform, it says "a task farm in which the master generates the initial conditions and the workers carry out the integration of the trajectories". Grids can be also used for master-worker execution, moreover this is the main way of using grids. Provide proper definitions for HPC and HTC. What do these mean in this context?
> - The second part of Section 5.1 (Starting with "It is worth emphasizing here that..." is one way of high level description of green IT, however this topic has nothing to do with the rest of the paper. It's not with the right tone for a scientific publication and disjoint from the rest of the paper.
> - Fig 11: How is it possible that the usage under 1 is zero? This means that nobody uses the applications that are compiled by the AU

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and SP.
> - In the Summary there is a sentense "... this is the first time that a study on the ... reaction has been performed using a single Grid Workflow" What follows from this? Without further explanation this statement is meaningless. (It is also possible that nobody did this before because it makes no sense. - just to give you an example)
> - In the Summary there is a sentence: "Results clearly show that GriF, ... , is well suited for ... " --> Which results show this? I do not see any sign of these results in previous sections of the paper.
>
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>
> Reviewer #5: The paper describes a chemistry-oriented gateway. Although it is a nice work there are significant number of issues that should be improved before the paper can be published in the journal.
>
> 1. There is no related work section in the paper. This is a must in a scientific paper. Its role is to show what is the contribution of the work described in the paper compared to the state-of-the-art. In such a related work section I would like to see two major issues discussed:
> a. Compared to other chemistry gateways in which sense GriF is better or implements new ideas. For example, papers like [1] and [2] (see at the end of this review) should be considered in such a comparison.
> b. Explaining why existing portal frameworks were not suitable to solve the problems raised by the COMPCHEM VO. Here I would like to see references and arguments compared to EngineFrame, Vine Toolkit and WS-PGRADE. The old P-GRADE is mentioned in the paper but not the new one that can be referenced by [3]. The paper mentions that "A comparison between the use of P-GRADE and GriF shows that the latter improves on the former in efficiency and by providing the users with better operational modalities based on friendly User Driven Services." Such a claim should be proven or not claimed in a scientific paper. Unfortunately, this claim is not proved in the paper which is a very bad scientific bahaviour that should be avoided.
>
> 2. The paper is basically and IT paper and not a chemistry paper so its contents should be useful for IT people rather than chemistry people. In that sense Section 2 gives too much chemistry details and only few

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IT details. The last paragraph is like an advertisement for GriF, describes a lot of nice features but does not explain how they were achieved, designed and implemented that would have been interesting for an IT reader. This is quite generic for the whole paper: it describes nice feature without explaining how they were achieved.
>
> 3. It is not clear from the paper what kind of workflow system is used. If it is a brand new one designed by the authors then a detailed description of this workflow language is necessary for the paper.
>
> 4. Section 4.2 on HTC farm again describes everything from the point of view of the chemists and not as an IT reader would be interested in reading it. The authors should decide to whom they write this paper. If for chemists then they have to withdraw the paper from this journal and submit to a chemistry journal. If they target IT people, then they have to significantly rewrite the paper, particularly sections 3 and 4.
>
> 5. I liked Section 5, it is a really new and interesting feature of this portal.
>
> 6. Reference list. An important scientific paper requirement is that whenever a scientific paper is available it should be used in the reference list and not a URL. A URL is not considered as an academic reference and hence the authors of the other IT products referenced by this paper cannot use this reference in their academic assessment. This means that the authors of the current paper do not pay respect to those authors developed the referenced products. For example, instead of reference 19 (Gromacs; http://www.gromacs.org, cited 13 Dec 2011), please, use [4] and instead of reference 23 (P-GRADE Grid Portal; http://portal.p-grade.hu, cited 13 Dec 2011), please, use [5].
>
> [1] Zhongwu Zhou, Feng Wang, Billy D. Todd: Development of Chemistry Portal for Grid-enabled Molecular Science, Proceedings of the Fourth International Workshop on Web Site Evolution (WSE'02), 2009
> [2] Georg Birkenheuer, et al: MoSGrid: Progress of Workflow driven Chemical Simulations, Grid Workflow Workshop, 2011
> [3] P. Kacsuk: P-GRADE portal family for Grid infrastructures,

Concurrency and Computation: Practice and Experience journal, Volume: 23, Issue: 3, 2011, pp. 235-245
> [4] Van Der Spoel D, Lindahl E, Hess B, Groenhof G, Mark AE, Berendsen HJ (2005). "GROMACS: fast, flexible, and free". J Comput Chem
> [5] Z. Farkas and P. Kacsuk: P-GRADE Portal: a generic workflow system to support user communities, Future Generation Computer Systems journal, Volume: 27, Issue: 5, 2011, pp. 454-465
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> Reviewer #1: Journal of Grid Computing
> On the Enhancing of GriF a Workflow-oriented Grid Framework combining High-level Services
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> The paper describes a Grid Framework, called GriF. From my point of view, the important innovation of GriF is the introduction of a rewarding system for VO "Developers" for contributions to the community.
>
> Summary:
> The aim of GriF is to allow an easy use of Grid services for not computer skilled scientists, facilitating optimal resource usage, optimal distribution of tasks and assemblage of applications, and the fostering the collaboration between experimentalist and experts.
>
> The framework consists of several components. The consumer is responsible for the job management. The provider is a container for web services and allows queue selection. The registry contains the available web services.
>
> Several ranking and quality evaluation methods should improve the work on the grid and reward engagement of VO members.
>
> The ranking of queues is done according to a metric of load and performance.
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> Quality of Service (QoS) and Quality of Users (QoU) are measures for the service and user performance. The Service QoS measure should fit to a wide area of web service purposes. The QoS properties are age, WS consolidation, diffusion, efficiency, production, social aspects, and green aspects.
> QoU should stimulate the competition between users and is build on collected and filtered implicit and explicit user information. Parameters are the number of compilations, job runs, number of success over failures, number of results retrieved over available, average amount of memory consumed, average elapsed wall time, and user specific feedback. Three types of users are distinguished, active user, passive user, and, software developer.
>
>
> Good:
> - The paper has a good concept and is well written.
> - The applied use case provides a conclusive motivation.
> - The framework allows a mix of local, HPC and Grid execution.
> - The reward system.
> - The framework is implemented and tested for the presented use case.
>
>
> Drawback of the approach:
> - As far as I see, there is no failure tolerance.
> - Users have to upload home build binaries. - Security issue.
>
>
> A few questions came to my mind that should be explained in the paper.
>
> - Only very few characteristics of the applications are mentioned. Are they sequential or parallel?
> - How does this affects 'ranking'?
> - Aim of GriF is minimal consumption of wall time. As far as I know, the runtime of the chemical simulations is be dependent on the molecules and difficult to guess. How does the framework estimate the runtime?
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> Reviewer #2: This is an interesting paper which describes the use of GriF as Science Gateway for molecular simulations.
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> Overall this is a well written paper which reads well and is easy to
> understand. The following minor modifications would enhance the clarity of the paper:
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> a) the authors should describe whether in the chosen context alternatives to GriF exist and describe them and why particularly they have chosen Grif
>
> b) figures like 3, 4 and 5 are hard to understand
>
> c) future work is not explained
>
> d) they report results for a nitrogen molecule. they should give an estimation on how difficult (or even feasible) or costly would the calculations be for more complex molecular systems; in other words, which kind of systems are amenable for working with this approach
>
> e) they mention that GriF can rank the grid services on the basis of users' profiles; in this aspect there should be comparison with other alternatives (for instance, pipeline pilot)
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> The paper is recommended for publication.
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> Reviewer #4: - The text in general needs proof reading. Long sentences should be broken up for better understanding. Avoid repeating words in the same sentence.
> - In the last paragraph of section 2 a "comparison between P-GRADE

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and GriF" is mentioned. Details about this comparison should be provided. Who carried out this work, what were the main aspects? It is also mentioned that GriF provides improved efficiency and operational modalities. Again some details about this should be provided: in what terms is it more efficient and to what degree?
> - First sentence of section 3 declares that "GriF has shown to be an extremely useful tool for the users because it facilitates an optimal usage of the memory, a reduced engagement of the cpu and a minimal consumption of wall time. From what aspect is it optimal? To what degree it reduces cpu engagement?
> - Next sentence: "On top of that, it leads to an optimized distribution of tasks over the network ..." Again, from what aspect is it optimal?
> - In section 3.2, after equation (3) is introduced, there are 5 cases described.
> - What happens if none of the are true?
> - Case 2-5 starts with Or (if no q matches this criterion) by this do you mean the above criteria?
> - It seems that letter q is used as a short for queue. In case 1 by qs you mean queues. This is quite misleading another notation would be more fortunate.
> - Equation (4) includes wt and ct representing wall time and cpu time. This notation is also misleading, the reader might think that these represent multiplications.
> - A section of similar solutions should be added that compares GriF with other workflow frameworks based on different aspects and focusing on the improved capabilities of GriF.
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> The Editorial Manager is at: http://grid.edmgr.com/