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D3.4 – Efficacy of Feedback Process

WP3: Consultancy & User Groups



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Executive Summary

This document is the fourth deliverable from WP3 *Consultancy and User Groups*. The project's structure requires that there is a good flow of feedback between end-users and the many activities spread amongst the project's work packages (WPs). It provides an opportunity to take stock and report on the efficacy of feedback in the project.

Overall, feedback in the project is good, but it is important to continue to monitor both external and internal feedback. With the former, we need to broaden the areas in which this occurs beyond the current scope, which is focused on the project's main codes. Internal feedback processes could be more explicit to maintain good feedback as the centre grows.

The document considers each work package in turn and depicts graphically the strength of feedback with other parts of the project and with external stakeholders. We look at the current state, a desirable future state, and then consider what could be done to reach the future state.

Feedback relating to WP1 (software) is broadly considered to be satisfactory, but there are links which could be improved, for example with WP2, the SAB, and particularly WP5. WP1 feedback directly with users through mailing lists and forums is good.

Strengths of WP2 (portable environments/workflows) in feedback relate to collaborations with organisations like ELIXIR and Open PHACTS. Possible areas for improvement were identified for all WPs except for WP6. WP2's work is approaching the stage where end-user feedback will become much more relevant

WP3 (user groups & community) generally has sufficient feedback, although possible improvements relate to WP2, WP5 and other infrastructures. WP3's strengths have been in supporting feedback to other WPs through provision of forums, webinars, IGs, etc.

WP4 (training & dissemination) feedback is broadly sufficient, but areas for improvement relate mainly to the technical WPs. Technical WP members already contribute to training, but coordination between these WPs' activities could be improved.

WP5's feedback to date has come to a great extent through WP3 and WP4. It is hoped that in future WP5 could connect more directly to other parts of the project, but that WP3 (and WP4) will still provide the main links with end-users.

WP6's feedback is sufficient. The similar future state for WP6 reflects the intention that WP6 should coordinate, but *not* act as a point through which most project communication and feedback should take place.

Areas for improvement are set out in Section 3. Decisions relating to which of these improvements can be actioned will ultimately fall to WP leaders and the EB, but WP3 will continue to track work being done to improve feedback through Task 3.7, *Feedback and Improvement*.

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1 Introduction and Context

1.1 Project Context

This document is the fourth deliverable from WP3 *Consultancy and User Groups*. From the outset of this project to establish the Centre of Excellence (CoE), it has been important that the centre should be user-driven. It is therefore important for us to be aware of how well the various feedback processes used by the project are working to meet the needs of users. The core activities of the Centre started early in the project and are ongoing: The project has been contributing to the development of the key codes (WP1), working on workflow systems and standards (WP2), running services for the wider community such as forums, webinars and events (WP3), running a set of pilot use cases (overseen by WP3 with much of the work happening in WP2 and WP1), offering training courses (WP4) as well as planning for sustainability (WP5). Feedback amongst different parts of the project is key to the success of a unified user-driven. This document therefore provides an opportunity for us to take stock, and to report on the efficacy of feedback in the project.

Overall, feedback in the project is good, however there are two areas that need to be monitored. Feedback to and from the centre's users is already taking place, particularly in areas where the centre is building on processes established by code owners, but there is scope for an increase in quantity and scope (for example, so that it adequately covers topics beyond the project's main codes). Current internal feedback processes rely to a great extent on the current size and make-up of the project. There are, at present, a fairly small number of people working on the project and much feedback occurs informally, as a result of key people working in multiple work packages, and alongside each other at meetings and events. As the centre grows, it is recognised that these approaches are unlikely to continue to scale, so one aim of this document is to understand the current state of project feedback so that we can ensure that it *remains* good as the centre grows.

In this document, we also want to make clear the ways in which feedback could be improved. Some of the improvements suggested here can be implemented quickly whereas others could require additional resources or more substantial changes to project processes.

1.2 Approach

We consider the different areas of the project and consider in particular how information flows (i.e. feedback and feed forward) between the project's work packages (WPs), and also how it flows between the project and external groups such as key stakeholders. There are some activities that cross multiple work packages, which complicates how the information flows between them. However information flow represented as graphs of nodes (groups of people), edges (relationships between them) with arrow heads (to show direction) is a simple approach to understand feedback now and in future, by completion of the project. Comparison between these two states enables us to identify improvement goals.

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We have used these information flow graphs as a mechanism to collect the information from each project work package to understand the relationships between them and important external groups. This enables us to present a systematic description of feedback in this document. We have created “now” and “future” state graphs for each work package, which is accompanied by an explanation. The “now” state graphs show how the project has been working to date where relationships are limited to sufficient, weak or missing. An example information flow graph is shown in Figure 1.

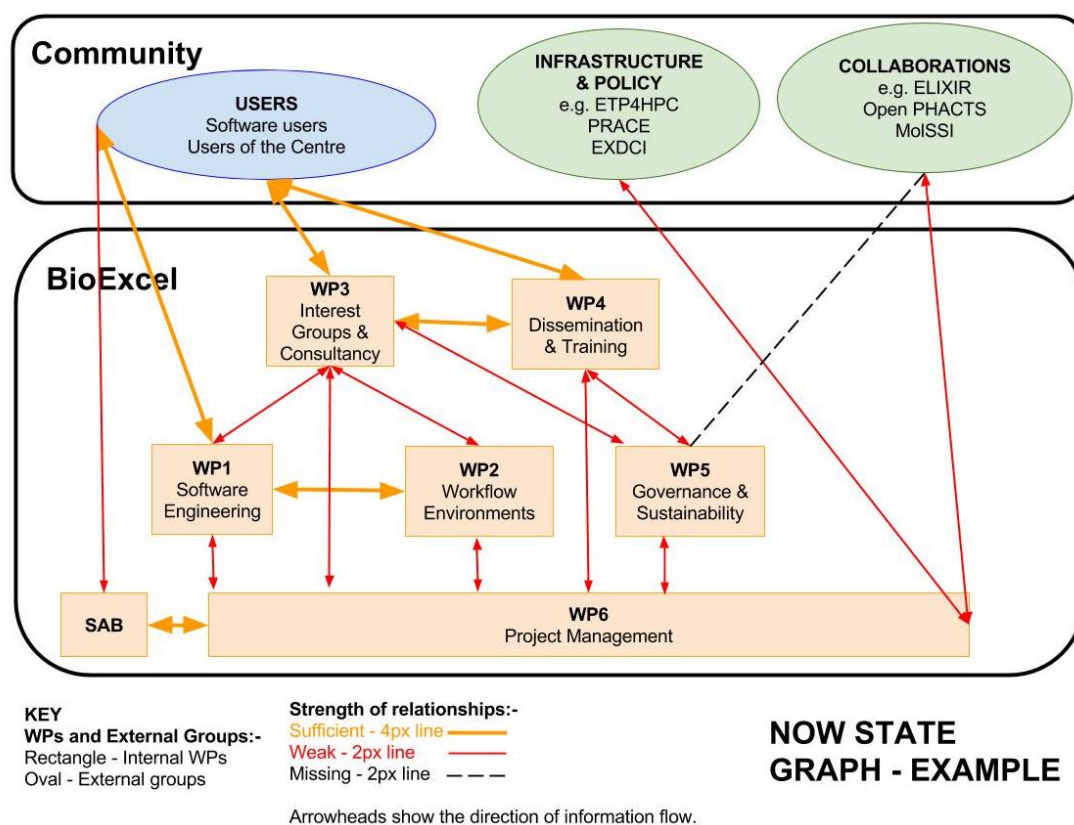


Figure 1: Example Information Flow Graph (feedback and feed forward)

In the “now state” graphs, we only allow three strengths of relationships: *Sufficient* relationships are those where we can demonstrate that feedback has been taking place, and that there are no obvious perceived problems with the quality of feedback. It will be seen that there are some relationships that could arguably considered to be *strong* already, but we reserve this strength of relationship for the Future State in order to make clear where we can see scope for improvement from already sufficient feedback relationships. *Weaker* relationships are those where we can identify issues with the quality of feedback, and can see ways in which these could be improved. In some cases, this reflects the current stage of the project; some activities are more advanced than others and those that have been built from scratch, for example, are not necessarily in a state where user-feedback makes sense. *Missing* relationships are those where it is difficult to demonstrate that there has been direct feedback to date, but where we consider that there should be feedback.

We have also depicted the “future” state as graphs (shown in Section 3) which are limited to sufficient or strong relationships. We consider the differences between the now and future state graphs to be the basis for realistic goals to aim for by the end of the current project phase (in 12 months’ time).

It should be noted that it is not necessarily problematic if there is a weak or missing relationship between nodes in the now state if current processes suffice for the size of the centre and the stage of the project (for example, if feedback is flowing indirectly through other parts of the project). It does, however, mean that these may need to be improved to a sufficient or strong relationship as the centre grows and matures.

Much of the input for this document has come from work package leaders. The basis for the current status of the project feedback is mostly self-evaluation by contributors working in different parts of the project.

In Section 2, we consider information flow in the project to date, and in Section 3 we look forward to the improvement in information flow to guide the future work of the CoE.

2 Project Feedback Flow So Far

2.1 WP1: Software Scalability and Usability

WP1 is aligned with both the *Software* and *Usability* themes of BioExcel. One important area of feedback are the existing support mechanisms of the codes in the project. BioExcel now contributes to these pre-existing support mechanisms. A significant proportion of developer contributions to mailing lists such as gmx-users and gmx-developers is made by developers of GROMACS¹ who are supported by BioExcel, as well as management of user feedback through the Redmine bug tracker used by GROMACS developers. It was decided in this case where there was a large and established user-base for these platforms, that it did not make sense to replace these with BioExcel infrastructure. On the other hand, in the case of HADDOCK² it was decided that moving existing users to a forum platform provided by BioExcel (*AskBioExcel*³) would be the best way to support these users.

Figure 2 shows the current state of information flow for WP1.

¹ <http://www.gromacs.org>

² <http://www.bonvinlab.org/software/haddock2.2/>

³ <http://ask.bioexcel.eu>

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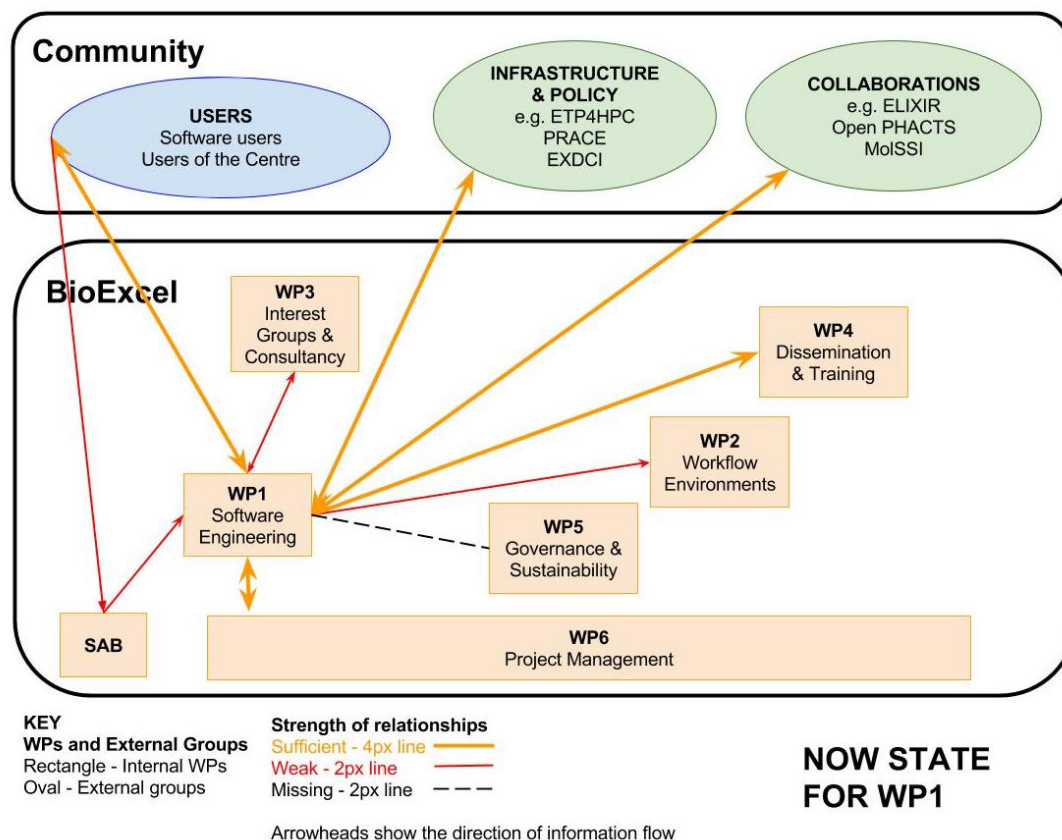


Figure 2: Feedback to Date: WP1

2.1.1 WP1↔Users - Sufficient

User communities for most of the WP1 software existed before BioExcel, and have been strengthened through the adoption of the *AskBioExcel* forum (based on the Discourse platform⁴). There is a good deal of feedback that takes place through the pre-existing mailing lists⁵ and bugtracker⁶ for GROMACS and the forum for HADDOCK. For the GROMACS mailing list, approximately 50 posts per month are made by BioExcel-supported staff, with further posts also coming from staff in the partners' groups who are in turn using infrastructure supported by BioExcel-supported staff. BioExcel supported staff also read the majority of the 500-800 posts per month which are made to the list. Figure 3 shows the number of posts per day on the HADDOCK forum. BioExcel-supported staff have made over 290 posts to the forum during the project.

Naturally, the more recent software development is only beginning to attract users, particularly, for example, in the case of QM/MM using the CPMD+GROMACS combination⁷. Information flows in both directions, normally in the form of usage questions and answers, advice on method design, feedback on missing or broken functionality, and requests for collaborations. Stronger connections with industry users would be beneficial, but would also require dedicated BioExcel personnel to maintain individual relationships. Privacy and

⁴ <https://www.discourse.org>

⁵ http://www.gromacs.org/Support/Mailing_Lists

⁶ <https://redmine.gromacs.org>

⁷ <http://bioexcel.eu/software/cpmd/>

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competitiveness considerations probably prevent some industrial users from engaging publicly, perhaps even for simple how-to questions.

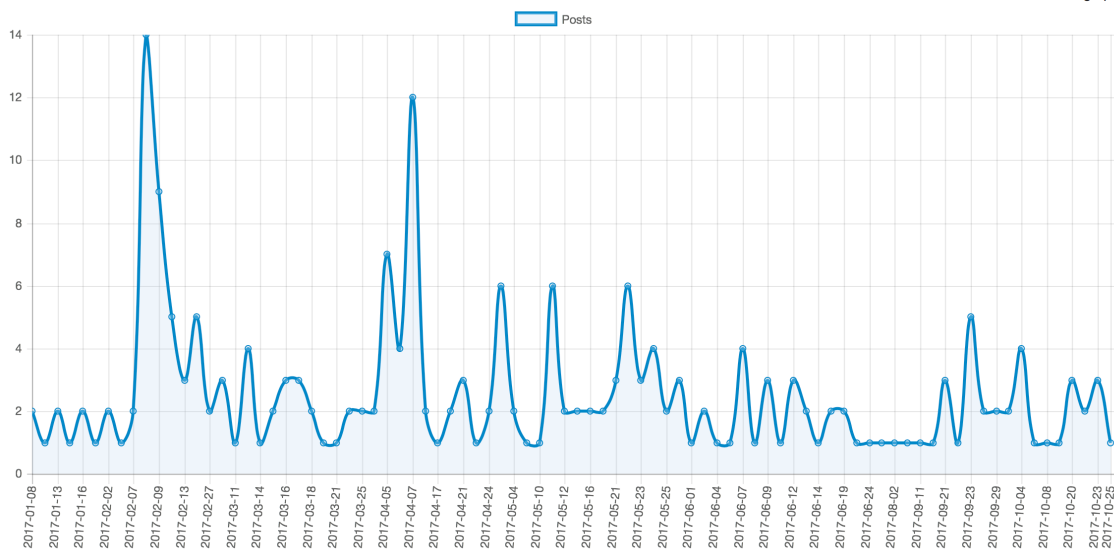


Figure 3: Posts per day on the HADDOCK forum

Figure 4 shows one of many examples in which user feedback has led directly to a change in the code. Here a conversation on a mailing list (which includes a developer supported by BioExcel) results in a bug report and then an update to the software (implemented by a developer supported by BioExcel).

Mailing list and forum feedback happens in both directions, with users being able to ask questions and make requests based on their circumstances, and with developers being able to communicate back to the users to offer assistance to the code users. The bug tracker allows users to make feature requests.

Much of this feedback to and from code users could be considered direct feedback between the code developers working in WP1 and the codes' users, but this is supported by WP3 through provision of services such as the Forum and through staff effort in contributions to code mailing lists.

2.1.2 WP1 ↔ Collaborations - Sufficient

Leaving aside the users of the scientific software, WP1 collaborations revolve primarily the teams that develop and maintain

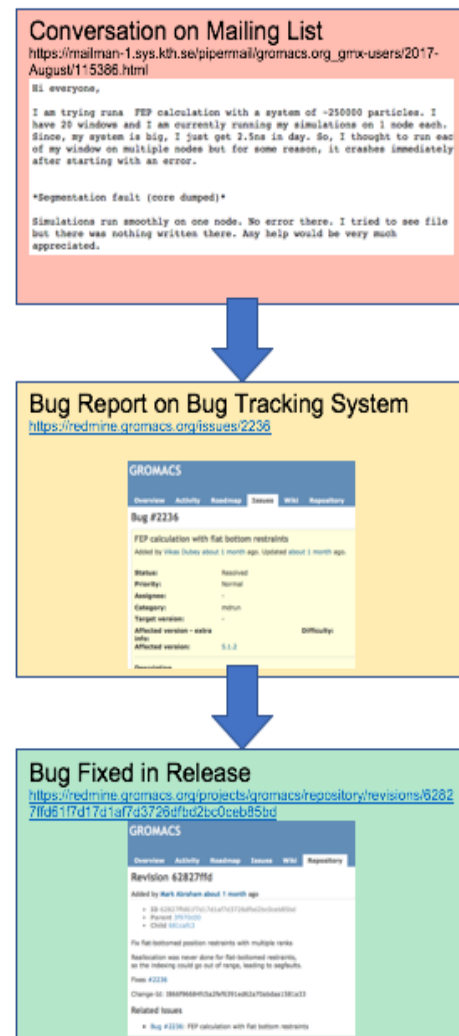


Figure 4: Feedback flow from code user to a code fix

the required software infrastructure, and the vendors of the hardware upon which it will run. Many of these collaborations were in place already for established projects (for example Intel, NVIDIA, AMD and IBM for GROMACS), and some are being extended (for example, the GROMACS team has built new relationships with ARM and Solaris, and is supporting the activities of the related MolSSI programme in the US). Information tends to flow both ways, as developers and vendors inform BioExcel about new capabilities, and we in turn advise them on what features the software would benefit from, and how best to extract highest performance from hardware and software once it is built.

2.1.3 WP1↔Infrastructure & Policy - Sufficient

WP1 is in direct contact with infrastructure providers such as PRACE⁸ and EGI⁹, making available benchmark suites, tuning advice, and supporting installation and documentation. Some of the work in WP1, particularly in GROMACS, could benefit from stronger relationships with providers of software infrastructure such as compilers, libraries, and software analysis tools. Information flows both ways, but often in different directions at different points of the life cycle.

2.1.4 WP1↔WP2 - Weaker

The pilot use cases connect the WP1 codes with the workflow-development activities of WP2, but so far little feedback has occurred. Workflow usage will probably illustrate areas where the underlying WP1 codes can improve, but there can be a long lead time before effect is felt, particularly where software has annual release cycles (such as GROMACS) and users adopt new versions irregularly as scientific projects start and end. Improving communication will require more effort from both ends.

2.1.5 WP1↔WP3 - Weaker

Interactions between developers of WP1 and WP3 interest groups have been of uneven strength, even though interactions with user communities have remained strong. Maintaining an interest group requires supporting a person who has the necessary breadth of scientific expertise to engage with multiple external projects, facilitating connections with developers and other members of the interest groups. This is challenging work that does not always offer clear benefits to the person engaged in it, and does not necessarily combine well with the skill set of software development. However, information has flowed to the interest groups in the webinar series. General interaction between WP1 and WP3 coordination has been effective in general, but links could be deepened. In some cases, IG leaders (WP3) are the same people as those developing the code in WP1, so in these cases little formal information flow is required.

2.1.6 WP1↔WP4 - Sufficient

The WP1 development teams have conducted training activities, and will continue to do so, particularly as projects complete and new feature support becomes available. As WP4 efforts at most partners are conducted by the same people as WP1 efforts, little formal information flow has been needed. WP1 could

⁸ <http://www.prace-ri.eu>

⁹ <https://www.egi.eu>

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benefit from increased lead-time for training events to make better use of personnel from WP1 who have the expertise required to deliver training.

2.1.7 WP1↔WP5 - Missing

Some information has flowed at all-hands meetings, but, for example, it is not yet clear if it will be possible to have a business plan that can support software development without a substantial component of public funding. However, there is not a large amount of information that should flow.

2.1.8 WP1↔WP6 - Sufficient

WP1 is represented at the fortnightly Executive Board teleconferences and has good communication with WP6 project operations. There is a bidirectional flow of information.

2.1.9 WP1↔SAB - Weaker

A role is envisaged for SAB advice on strategic direction to the WP1 developers, and suggestions have already flowed. Naturally those have been of large scale, such as replacing existing commercial products' MD engines with GROMACS. These offer exciting possibilities, but are risky activities. There is a large risk that an attempt to persuade an existing product to switch dependencies (and risk its customer base) will produce no result for a long time (or ever).

2.2 WP2: Portable Environments for Computing and Data Resources

This work package is closely aligned with the *Usability* theme of BioExcel. There are some obvious links with other parts of the project; for example, the project's pilot use cases (coordinated in WP3) form the basis for the workflows investigated in this work package¹⁰.

Figure 5 shows the current state of information flow for WP2.

¹⁰ See, for example, BioExcel Deliverable D2.2, *First release of workflows blocks and portals*, <https://doi.org/10.5281/zenodo.263965>

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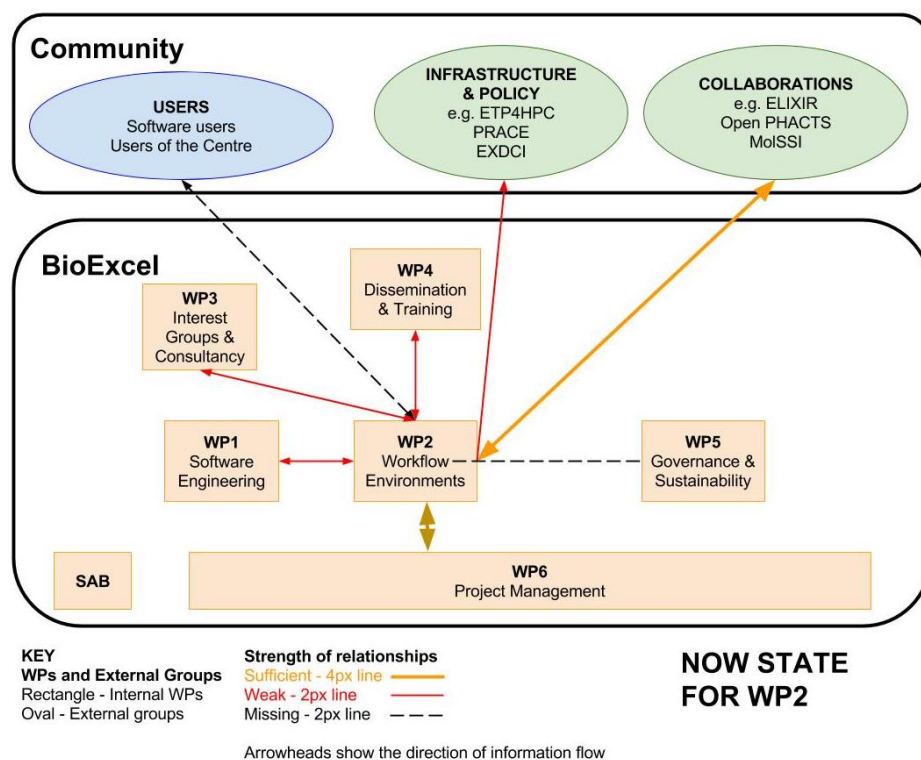


Figure 5: Feedback to Date: WP2

2.2.1 WP2↔Users - Missing

In this section, we consider users to be users of the workflows and components worked on in WP2. Connection between WP2 developed workflows/VMs and BioExcel users is missing. However, almost all the needed infrastructures are now up and running (portal, tools registry, VMs database, service providers), so we expect to have them opened in the coming months. This should become a bidirectional relationship, although of course there hasn't been any external feedback so far, as tools are not publicly available yet. More general feedback to and from users does flow through WP3.

2.2.2 WP2↔Collaborations - Sufficient

WP2 is one area of the project in which collaborations have been strongest. WP2 has active collaborations with ELIXIR¹¹, EGI, CWL¹², Open PHACTS¹³ as well as partners in the pilot use cases such as Nostrum BioDiscovery¹⁴ (a pharmaceutical spin-off from the Barcelona Supercomputing Center) and the Institute for Genetic and Molecular Medicine (IGMM)¹⁵ at the University of Edinburgh.

WP2 has been working with ELIXIR on *bio.tools*¹⁶ interoperability and AAI. The interaction here has been in both directions, as BioExcel workflow descriptions (using CWL) and a Python wrapper library were presented and accepted as a use

¹¹ <https://www.elixir-europe.org>

¹² <http://www.commonwl.org>

¹³ <https://www.openphacts.org>

¹⁴ <http://nostrumbiodiscovery.com>

¹⁵ <http://www.ed.ac.uk/igmm>

¹⁶ <https://bio.tools>

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case in the ELIXIR tools and interoperability platform. The ELIXIR interoperability platform suggested a set of best practices (ELIXIR EXCELERATE¹⁷ WP5) to register, describe, make interoperable (and, when applicable, FAIR¹⁸), and maintain provenance information. The BioExcel *Model Protein Mutants* workflow prototype is used as an example (use case) of how to follow this set of recommended best practices and the benefits of applying them.

Collaboration with Common Workflow Language (CWL) was also started and has good momentum, with the description of the workflow prototype. New workflows to be implemented in BioExcel will be also described with CWL and visualized with the CWL viewer¹⁹.

Collaboration with Open PHACTS was started thanks to the *Virtual Screening* use case. The same use case is being also designed and implemented in collaboration with Nostrum BioDiscovery.

2.2.3 WP2↔Infrastructure & Policy - Weaker

WP2 is in direct relationship with the Barcelona Supercomputing Center (BSC) and its supercomputing facilities, in particular the new Marenostrum 4. Workflow prototypes have been tested here, but we would like to test them also in other supercomputer infrastructures such as ARCHER²⁰ at EPCC or Juqueen²¹ in Jülich, both installed in BioExcel partners' premises.

2.2.4 WP2↔WP1 – Weaker

This relationship has been described already and here is the WP2 view:

There is an existing relationship between WP2 and the GROMACS code, as the workflow prototype is using it for the molecular dynamics section of the pipeline. However, we expect to have more profound discussions once the workflow is completed.

Relationships with the other WP1 codes (HADDOCK, CPMD, PMX²²) is established thanks to the project pilot use cases. The relationship should be bidirectional by the end of the project, but so far its strength is weak in both directions.

2.2.5 WP2↔WP3 - Weaker

The relationship between WP2 and WP3 is expected to grow once the different workflows and VMs that are being implemented will be accessible. Interest groups such as the *Entry Level Users* IG and the *Workflows* IG will benefit from the work published by WP2, increasing the visibility, easiness of usage and portability of these computational biomolecular pipelines. So far, WP2 and WP3 have been working together on the organization and presentation of a couple of

¹⁷ <https://www.elixir-europe.org/about-us/how-funded/eu-projects/excelerate>

¹⁸ <https://www.nature.com/articles/sdata201618>

¹⁹ <https://view.commonwl.org/>

²⁰ <http://www.archer.ac.uk>

²¹ http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html

²² <http://pmx.mpibpc.mpg.de/>

webinars for the *Entry Level Users* interest group showing web servers running molecular dynamics and analysis workflows, and another one presenting a project pilot use case workflow (Virtual Screening) that is currently being implemented in collaboration with the Open PHACTS platform. All of these points are also strongly related to the training, discussed in the next section. This interaction has been bidirectional.

2.2.6 WP2↔WP4 - Weaker

We expect the relationship between WP2 and BioExcel training and outreach WP4 to increase in the last year of the project, once the different workflows and VMs that are being implemented will be accessible. However, we have been working together in the organization of the BioExcel workflow training for computational biomolecular research²³, and in a couple of webinars prepared for the *Entry Level Users* interest group presenting web tools running molecular dynamics and analysis workflows. Feedback has been bidirectional.

2.2.7 WP2↔WP5 – Missing

This missing relationship has not been relevant to date but is expected to become more important in future.

2.2.8 WP2↔WP6 - Sufficient

WP2 is present in all the fortnightly Executive Board teleconferences and has a fluent and bidirectional communication with WP6 project operations.

2.3 WP3: Consultancy & User Groups

This WP is one of the more user-facing work packages. As described below, some of the work undertaken in this work package is carried out in conjunction with the technical work packages. The individuals who are contributing to this work package from many of the partners are also directly involved in technical work. An important part of the work of this WP has been to set up activities and events (e.g. webinars, interest groups, meetings, forum) that are of direct relevance to users and also used by project partners to interact with external users.

Figure 6 shows the current state of information flow for WP3.

²³ <http://bioexcel.eu/events/bioexcel-workflow-training-for-computational-biomolecular-research/>

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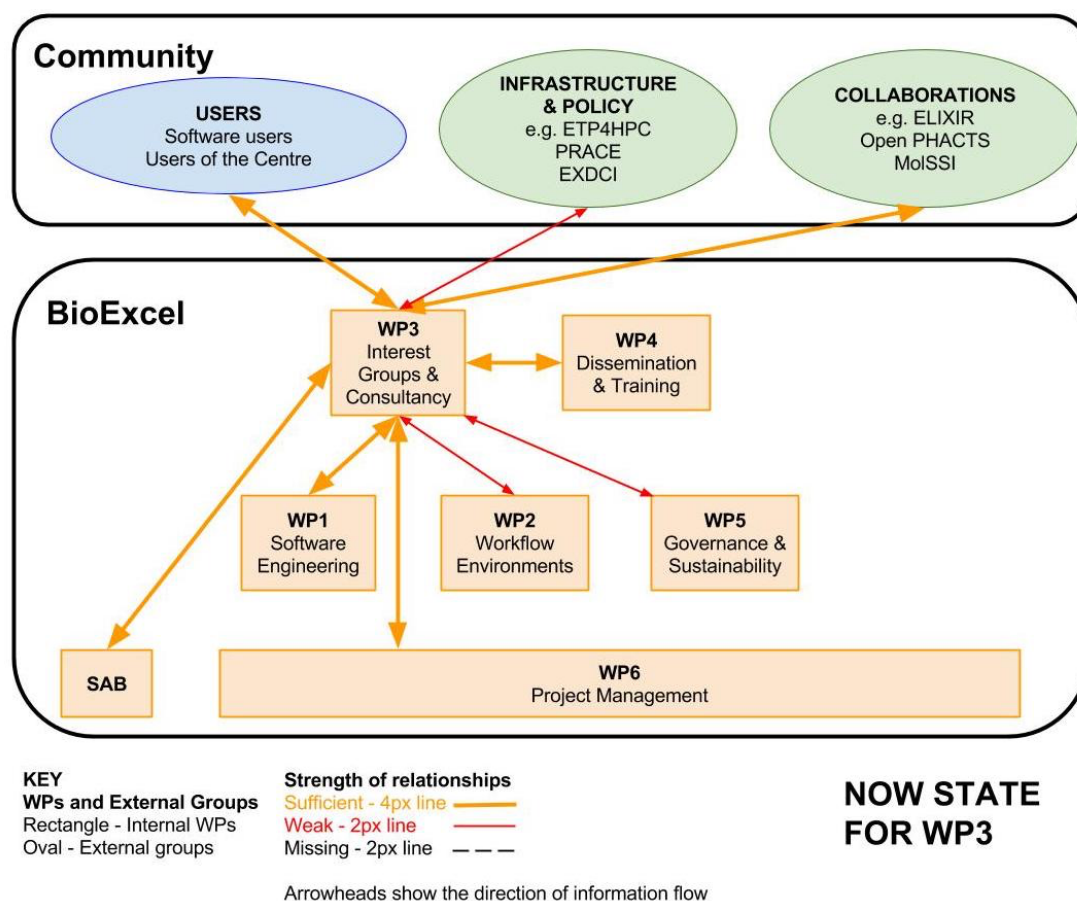


Figure 6: Feedback to Date: WP3

2.3.1 WP3↔Users - Sufficient

A considerable amount of groundwork has been done to establish feedback between users of the CoE and the project. Whilst the level of feedback between WP3 and users is probably sufficient for this stage in the project, there is work to do to continue to improve this.

The webinar series organised by WP3 has delivered 16 webinars²⁴. This successful mechanism has disseminated information about work underway in the project, and also to allow others in the community to share information on their work. Recordings of the webinars are made available afterwards, and to date there have been over 3,400 views of these webinars, showing that it is a resource valued by our users.

The *AskBioExcel* forum provides an informal mechanism to support users at any time which has been used very successfully in some cases. To date, there have been over 12,500 pageviews from logged-in users (spread over ~1,700 visits) and over 78,300 pageviews from users who are not logged in. A total of 683 posts have been made in 179 different topics/threads. By some margin, the most active forum is that related to the HADDOCK code.

Interest Groups (IGs) are an important mechanism for interaction with our users. They were established early in the project and they provide valuable feedback

²⁴ <http://bioexcel.eu/category/webinar/>

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and interactions with our users. Individual IGs have organised particular webinars and some have devoted pages on the BioExcel website.

The *Integrative Modelling IG* produces regular newsletters which highlight relevant activities and events within the project and the wider community. The *Practical Applications for Industry IG* meets occasionally through interactive conference calls which host discussion of relevant use cases, shared challenges and resources. The *Hybrid Methods IG* organised a session at a face-to-face meeting in Cagliari, and this provided a good opportunity to foster further links with this community. Attendees at this meeting have subsequently contributed to BioExcel's webinar series²⁵. At this meeting *BioExcel* was able to share information on work that is being done in the project related to QM/MM calculations with CPMD. The *Free Energy IG* helped to promote work going on in the project including the publication of the pmx webserver manuscript²⁶ and the joint BioExcel/CompBioMed workshop on free energy calculations²⁷. At this meeting, there were discussions on topic of interest to IG members including standards for reference datasets and blind predictions and best practices for free energy calculations. Examples of information learned from this IG include reproducibility issues between software packages and versions experienced by novice users and the importance of increasing awareness of the need to apply sanity checks in free energy calculations. The IG has also facilitate knowledge exchange between members on topics such as charge changing modifications and parameterisation of non-standard molecules.

Whilst there have been some notable successes in activities related to IGs such as webinars, there remains some inconsistency. As would be expected, some IGs are working better than others. Since the service offering of the CoE is still relatively limited (webinars, IGs) the concept of what a “user” of the CoE is not as clear-cut as it would be, for example, for users of a computer system or piece of software.

2.3.2 WP3↔Collaborations - Sufficient

WP3 has been involved in design of agreements for strategic and collaborative partnerships. It has been directly involved in establishing particular partnerships with ELIXIR and Open PHACTS. However, as expected, most of the interaction with these organisations has been with the project's more technical WPs. WP3 has been involved in organising webinars by speakers from these organisations²⁸.

²⁵ Webinar: *NAFlex, a web server for the study of nucleic acid flexibility (2017-07-20)*, <http://bioexcel.eu/webinar-naflex-a-web-server-for-the-study-of-nucleic-acid-flexibility/>

²⁶ Gapsys and de Groot, *pmx Webserver: A User Friendly Interface for Alchemy*, *J. Chem. Inf. Model.*, **2017**, 57 (2), pp 109–114, <http://pubs.acs.org/doi/abs/10.1021/acs.jcim.6b00498>

²⁷ <http://bioexcel.eu/events/free-energy-calculations-from-molecular-simulation-applications-in-life-and-medical-sciences/>

²⁸ Webinar: *“BioExcel and OpenPHACTS: Building pharmacological workflow blocks for virtual screening” (2017-07-17)*, <http://bioexcel.eu/webinar-openphacts/>

2.3.3 WP3↔Infrastructure & Exascale - weaker

There is interaction between the *Training* IG and training providers in PRACE and ELIXIR. The *Training* IG Leader is part of the HPC "subgroup" of the ELIXIR Training Coordinators Group.

2.3.4 WP3↔WP1 - Weaker

This relationship has been described already and here is the WP3 view:

WP3 has provided some infrastructure (such as the forums) that has facilitated direct communication between code owners and users. Information has been the initial BioExcel survey has been passed back to WP1, but the findings from this were not sufficiently insightful to lead to any change in direction of development by WP1. On the other hand, the HADDOCK forum has generated user feedback and feature requests. WP3 has also advised on intellectual property and security aspects of licensing agreements for software usage by commercial organisations in industry, for example for HADDOCK.

2.3.5 WP3↔WP2 - Weaker

This relationship has been described already and here is the WP3 view:

The main interaction between WP2 and WP3 has been in the context of the pilot use cases. WP3 has collected information from the pilot use cases, and also helped to coordinate the revision of the pilot use cases earlier in the project. These use cases are used as the basis for some of the WP2 work on workflows.

2.3.6 WP3↔WP4 - Sufficient

WP3 has supported WP4 through the Training Interest Group and associated webinars. WP3 has worked closely with WP4 on forming IGs and publicising them through the website, newsletters and conference stands and posters. Representatives from WP3 have also contributed to discussions about classifying training participants and development of the competency framework. Feedback has been mostly through informal discussion (some face-to-face) between WP leaders.

2.3.7 WP3↔WP5 - Weaker

Earlier in the project, interaction between WP3 and WP5 was mostly through the writing of deliverables (such as D3.2 and D3.3) that were designed to inform the work of WP5. More recently, the WP3 leader has been attending regular WP5 meetings to offer advice from a WP3 perspective.

2.3.8 WP3↔WP6 - Sufficient

Feedback to and from WP6 occurs during fortnightly EB meetings, but there is also frequent communication (email, Skype) about matters relating to the wider project. This relationship works sufficiently well.

2.3.9 WP3↔SAB - Sufficient

The *Practical Applications for Industry* IG has recruited a user from industry (Zara Sands at UCB) who has joined the project's Scientific Advisory Board.

2.4 WP4: Dissemination & Training

The *Dissemination & Training* work package has been working with multiple parts of the project. WP4 receives interaction directly through WP4 relationships but additionally through the WP3 *Training* Interest Group. This second set of relationships is primarily used to maintain contact with external initiatives that have a strong interest in training or individuals involved in training. Current relationships are strongest where personal contacts are well established. This has allowed us to build good relationships quite fast but needs to be replaced by more structured channels to scale to a larger CoE and become less dependent on individuals.

Figure 7 shows the current state of information flow for WP4.

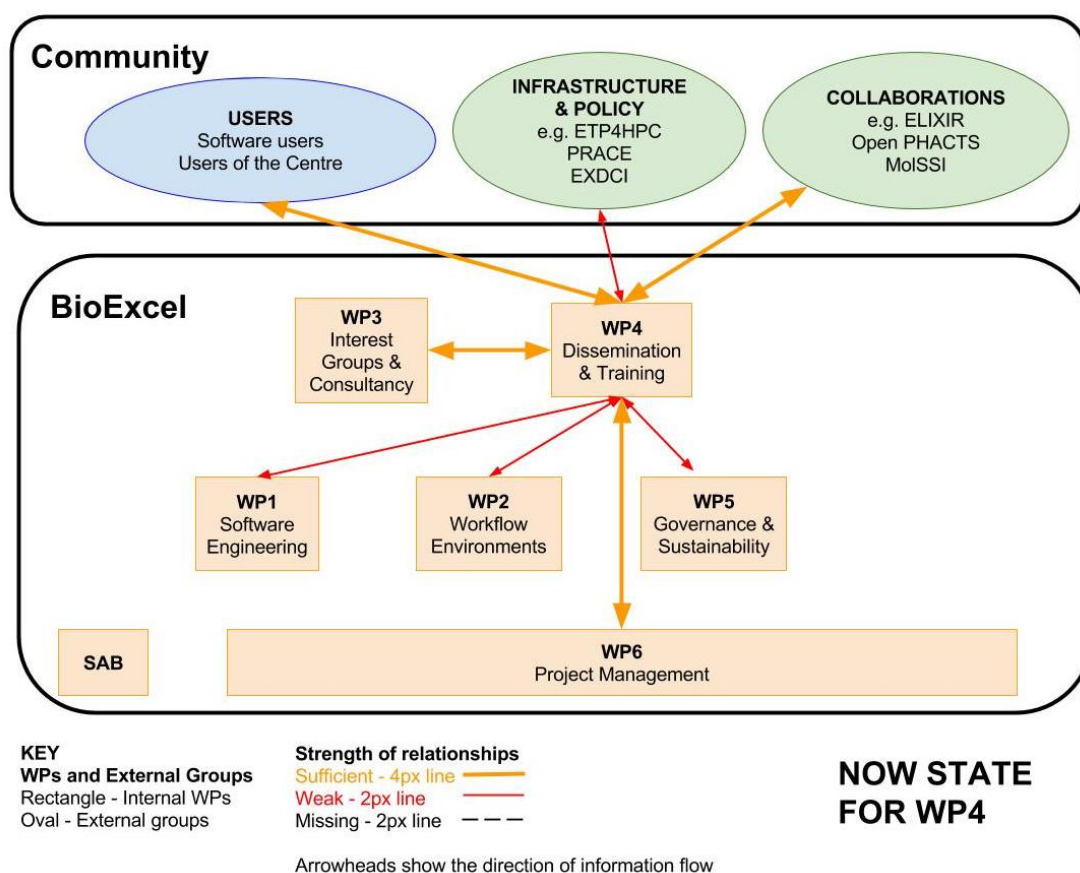


Figure 7: Feedback to Date: WP4

2.4.1 WP4↔Users - Sufficient

Interaction with users runs through a multitude of channels. With the prospective/current/previous course participants, information from the users to WP4 flows through course application documents, post-course feedback forms (post-event and long-term), and impact interviews with selected participants. The strongest flow of information is the social interaction during a training course, these take place primarily during introduction sessions where discussions with participants highlight use cases and bottlenecks but also through discussions at coffee breaks and dinners. Elements of the centre’s work are influencing the training offered, and in this way WP4 is providing a bridge in

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a similar way that WP3's activities are connecting users to the technical work in the project.

From WP4 to users, information additionally flows through the website, conference participation, LinkedIn and Twitter. Though these channels are primarily to the user, interactions do take place, especially during conferences and on social media. Many of the WP4 KPIs track this information, though they are not very strong in indicating the level or strength of the bidirectional information flow.

WP4 already has some direct interaction with the centre's users. Elements of the centre's work are influencing the training offered, and in this way WP4 is providing a bridge in a similar way that WP3's activities are connecting users to the technical work in the project. Trainees are feeding back informally through discussions with trainers at events, and more formally through post-course questionnaires.

2.4.2 WP4↔Collaborations - Sufficient

The WP4 outreach channels such as LinkedIn and Twitter are used to communicate with external initiatives. This primarily involves advertising each other's events and tagging into relevant posts.

Strong contacts with training collaborators are maintained through the *Training* IG, an example of this is the *Training* IG leader's involvement in the ELIXIR training coordinators group teleconferences and all-hands meeting.

2.4.3 WP4↔Infrastructure & Policy - Weaker

WP4 has organised two joint training courses with PRACE (one completed and one pending), through the KTH and UEDIN partners. In addition, contact with PRACE is made through the WP3 *Training* IG. Contact to other initiatives is substantially weaker, and runs through WP6, therefore this relationship is considered weak.

2.4.4 WP4↔WP1 - Weaker

This relationship has been described already and here is the WP4 view:

There is a personnel overlap for WP1 and WP4, which contributes to the success of the training activities. The reason this relationship is considered weaker is that the different WP4 activities are not joined up sufficiently. The feedback from WP1/WP4 to WP4 and vice versa is not as rich as it could be.

2.4.5 WP4↔WP2 – Weaker

This relationship has been described already and here is the WP4 view:

The relationship between WP4 and WP2 has been sporadic and centred around specific joint events, such as the "BioExcel workflow training for computational biomolecular research" event in Barcelona, October 2016. The relationship is considered weaker due to the sporadic nature, during the joint event organisation the relationship was sufficient. We anticipate a closer relationship once WP2 will be reaching out to the user to test and use the implemented workflows and VMs.

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2.4.6 WP4↔WP3 - Sufficient

This relationship has been described already and here is the WP4 view:

WP4 has joined the WP3 biweekly teleconferences from the beginning of the project. In addition, the training interest group is a major source of information for WP4 and the main channel through which WP4 maintains contact with external training initiatives. The WP4 leader is the training interest group leader and joins the WP3 IG leaders TC. Joint event organisation and overlapping personnel in WP3/WP4 have made for strong relationships. *Ad hoc* teleconferences are organised to discuss specific issues.

2.4.7 WP4↔WP5 - Weaker

To date, there has been little direct feedback between WP4 and WP5. A WP4 representative has now joined the regular WP5 calls. This should improve the flow of information in the future.

2.4.8 WP4↔WP6 - Sufficient

WP4 attends the biweekly EB teleconferences. Overlapping personnel between WP6 and WP4 allow for close collaboration. *Ad hoc* teleconferences are held when necessary, predominantly on WP4 KPIs/Risks and all outreach elements including website content.

2.5 WP5: Sustainability

Figure 8 shows the current state of information flow for WP5.

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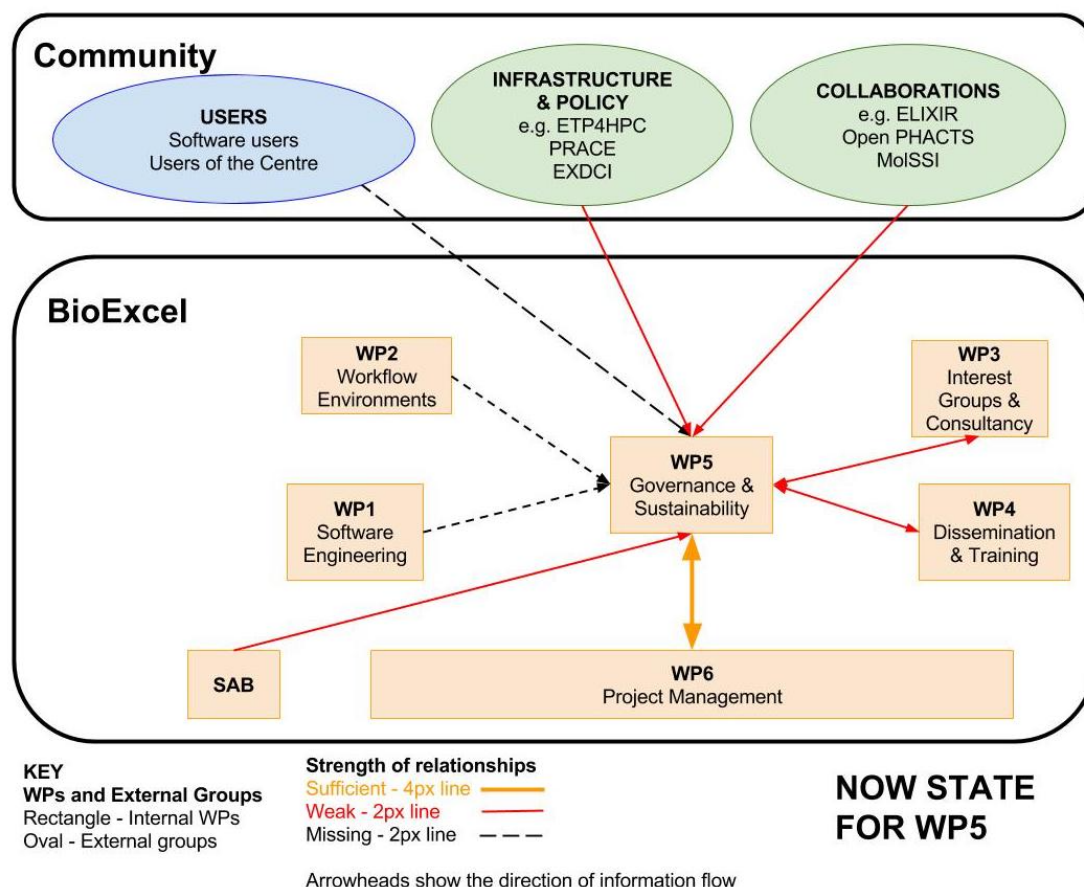


Figure 8: Feedback to Date: WP5

2.5.1 WP5↔Users - Missing

To date, there has been no direct feedback from users into the sustainability work of the centre. All user feedback and needs analysis has been obtained indirectly through user contact in the other work packages.

2.5.2 WP5↔Infrastructure & Policy - Weaker

WP5 does not possess the technical expertise that is inherent in e.g. WP1. Therefore, WP5 has relied upon judgement from other WPs to stay up to date with developments and trends in this field. Feedback from HPC infrastructure providers has been collected to a small extent, and is complemented through work in WP3 (particularly in the case of D3.3²⁹). Expected future priorities of funding bodies such as the Commission have been communicated by WP6. Policy have been investigated during D5.1 and D5.2 when taking European legislation and market studies into account for sustainability planning.

2.5.3 WP5↔Collaborations - Weaker

New MoUs are shared with all partners for comments, and are stored for reference. However, there is not always clear feedback as to if or when an MoU results in substantial collaboration, and what is then done.

²⁹ BioExcel Deliverable D3.3, *Consultancy Modalities and Funding Options, Half-time Update*, <https://doi.org/10.5281/zenodo.574613>

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WP5 organised a sustainability workshop with other organisations including WestLife³⁰ and the MaX CoE³¹ to discuss sustainability planning, including options for establishing a legal entity.

2.5.4 WP5↔WP1/WP2 - Missing

This relationship has been described already and here is the WP5 view:

Information has been received on request, although this has sometimes been brief, particularly when required at short notice. No considerable information flow between WP2 and WP5 has taken place to date. Strategic planning decisions and priorities affecting the codes in response to factors outside the project have not been transmitted very well from WP1 and WP2 to WP5, possibly since there was no explicit request for this information. At the current stage of business planning, there is not yet considered to be information that needs to be conveyed directly to WP1 and WP2, as their current work plans are defined by the existing project Description of Action. Beyond Q4 2018, more detailed dialogue between WP5 and WPs 1 and 2 will be required, particularly where technical and software development aspects for the business plan are to be considered.

Currently, WP5 gathers most information from WP1 and WP2 by reading their deliverables, and through conversations during EB meetings and project events.

2.5.5 WP5↔WP3 - Weaker

This relationship has been described already and here is the WP5 view:

Communication between both work packages is weaker than it needs to be. Information has been passed through the process of reading (and also reviewing and contributing to) deliverable documents. More recently fortnightly WP5 meetings have been established which includes a representative from WP3 attends.

2.5.6 WP5↔WP4 - Weaker

This relationship has been described already and here is the WP5 view:

Information about WP4 efforts is obtained primarily from WP4 deliverables and through direct correspondence with the WP4 leader as required. This weaker information flow also tends to be rare, but is about to be enhanced by involving a representative from WP4 in the fortnightly WP5 meetings.

2.5.7 WP5↔WP6 - Sufficient

Communication through fortnightly EB meetings and regular email correspondence is sufficient.

2.5.8 WP5↔SAB - Weaker

Direct communication has taken place, including a telephone conference with some SAB members; input was good, but not sufficiently detailed to significantly influence strategy. To make use of the SAB, WP5 would need to define clearer

³⁰ <http://west-life.eu>

³¹ <http://www.max-centre.eu>

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questions and topics that are for discussion, to which the SAB can take position. Interactions here could benefit from a more formal process.

2.6 WP6: Management

Figure 9 shows the current state of information flow for WP6.

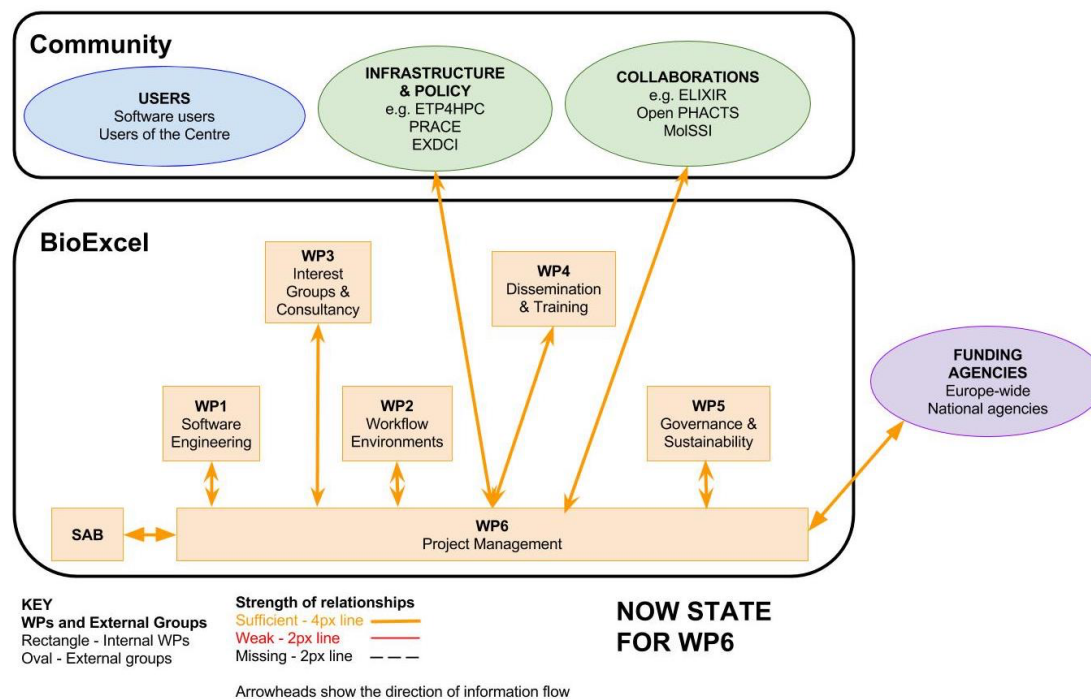


Figure 9: Feedback to Date: WP6

2.6.1 WP6↔WP1-WP5 - Sufficient

These relationships have been described already and here is the WP5 view:

Early in the project WP6 established procedures along with a selection of tools to enable efficient and sufficient communication within the consortium in general, and with the WP leaders/deputies in particular. Those were described in detail in the D6.1³². Via regular virtual meetings, WP6 is receiving feedback regarding the progress of work in the different WPs. Quarterly reports summarize the progress of each partner in the given period, while KPIs are used to monitor the progress towards the goals of each WP, as described in D6.2.

WP6 organises bi-annual meetings with all members of the consortium during which the progress of the project is presented and openly discussed. WP6 also organizes strategic meetings with core partners and the Project Management Board.

2.6.2 WP6↔SAB - Sufficient

The Scientific Advisory Board was established in the first months of the project, and its members attend our bi-annual meetings. At the end of those meetings they provide feedback regarding the progress and recommendations for future development.

³² BioExcel Deliverable D6.1, *Management Plan*. <https://doi.org/10.5281/zenodo.263933>

3 Possible Improvement Goals and Implementation

In this section, we consider areas in which we would aim to improve feedback by the end of this phase of the project.

3.1 WP1

Figure 10 shows the desired future state of information flow for WP1.

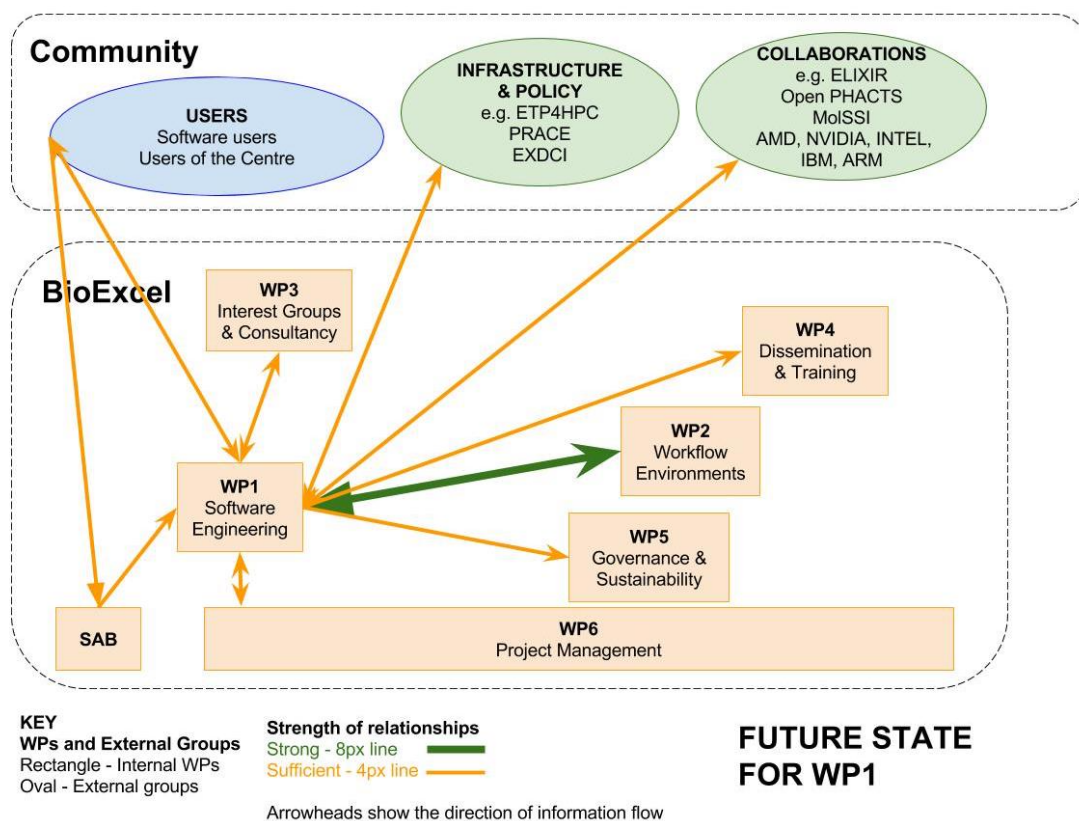


Figure 10: Future Feedback: WP1

WP1 has identified that they would like to improve feedback between WP1 and WP2, WP3, WP5 and the SAB.

When the workflows being looked at in **WP2** are run, this could identify areas in which WP1 codes could improve. Issues are likely to relate to interfaces and configuration, that is, issues related to usability more than those related to performance. To give an example of past feedback of this type, a partner's past experience with developing the Copernicus workflow engine showed that there was a need for (more) auto-tuning code in order to use *mdrun* efficiently in a workflow. Feedback in WP1 and WP2 benefits from the developers wearing hats from different roles elsewhere in the project.

Workflows from WP2 that involve the main project codes could have immediate value to the code development taking place in WP1 in that they could be used for quality assurance processes, to demonstrate that WP1 codes both continue to function as expected, and that they remain useable as part of common workflows.

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Further work could be done to better communicate the value of those workflows in WP2/3 that do not use GROMACS, HADDOCK or CPMD, although it might be that their value to the project is of less immediate interest to WP1.

From **WP3**, WP1 could potentially learn more about how their codes are being used at the moment, and how users would hope to use them in the future. This information could include which code functionality is most commonly used (so that its performance could be optimised), additional functionality that would be useful (as perceived by users and/or potential users), the areas in which users are applying their codes, the systems on which people are running their codes, and the sizes of jobs/systems that people are currently using. Feedback could also be obtained about willingness to pay for services or bespoke development related to the codes. For all the information listed above, feedback could come from questionnaires to groups identified by WP3, through consultation with IG members at events such as the upcoming Community Forum, or in response to discussion points on *AskBioExcel*. As can be seen, much of the feedback described above ultimately comes from users, but WP3's involvement would come in the support for the IGs, forum and preparation and analysis of questionnaires.

It is also possible that WP3 could broaden the available sources of feedback from existing code users to other potential users of the code. This could help to understand users' choice of code(s) and how GROMACS, for example, is perceived in comparison to other MD codes, but code developers already have an understanding of important factors affecting code choice. This depends, to a great extent, on familiarity of code with colleagues/collaborators. Availability of training opportunities and feature support dominate choice of MD software. One aspect that might benefit from further analysis is the impact of a lack of confidence in new versions, and whether there is a need more transparent testing and reporting.

WP1 would also continue to build on existing feedback to users, via WP3, through webinars and attendance at face-to-face meetings. WP1 could provide more feedback to WP3 by providing more suggestions for possible face-to-face meetings, based on their existing knowledge of their codes' users.

As the business plan for the CoE is refined in **WP5**, relevant information should be communicated directly to WP1. In particular, if there are any priorities in terms of audiences, application areas or job types that would help the centre respond to a business opportunity, then these should be passed to WP1. In response, WP1 should feedback to WP5 the viability of making changes or adding functionality in response to these opportunities. The viability of responding to this feedback will depend on several factors, including the fact that the codes are not "owned" by BioExcel, and the priorities of the codes' developers (and others funding the code's development) may sometimes differ from those of BioExcel, however BioExcel should be in a good position to influence the direction of development and to have a good understanding of the roadmap for future developments that could influence BioExcel's business plan.

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WP1 could benefit from a clearer view on the likely distribution of funding sources for the CoE in the future as sources of funding do influence the emphasis places on different aspects of code development. There are some key viewpoints that WP1 partners would want to make sure were fully taken into account in a future business model, such as the importance of general support for the code as a whole (including testability and maintainability), and not just tagging on additional functionality. This is a key benefit that having a CoE support the development of a code. It is thought that the current model for software development is unsustainable. A funding model for a code needs to be based on understanding that you cannot just keep relying on PhD students, who often still need to learn much in all of the domain science, programming and software engineering. The cost of development (in time and money) depends very much on the calibre of the person hired; hacking the code to work is easy, but building something maintainable and extensible requires that development effort also goes into avoiding technical debt. Functionality is always the desired outcome, but the code that expresses it is always a liability.

WP1 could prepare a short statement for WP5 to highlight important points, such as those described above, to ensure that these are taken into account. WP1 would benefit from a business plan that gives software developers an idea of what funders would agree to pay for, and over what time scale.

There is scope for project all-hands meetings to place a greater emphasis on cross-WP work.

3.2 WP2

Figure 11 shows areas to target for improved information flow by the end of the project.

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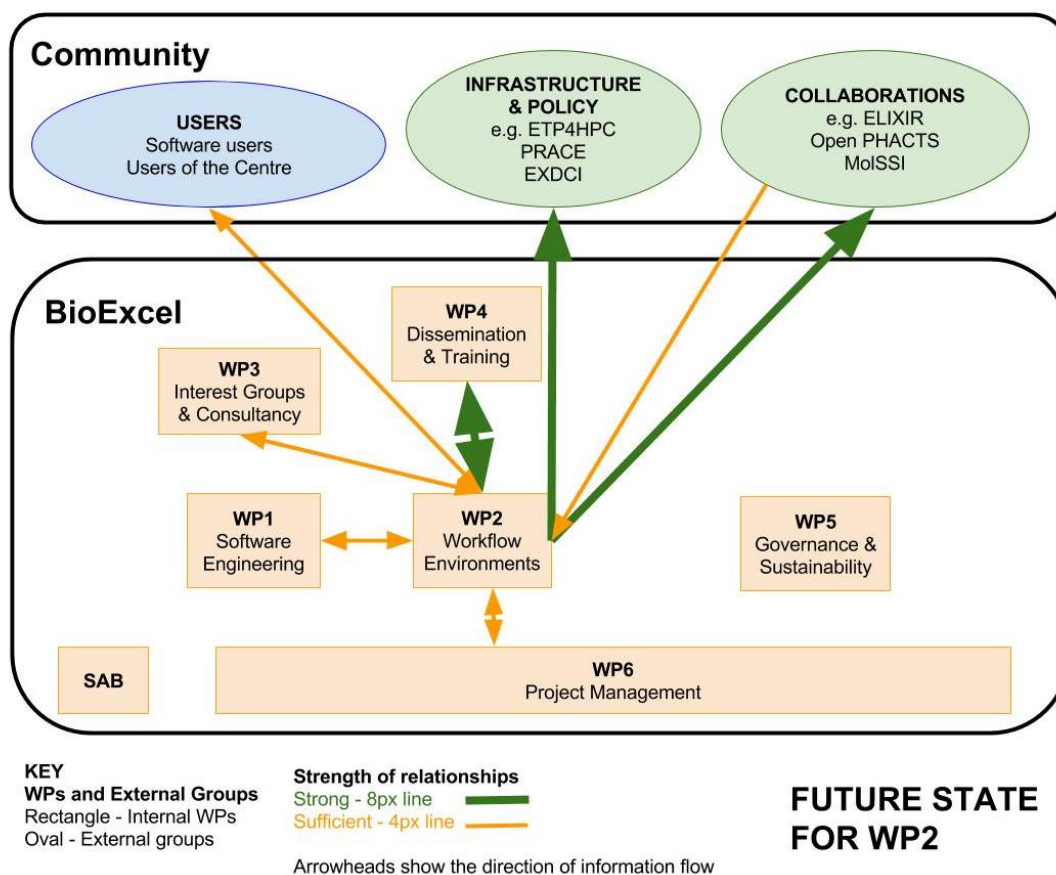


Figure 11: Future Feedback: WP2

Areas where it is considered important to have strong feedback links are with WP4, with infrastructure providers and with collaborating organisations. Links to WP1, WP3 should also be strengthened as they are currently weaker feedback channels.

Aspects of the links between **WP1** and WP2 have already been mentioned above. The main connection here is through the pilot workflows. All of the main WP1 codes are involved in at least one of the pilot workflows, and WP2 will aim to feedback in each case about issues relating to the usability of the main codes in a workflow context. Feedback from WP1 to WP2 is likely to come in the form of experience of how the codes are typically used, so that the workflow components developed in WP2 are suitably configured to maximise their usefulness.

There are various different aspects of **WP3**'s work into which WP2 could feed. In terms of Interest Groups, both the *Entry Level Users* and *Workflows* IGs are particularly relevant. It is expected that IG meetings and webinars will be used to communicate the work being done in WP2 so that the WP's outputs can be promoted as widely as possible. There is also a link in terms of the pilot workflows that are coordinated through WP3, and this is expected to strengthen once all of the associated workflows and components are accessible. WP3 will aim to help establish from the wider community what the take-up is of these workflows and components and feed this back to WP2.

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Towards the end of the first phase of the project, a number of workflows and virtual machines (VMs) are expected to be made available by WP2. These could be incorporated into training activities organised by **WP4**. Also, as these are made available, the centre will have more concrete outputs to promote, and so there will be increased communication with WP4 to ensure that that WP2’s work is disseminated through all channels. The offering should also be clearly communicated to **WP5** so that they can consider any implications for the centre’s business plan.

In terms of strengthening feedback to and from **infrastructure** providers, one of the pilot workflows is about to be evaluated on additional PRACE platforms. Although this is currently indirect collaboration with PRACE, any outcomes can be fed back to PRACE. The capability of service providers (such as EUDAT and Globus Transfer) will be assessed for their suitability to provide data movement and replication functionalities. It may also be necessary to test data services from EGI to test larger executions of the WP2 workflows. Outcomes will be fed back to the infrastructure providers.

As described above, WP2’s links with **collaborators** are already good. The strengthening of the feedback with these partners is likely to arise naturally from having longer-standing relationships.

3.3 WP3

Figure 12 shows how WP3 aims to improve information flow going forward. WP3 has identified that it wishes to establish stronger relationships with Users, WP4 and WP5. All the other relationships with WP3 need to be sufficient.

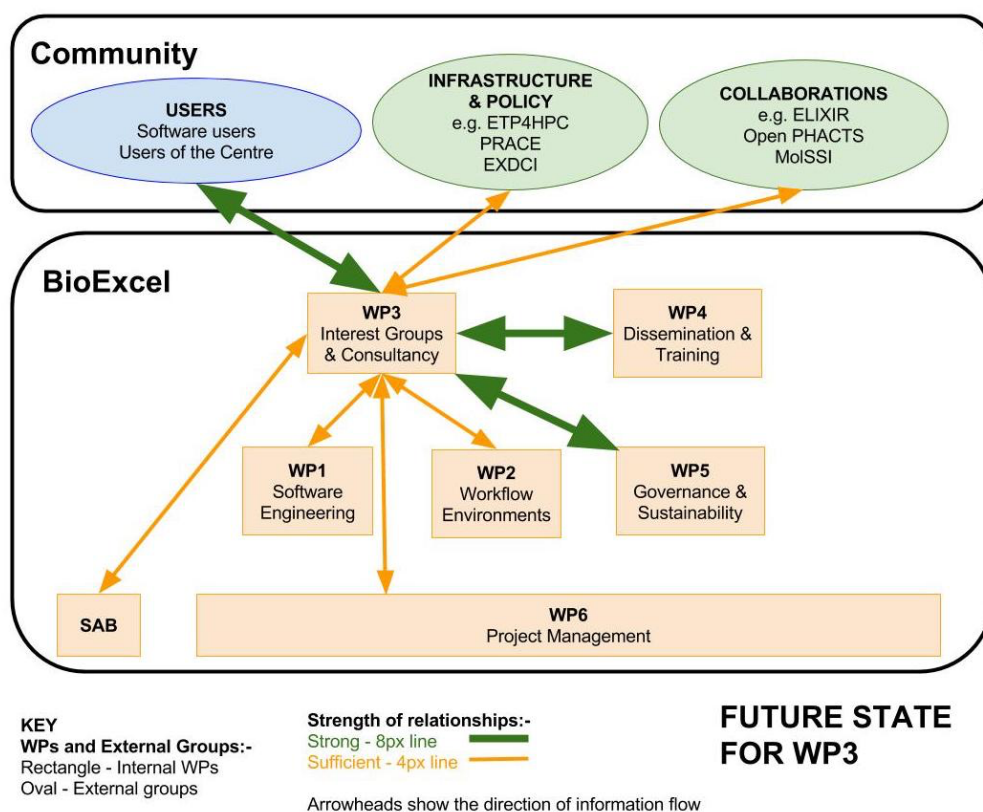


Figure 12: Future Feedback: WP3

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As discussed above, there are areas in which feedback between WP3 and the **users** is good, but in order to progress to a strong feedback relationship it would be useful to:

1. increase consistency in feedback levels in the different interest groups,
2. make more use of face-to-face meetings to gather feedback,
3. make more use of questionnaires to collect feedback,
4. aim to collect specific feedback of immediate use to other parts of the project, and
5. make better use of the data we already have stored in disparate systems in the project in order to inform project decisions.

Feedback levels in the different interest groups vary significantly. There are many reasons for this (the size of the group, the length of time that the IG has been running, the size of the wider community from which the IG members have been drawn, to name a few) and it is therefore neither likely nor necessarily desirable to have the same level of feedback from each IG. Having said that, there are activities that have been undertaken by some IGs that could be taken up by others in order to promote more feedback.

One (possibly longer-term) improvement to WP3's ability to understand the centre's users would be to register named users in a central repository. This would enable us to support registered users to understand how they use the centre, including context for feedback. At present, we have user information stored in a variety of systems and services: mailing lists and IG lists are stored in the *MailPoet* plugin to *WordPress* on which the project's web site is built, forum posts and sign-ups are stored in the *Discourse* instance underlying *AskBioExcel*, event sign-ups are stored in more than one place (including partner's platforms (e.g. for PRACE courses) collaborator's systems for joint events, and *EventBrite*), and webinar data is stored in *GoToWebinar*. Looking forward, we will want to ensure that the central repository is implemented in an appropriate storage and tracking system which is compliant with upcoming changes to data protection legislation in the form of the GDPR.

As discussed in more detail below in the next section on **WP4** (Section 3.4), we will aim to improve interaction with WP4 by collaborating more closely to understand our relationship with individual users, to implement the user personas, and to share feedback forms, etc. as appropriate.

The relationship with **WP5** will become even more important as the project progresses. This need to improve considerably from weak to strong. Feedback that could be improved here includes:

1. Coordinate and collaborate on activities through regular meetings between WP3, WP4, WP5 and WP6 to develop the sustainability plan.
2. Collaborating on a questionnaire to find out more about users' needs (work already underway). This also helps improve feedback from users to WP3.

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- WP5 could make it clearer to WP3 what information from users and the wider community would help to inform business planning (this may be addressed through point 1 above). WP3 could then collect this and feed this back to WP5.
- Once more concrete service proposals are in place, these could be evaluated by a focus group (or similar) drawn from a cross-section of users that WP3 interacts with.

3.4 WP4

The future state graph for WP4 is shown in Figure 13. It can be seen that the *weaker* feedback with infrastructure and WP1 should be increased to *sufficient*, and that with WP2 and WP5 should be increased to *strong*. Feedback channels with WP3 and users, whilst already *sufficient*, should also be brought up to *strong*.

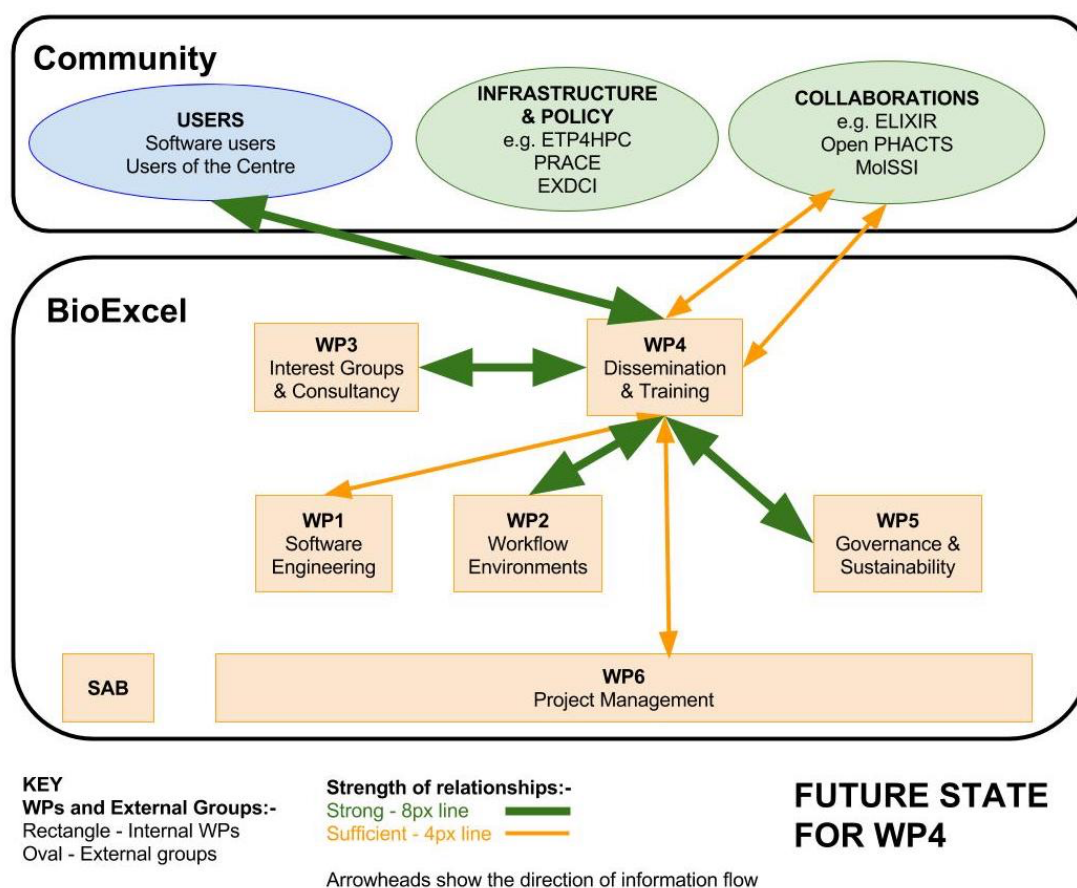


Figure 13: Future Feedback: WP4

Whilst feedback to and from users from WP4 is already considered sufficient, this channel could be further strengthened. Additional mechanisms have been identified to build on the **WP3/WP4** interaction to each other and the users; for example, joint feedback mechanisms and a combined contact database, as described above. This corresponds to a strengthening of feedback between WP3, WP4 and users to build the strong triangle shown in the graph. To date, there has been little work done to try to correlate, for example, people who have attended training courses and people who are members of, or who have subsequently

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joined Interest Groups. Analysis of this kind is planned for the next 12 months. This kind of analysis would be aided by a centralised register of users, but could be undertaken independently of this, with experience from this process possibly feeding into the design of such a register.

Through the *Training* Interest Group, WP3 is providing a link between WP4 and users, but also to infrastructure partners and project collaborations who are also involved in HPC-related training. As this IG becomes more established, this is also expected to strengthen feedback with WP3. WP4 has feedback mechanisms in place for training courses. We need to discuss with WP3 whether the WP4 templates could be amended and used for WP3 (for example, for IG-related events) or if alternative mechanisms need to be put in place. The interest group activities are ramping up at this phase of the project, if we can maintain the relationship between WP3 and WP4, and make sure this includes the IG leads, this could result in a rich information flow centered around user needs.

In terms of feedback from **users**, WP4 has some mechanisms in place (including standard feedback questionnaires for training participants); at this point the system needs time to grow. We would like to see more information flowing from the user to WP4. We will try to encourage this by spreading the word about BioExcel CoE at different community events and by getting involved in discussions in the community (partially through the *Training* IG in WP3).

An analysis is needed with WP6 to see if additional interaction between WP4 and other **infrastructure** and exascale initiatives would provide added value to the CoE. Resources are limited so it is justified to prioritise interaction with external partners where the most added value can be identified (e.g. PRACE). However, this decision needs to be based on evidence where it is currently based on where relationships have naturally grown during the first part of the project.

To increase feedback levels with **WP1** from weaker to sufficient will required increased direct communication with WP1, particularly through WP4 participants from the partners involved in WP1. We will need to carefully consider how to increase the information flow without imposing an unnecessary time burden on WP1 staff which could detract from development time.

There will be a need to incorporate the accessible workflows and VMs from **WP2** into WP4 training activities and to promote their availability through the Bioexcel outreach channels. WP4 will be able to provide user feedback to WP2. We will likely organise a series of WP4/WP2 teleconferences to streamline these activities, as was successfully done during the joint “BioExcel workflow training for computational biomolecular research” event in Barcelona, October 2016.

WP4 has now joined the regular **WP5** teleconferences. This should improve the flow of information in the future. In conjunction with WP3, WP4 can provide information about the centre’s users to WP5; this includes what use cases they are trying to solve, what their pain points or bottlenecks are, and what services they would like from the CoE.

3.5 WP5

Figure 14 illustrates what WP5 information flow should look like in the future.

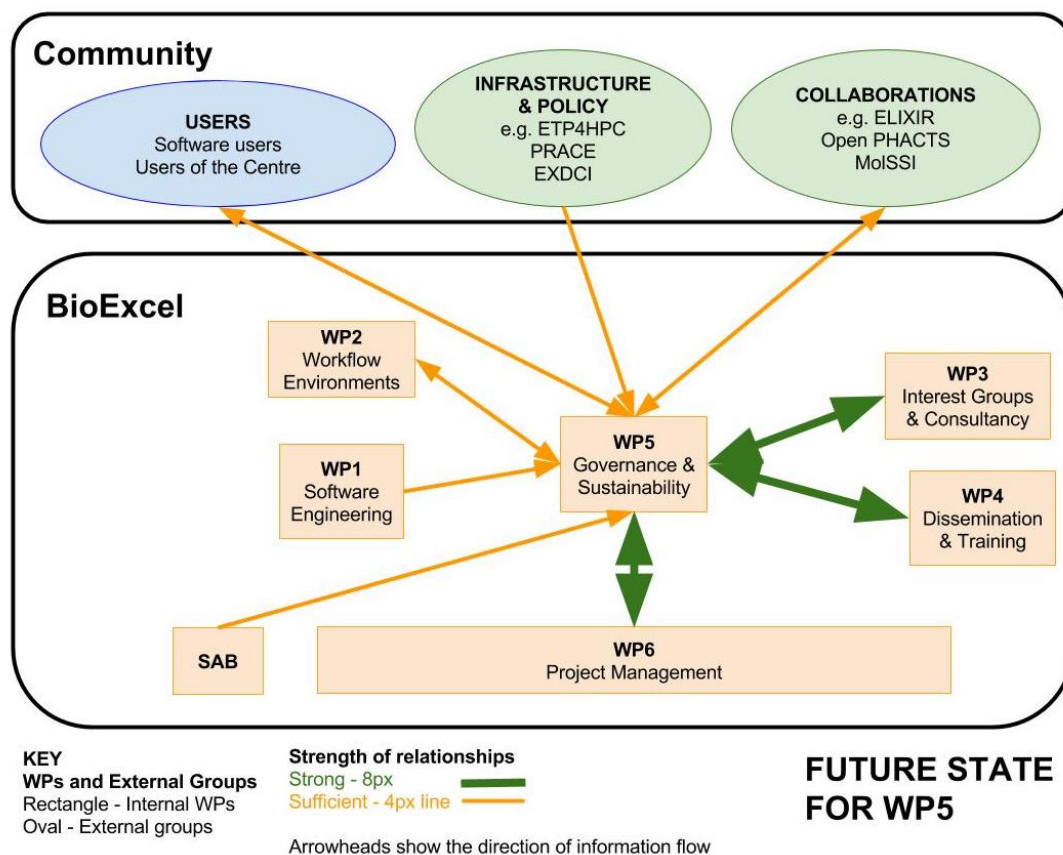


Figure 14: Future Feedback: WP5

With **users**, information could flow in both directions. Communication from WP5 to users could take the form of pitches for our service and product offerings to help promote sustainability. The actual communication would then likely flow through direct contact points in WP1, WP2 (developers) and WP3, WP4 (user training) and WP6 (main webpage). Consistency of our communication messages throughout the above-mentioned channels must be ensured however, and it would make sense that WP5 guides the development of a coherent communication strategy that is aligned to our sustainability plan. This is something that still needs to be done.

In terms of feedback from users, more use could be made of questionnaires, which not been used widely in the project to date. Most information about our existing and prospective users was more ad-hoc, and provided from partners with direct user contact, as well as from accessible market studies and other similar types of desk-based research. A process for regular collection of technology-related user feedback from WP1/WP2 and usage-related user needs from WP3/WP4 would be useful. It is fine and useful to have decentralized information gathering, but the collection, merging and reprocessing of different inputs would require a formal process to be established.

D3.4 – Efficacy of Feedback Process

In terms of **infrastructure and policy**, WP5 could potentially benefit from more feedback regarding hardware trends and technology shifts, but this could come via other work packages (see below). A possible improvement to feedback approaches in this area would be for WP5 to more actively investigate future priority areas for funding bodies, although this could be done in conjunction with WP3 (in the context of D3.5).

WP1 and **WP2** could help WP5 contributors gain a deeper understanding of the reasons and potential consequences of such technology shifts, might they be need-driven, technical or political nature, is needed for WP5.

Now that a representative from **WP4** is regularly attending WP5 calls, it is hoped that WP4 can increasingly influence the sustainability planning, particularly with respect to user training and project communications.

In terms of **collaborations**, WP5 could benefit from a monthly/quarterly status report of all ongoing actual collaborations would be useful to allow identifying e.g. matchmaking opportunities or projects of relevance for attraction of funding.

3.6 WP6

The future feedback graph for WP6 is shown in Figure 15. Comparing this with the current position (Figure 9) it can be seen that the most significant difference, namely a stronger feedback channel with funding agencies, which could become strategically important when understanding how the Centre fits into the wider HPC and Computational Biomolecular Research landscape. As the project moves towards the end of the first phase, it could be beneficial to strengthen external feedback with other infrastructures and policy makers and internal feedback with WP5 to ensure that business plans developed in WP5 align with operational plans for the project.

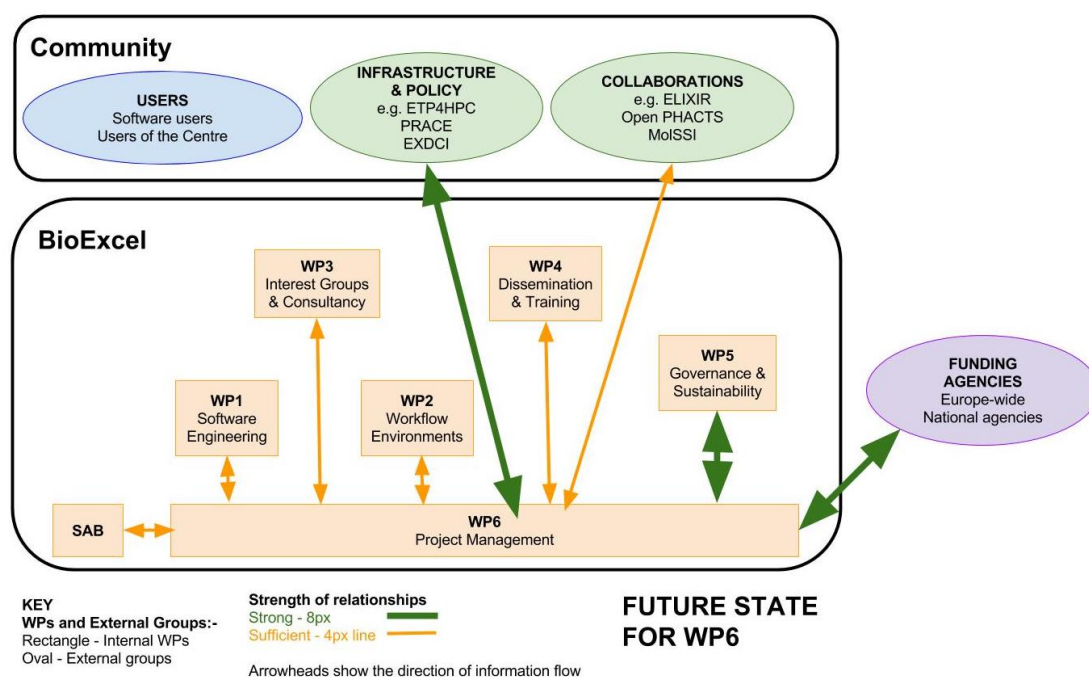


Figure 15: Future Feedback: WP6

D3.4 – Efficacy of Feedback Process

In terms of other aspects of the project, the future state shown here reflects the idea that WP6 should not act as a general channel for detailed feedback amongst WPs, and that these should communicate directly. WP6 will continue to support and chair regular EB meetings at which all WPs are represented. This provides a mechanism to escalate important issues that affect multiple WPs, but non-exceptional feedback need not be considered at management level.

Alongside the update and implementation of the business plan developed in WP5, WP6 will work towards increasing the outreach towards **funding agencies** (Europe-wide, National etc.) to highlight the benefits of the work done by the center. By provisioning such input, we would expect to increase the possibilities for attracting additional operational funding.

4 Conclusions

Feedback processes in the BioExcel project are judged to be fairly good, but there are many areas in which improvements could be made. In particular, feedback from users and potential users of the centre needs to be put to better use in the project. Until recently, much of WP3's work has been establishing interest groups, building communities in some areas, and making links with existing communities in others. Only in recent months have membership levels of IGs reached a level where feedback from these groups could be considered to be representative. Now that these communities and groups are more established, WP3 can place more emphasis on ensuring that feedback to and from users is flowing as described in the future states described in this document.

The project has taken a (possibly over-) cautious approach in avoiding bombarding new users of the centre with questionnaires and requests for feedback when, at this stage, we have less to offer in return than we will as the project proceeds. This will need to change; as the centre grows we will need to have a clearer picture about who our users are, and what they would like to get from the Centre.

Sustainability will continue to be an important piece of this three-year project, and it is important to ensure that this WP does not become isolated from more technical and user-facing aspects of the project. Recent moves to bring WP3 and WP4 representatives into regular WP5 meetings should help to improve this aspect, but the technical work packages should also ensure that they are giving and requesting suitable feedback directly to and from WP5.

As work in WP2 progresses to a stage where products are made available to end-users, feedback will become increasingly important, and as the development plans laid out in the original project plan move to completion, there will probably be a greater need for feedback to ensure that technical development is aligned with the Centre's strategy.

The general high-level structure of the project is considered good, and seems to facilitate good information sharing and feedback but care will need to be taken to ensure this continues to work as the centre grows. This may require some

D3.4 – Efficacy of Feedback Process

further formal procedures, but incremental improvements are likely to continue as the project learns from experience.

Decisions relating to which of the improvements detailed in Section 3 can be actioned will ultimately fall to WP leaders and members of the EB, but WP3 will continue to track work being undertaken to improve feedback in the context of Task 3.7, *Feedback and Improvement*.