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D3.3 – Consultancy Modalities and Funding Options, Half-time Update

WP3: Consultancy & User Groups



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Executive Summary

In the BioExcel project, we are establishing a Centre of Excellence (CoE) for Computational Biomolecular Research. We expect the centre to interact with its users in many ways, and part of our work in the “Consultancy and User Groups” work package is to inform the project about ways in which the centre could usefully work with its users and the wider biomolecular community.

This document describes work to date on the evaluation of possible consultancy *modalities* (that is, *ways* in which we can offer consultancy) and funding options for these modalities. This document focuses primarily on the former, although it also includes a basic classification of how different modalities could be funded. A second version of this document, due in project month 36, will be more conclusive, and will have a greater emphasis on funding considerations.

Core services, for the wider community are likely to be made available free at the point of use, such as services that are accessed primarily through the project’s web site. Some of these are already offered by the Centre such as discussion forums and a webinar series; others, such as a more formal helpdesk could become more important as the Centre becomes more established. These online services can act as a gateway to more in-depth consultancy.

Face-to-face meetings with users provide a means to interact with users to provide consultancy, and to listen to the community’s priorities. These include interest group workshops, larger community events and training courses.

With partnerships and collaborations, the Centre would have an agreement with the partner to work together, with both parties making some contribution. In this modality, BioExcel engages with a partner over an extended period of time. This can be through partnerships of varying degrees of formality, through to projects in which BioExcel or its partners apply for funding to work together in a larger project. BioExcel’s consultancy services could also be offered as calls to which users apply, consultations or drop-in services.

Professional services for paying customers provide a means to offer more expensive and more tailored services to companies and other organisations. The *customer* relationship differs from that for the wider community. These forms of consultancy must offer clear business value underpinned by a legal contract, and therefore often need to be more targeted towards individual customer organisations. These include tailored technical and scientific support services.

Industry partner programmes, software management collectives and pre-competitive collaborative alliances are also described.

Work in this area will continue throughout the project, and over the next 18 months we will work with WP5 and ensure that feedback from the Centre’s users and pilot projects feed back into the decision-making processes that will define the Centre’s business plan, and service offering.

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1 Introduction

In BioExcel, we are establishing a Centre of Excellence (CoE) for Computational Biomolecular Research. We expect there to be a number of different ways in which the centre will interact with its users and part of our work in the “Consultancy and User Groups” work package is to help to inform the project about ways in which the centre could usefully interact with its users and the wider biomolecular community. As discussed in D3.1¹ the communities with which we wish to work are diverse, and it is therefore likely that we will have to offer our services in different ways to different groups. D3.2, which is published alongside this document lists activities in which BioExcel’s partners are currently involved, and proposals in which the partners have been involved. Most of these activities fall under the scope of §2.4.4 below, in which the Centre’s partners apply for funding with collaborators to undertake projects, but it is expected that as the CoE grows, there will be scope for a wider range of consultancy modalities such as the ones laid out below.

One area in which the project is currently working with others is through a number of pilot use cases. These five use cases cover several different application areas and complement the work being undertaken in the project’s two technical workpackages². The use cases involve collaborators external to the project, and the activities themselves are not funded directly by BioExcel. WP3 is therefore not *managing* these use cases, but is acting as a bridge between the collaborations and the Centre itself. These use cases can be viewed as mini projects which are running for an extended period of time, throughout the initial three-year project. Through these use cases we are exploring one way that the Centre can work with the wider community in the future. As described above, however, it is expected that in the longer term, the centre will need to consider a number of different interaction models or, as we refer to these here, *consultancy modalities*.

This document describes work to date on the task of evaluating possible consultancy modalities, and funding options for these modalities. This document will focus primarily on the former, although it will also include a basic classification of how different modalities could be funded. A second version of this document, due in project month 36, will be more conclusive, and will have a greater emphasis on funding considerations. It should be noted that we are not recommending that the Centre adopt all the modalities that are listed here, but they are included here to reflect the fact that these options are all possible things that a CoE could be involved in.

Input has been gathered from multiple sources including interviews with representatives from ARCHER and the SSI³ in the UK and NBIS⁴ in Sweden.

¹ BioExcel Deliverable D3.1, *Selection and Establishment of User Groups*, <https://doi.org/10.5281/zenodo.264011>

² WP1, which focuses on three pilot applications, and WP2 which focuses on workflows and usability.

³ The Software Sustainability Institute, <https://www.software.ac.uk>

⁴ National Bioinformatics Infrastructure Sweden, <http://nbis.se/>

The material in this deliverable is complementary to two other deliverables submitted at project month 18, as follows: "D3.2 - Consultancy proposals" describes in what other proposals/project the partners are involved. We argue that there are multiple funding streams for separate activities done by the partners but in order to ensure a European leadership in the field, there is a crucial need for funding for coherent joint efforts. "D3.3 - Consultancy Modalities and Funding Options" describes what services and in what ways (i.e. modalities) they can be offered by the centre. We give examples of existing services provided by institutions at the partner countries. Finally, "D5.2 - Revised Business Plan" describes how those services will be financed and what governance structure will be able to support those offerings.

1.1 What we mean by “consultancy” and “modality”

We use the term *modality* here to describe *how* consultancy services are offered, as opposed to what the services actually offer. There are also different possible definitions of *consultancy*, from the very broad (which could encompass activities such as training) to the very narrow (which could exclude everything other than offering advice in very specific areas in which we have expertise). In this document, we consider consultancy fairly broadly to encompass all the different services through which people would seek help from the centre, either to gain knowledge, or to get the centre to undertake work on their behalf. We do not go into detail about training activities as these are considered in more detail in Work Package 4, although it will be seen from the following discussion of modalities that training activities can be considered to fall at one end of an axis in a space of possible modalities, and so we do include here an overview of possible types of training. We also exclude services which are focused primarily on the provision of infrastructure (such as compute hardware and storage) which are not the primary focus of the CoE.

1.2 Types of Consultancy Modality

We have considered different types of consultancy modality either as core or professional consultancy services according to the target audience and relevance to BioExcel resources in Table 1.

In the next two sections, we consider the two broad categories of consulting service in more detail. The second category for paying customers will be additional to those modalities in the first category for the wider community.

In Section 2 we describe core consultancy modalities for the wider community. In general, they will be free-at-the-point-of-use, they are more likely to be publicly funded, and they are more likely to appeal to academic users.

In Section 3 we describe professional consultancy modalities for paying customers. In general, they will be paid for, by the customer, at the time of use, or in advance by contractual arrangement.

In Section 4 we describe other relevant modalities like an industry partner programme, and pre-competitive, collaborative alliances.

Future plans in Section 5 conclude the deliverable.

Table 1: Types of Consultancy Service Modality

<p>Target audience: Free* to wider community</p> <p>Web site & online resources Home pages Discussion & feedback forum Helpdesk Workflow portal FAQ resource White papers & best practice guides Webinars Online Interest Group Meetings Remote training</p> <p>In-Depth Remote Consultancy</p> <p>Face to Face Meetings with users Interest Group workshops Community Conferences Training courses & schools</p> <p>Partnerships & Collaborations Strategic partnerships Collaborative partnerships Consortium Contacts Joining Projects as a Partner</p> <p>Consultations & Drop Ins</p> <p><i>* as noted below, these modalities are often offered free, but do not need to be free</i></p>	<p>Target audience: Paying customers</p> <p>Technical support Field specialist</p> <p>Scientific support Application expert</p> <p>Bespoke training Training expert and material</p> <p>Matchmaking alliances Big challenges</p>
	<p>Target audience: Institutional or Project Collaborators</p> <p>Industry Partner Programme</p> <p>Software Management Collective</p> <p>Pre-Competitive Collaborative Alliance</p>

2 Core Consultancy Services for the Wider Community

As mentioned above, the modalities described in this section are often provided free-at-the-point-of-use. It should be made clear that this *need not be the case* and access to some modalities could be limited to fee-paying members, or there could be a fee charged for the service. The division is therefore not entirely clear-cut. For example, the Task Based Support described below in §2.5.1 is similar in many respects to the Science Support Service described in §3.2; the offering could be very similar, but it could be offered for-fee, or it could be offered for free as part of a call (which may still have eligibility restrictions). A discussion of what would be the most appropriate funding model for the CoE can be found in D5.2, and a further discussion of which approach is likely to work better is reserved for D3.5 “Consultancy Modalities and Funding Options, Final Update” due in M36.

2.1 Website & Online Resources

2.1.1 BioExcel and Core Applications home pages

BioExcel's web site provides information about the Centre's services and activities. It also provides an overview of the software that the Centre is developing. A web site would not normally be considered consultancy, but it remains an important channel through which we can provide useful material to the community, and the gateway to any services which BioExcel offers.

2.1.2 Online Discussion / Feedback Forum

A simple but potentially effective mechanism to offer basic consultancy is provided by an online discussion forum that allows people to have conversations with each other and experts from the Centre. BioExcel has already launched such a platform at *ask.bioexcel.eu*. Members of the centre subscribe to particular forums and contribute to discussions. The forum also helps the Centre to understand the needs and priorities of those members of the community who post on the forums. These forums have the advantage that as well as providing users a means of communicating directly with the Centre, the discussions are visible online meaning they become a useful reference resource for others in the future.

2.1.3 General Helpdesk

A helpdesk service allows people to ask quick questions to the centre. A basic form of this type of offering is provided by the current *ask.bioexcel* forums, but this type of service could offer:

- (i) more than one contact mechanism, e.g. phone, email, web page, and
- (ii) an expected response time for every query/ticket
- (iii) an expectation of confidentiality compared to an open forum

This type of helpdesk could answer questions that do not require any in-depth analysis of a problem. Queries that would take longer to answer could be referred to an in-depth support channel. A more detailed description of how this modality can be offered is included in Appendix 1.

Examples

ARCHER operates a helpdesk as part of its offering to users. Two parts of this helpdesk service are actually offered under two different contracts between the ARCHER service providers and the research councils which fund the service. The front-line (helpdesk management and the operators who monitor the helpdesk) is paid for as part of the Service Provision contract (which also covers, for example, system administration). The people who respond to the queries are funded under the Computational Science and Engineering support contract which also funds other support activities, such as contacts for key scientific consortia, technical assessments for applications to the use the service, etc. Helpdesks are common for large-scale HPC systems.

2.1.4 Workflow portal

Complementing consultancy offerings that are based on giving advice, a workflow portal can offer concrete realisations of processes of use to the wider community that can be downloaded and executed directly by the end-user. This increases the

usability of software. As described in BioExcel Deliverable D2.2⁵, BioExcel plans to offer a workflow portal. This portal will provide access to workflow components and will therefore provide another channel to share more widely outputs such as software components and pipelines from other collaborations in the project.

2.1.5 Online FAQ resource

A FAQ (Frequently Asked Questions) section online can be a good way to collect common questions and answers so as to reduce the need for individual support. It does require some effort to establish, but it is likely to grow in usefulness over time. It would typically be populated based on input from other sources, such as questions asked of the helpdesk, questions asked at webinars, etc. In the case where the questions relate to constantly changing software and methods, it could be that additional effort would be required to clean up the FAQ to keep it up-to-date. Both GROMACS and HADDOCK have existing FAQ pages online, but there would probably be value in having either a central resource, or a page to cover questions not related to a specific code.

2.1.6 White Papers and Best Practice Guides

As a step up from an FAQ, white papers and best practice guides can be created for users based on common user questions, or community input (perhaps at the request of, or created in conjunction with Interest Groups). The white papers can take some time to research or investigate so can require some effort to create, but they are typically useful to a wide number of users after they have been created.

Example

This is one way in which the PRACE Application Enabling team supports users of PRACE resources (see also §2.5.1).

2.1.7 Webinar series

Webinars provide another way to engage with the wider community. The presenters can be either Centre staff, or experts invited from the wider community. Since webinars are live and interactive, they allow viewers of the webinar to ask questions to the presenter, so while most of the session is one-way communication of information, the Q&A sessions allows people to ask questions directly to experts, both from the centre and elsewhere.

BioExcel has been running a successful webinar series⁶, with 13 webinars delivered to date, and several others in the pipeline. The webinars are also posted online afterwards on YouTube (and *bioexcel.eu*), allowing the material to be accessed at a later date, with links back to the *ask.bioexcel* forum, so that viewers who cannot ask questions live can pose questions at a later date.

There are a number of tasks related to running webinars, and there is a small cost associated with the GoToWebinar account that we use, but the webinars offer a good way to reach out to the wider community. We have also linked these

⁵ *BioExcel Deliverable 2.2 – First Release of Workflow Blocks and Portals*, <https://doi.org/10.5281/zenodo.263965>

⁶ www.bioexcel.eu/webinars

webinars to our Interest Groups to help attract new members, and to share information of interest to the groups.

2.1.8 Online Interest Group Meetings

Online Interest Group meetings allow (usually) small groups of people to meet online to discuss matters of common interest. Unlike webinars which usually have one main speaker, online meetings can be chaired by a BioExcel member, but they take the form of a discussion.

BioExcel is using this type of meeting with the Industry Interest Group.

2.1.9 Remote training

BioExcel has an entire Work Package dedicated to training, so we do not cover this subject in detail. We include Training here to show how it could fit in with other consultancy offerings. As a consultancy modality, online training provides an alternative means for users to engage with BioExcel's training activities without attending courses in person. Remote training might take the form of videos or tutorials which can be accessed at any time convenient for the user or they can be live interactive training sessions delivered using videoconferencing or webinar technology. Most free training will be set courses that people can sign up to attend (in person, or online). Bespoke training is covered in Section 3. Further details of BioExcel's training plans are given in D4.5⁷.

2.2 In-Depth Remote Support / Consultancy

This kind of support is related to the helpdesk support described in §2.1.3 and access to this kind of support or consultancy would normally be provided as an escalation of a query to a standard helpdesk. In this case, the user would be put in touch with an expert and would work with the expert on a problem for a more extended period (weeks/months) to work on some specific issue. This could be to resolve an immediate problem, but this also encompasses longer-term application enabling work. It is similar in nature to modalities offered as professional services (see, e.g. §3.1 and §3.2) but access to the consultancy will typically be through different means and is likely to be free at the point of use, although it could be limited to a subset of qualifying users.

Example

This kind of support is offered by the PRACE High Level Support Teams that “provide users with support for code enabling and scaling out of scientific applications / methods, as well as for R&D on code refactoring on the Tier-0 systems”⁸. Access to this kind of support is usually through the helpdesk for the Tier-0 machine and whilst it is normally open to all users, these will typically already have been through a competitive peer-review process to gain access to the service.

⁷ BioExcel Deliverable 4.5, *Training report and updated plan* will be published alongside this deliverable and will be available from zenodo.org.

⁸ *PRACE 2: growth in capacity for growth in excellence* <http://www.prace-ri.eu/prace2-council-ratification/> (Accessed 2017-04-26).

2.3 Face-to-Face Meetings with Users

Face-to-face meetings with users, arranged by the project, provide a means to interact with users to provide consultancy, and also to listen to the needs and priorities of the different communities,

2.3.1 Interest Group workshops

Face-to-face Interest Group workshops can take place either as stand-alone events organised by BioExcel, or in conjunction with other community meetings. They allow for longer periods of discussion than could be offered by online meetings, and tend to be better places for establishing business relationships as well as simply opportunities to communicate information.

BioExcel has already run two face-to-face meetings, one as part of a workshop on Workflows and another as part of a community meeting on Hybrid Methods⁹.

2.3.2 Community forum Conference

As a step up from small, single-IG meetings, larger events can bring together members of different interest groups to share experience and discuss the bigger picture.

BioExcel is planning such a community forum event for November in Amsterdam, which will be open for registration in early May.

2.3.3 Training courses/schools

Face-to-face training events that could last anything from a few hours (possibly as part of a wider event) up to a week (such as a summer school). BioExcel and the project's partners have already delivered both kinds of course. More details are given in D4.5¹².

2.4 Partnerships & Collaborations

These types of “consultancy” are more symmetric, in that the Centre would have an agreement with the partner to work together in some way, with both parties making some contribution. In this modality, BioExcel engages with a partner over an extended period of time.

2.4.1 Strategic Partnership with numerous relevant third parties

In this case the Centre makes a public agreement with a third party to work towards a common set of goals in a particular area. In some cases, these partnerships could be made more formal, but in most cases, there is no contract, only a statement of intent to collaborate. BioExcel has already established such partnerships with ELIXIR¹⁰ and the Open PHACTS Foundation¹¹ and a partnership with MolSSI is being finalised at the time of writing. Descriptions of these partnerships are included in Appendix 1.

⁹ *First Workshop on Hybrid Methods in Molecular Simulation*, Cagliari, April 2017, http://www.fz-juelich.de/ias/ias-5/EN/Conferences/Hybrid_Methods/Home.html

¹⁰ *BioExcel announces ELIXIR Partnership*, <http://bioexcel.eu/bioexcel-announces-elixir-partnership>

¹¹ *Partnership between BioExcel and Open PHACTS Foundation*, <http://bioexcel.eu/partnership-between-bioexcel-and-open-phacts-foundation>

2.4.2 Collaborative with a few highly relevant third parties

Similar to the strategic partnership above, but in this case, there would be a more specific agreement to work on specific tasks together.

2.4.3 Consortium Contacts

In this model, users of the centre could group together into consortia (either through self-organisation, or with definition of and membership of the consortia controlled by the funding body. Recognised consortia would then be appointed a consortium contact who can provide support and consultancy, free at the point of use for the end-user.

Example

This is another modality used by ARCHER. In the case of ARCHER, there are 10 consortia¹² and each consortium is allocated a contact in the centre (who is funded at 0.1 FTE) to offer support and consultancy. The contact has knowledge of the system, but also has some familiarity with the subject area of the consortium. In the case of ARCHER, the consortia have a wider role than shared access to a consortium contact; they also pool CPU resources on the machine itself and must demonstrate their scientific output to the research councils to continue to receive funding.

2.4.4 Joining Projects as a Partner

The centre (if it ultimately becomes a legal entity) or its partners (if not) could join other projects (funded through other calls) in order to provide certain expertise and support. With a CoE providing continuity and possibly with some core funding to support the application process, it could be possible to involve even a fairly small fraction of an FTE on a project to offer consultancy (or as a main partner to contribute to the main project work).

Example

This is another example of a modality that is used by the SSI. In this case the SSI has a policy that for these kinds of projects it aims to support in the early stage of a project, or during an initial funding round with a view to leaving the other project partners with sufficient expertise to move forward without the SSI's involvement in the longer term.

2.5 Calls for Access to Expertise

The modalities described in this section are similar to some of the professional consultancy services described in Section 3. The different here is that these calls would provide access to experts from the CoE which would be free to the end-user. It is likely that such calls would offer access to services defined or prioritised by the funders but delivered by members of the CoE.

2.5.1 Task-Based Support

In this modality, we consider the possibility that through a call, the Centre could offer a specific service, such as performance tuning. In this case a user could apply to a call with a request for help in performing a certain task, such as tuning the

¹² <http://www.archer.ac.uk/community/consortia/>

performance of a code on a given machine. The Centre would look at the responses, and select those where it could have most impact (for instance, where the code will be used by many people, or by a new community, or in some particularly high-profile research) and then a member of the Centre could, at a mutually convenient time, work with applicant to undertake the task.

Examples

The Software Sustainability Institute in the UK (SSI) have widely-advertised, competitive calls for consultancy on a set topic, namely “code development and release”. These calls provide access to staff effort (normally, although not exclusively, SSI staff). In a conversation with the SSI’s director, it was stated that from their experience, they found that providing access to staff effort was more effective than offering money.

This kind of support/consultancy is sometimes offered as part of a package. For example, as part of the Preparatory Access (“Type C”) mechanism¹³ for getting access to PRACE resources, it is possible to request up to 6 person-months of effort for application development and optimisation work which is provided by the PRACE Application Enabling team.

2.5.2 Embedded Support

This modality offers effort to support specific activities, such as software development. Applicants would request some fraction of the time of one of the Centre’s software developers. The centre administers this programme and coordinates the application process; applications would likely be independently reviewed against guidelines agreed between the centre and funders.

Example

ARCHER offers a service like this which is very popular with ARCHER users. In ARCHER’s case, this accounts for about 14FTEs of effort. In the case of ARCHER, most of the effort is allocated to members of the ARCHER team to work with external groups, but applicants can also apply for funding to employ experts directly at the applicant’s institution.

2.6 Consultations & Drop-Ins

2.6.1 Consultations

In this modality, the user would apply online and would be granted a meeting to speak with an expert from the centre. These would normally be fixed in length, but could also act as a gateway to more in-depth consultancy. In the context of a distributed Centre of Excellence, it could be that such a consultation is offered online. If all applications for consultation are accepted, the effort required here is limited mainly to the length of the consultation. If these were popular, availability would be constrained by the availability of experts.

Example

NBIS offers 1 hour consultations. These are free to users.

¹³ PRACE Preparatory Access, <http://www.prace-ri.eu/prace-preparatory-access/>

2.6.2 Drop-Ins / Surgeries

These are similar to consultations, the difference being that these take place at fixed times in a fixed location (or possibly online). Here an expert makes themselves available in an open place to answers questions from users. These could either be private (in which case, users would have to queue and be seen on a first-come-first-served basis) or they would be open, which whilst possibly less attractive to some users, it would mean that other attendees can learn from the session, and the expert can address common questions more efficiently.

Example

NBIS offers these sessions at 6 Swedish universities, and this is a sought-after service.

3 Professional Consultancy Services for Paying Customers

In this section, we describe a number of modalities that are exclusive to paying customers. The *customer* relationship differs from that for the wider community as described in the previous section. The forms of consultancy described in this section must offer clear business value underpinned by a legal contract, and therefore often need to be more targeted towards individual customer organisations. We are not going to detail the possible variations in funding structure for how customers, or more likely, their organisations will be charged. Suffice to say that this is likely to be through pre-payment of consulting time (days or hours) or by delivery milestone to trigger payment.

3.1 Technical support service

The scope of this service is likely to cover technical installation, tuning, maintenance and troubleshooting for BioExcel application and workflows. This service could be a planned site visit or an appropriate response to a trouble shooting call routed through a support helpdesk. This level of technical support service will be in addition to the remote mechanisms of support available to the wider community.

Example

Technical support services are commonly found among commercial instrument or analytical platform vendors, for example, GE Instruments¹⁴ and Cardio Analytics¹⁵.

3.2 Scientific support service

This service will provide scientific support for the core software and workflows which are being used in a customer setting for a particular business process such as virtual screening or antibody engineering. The scope is likely to encompass design, development and production phases for an agreed project of sufficient business value. It is like to involve bespoke solutions for particular projects. An

¹⁴ <http://www.geinstruments.com/support/technical-support>

¹⁵ <http://www.cardioanalytics.com/support/technical>

application expert is likely to deliver this service through site visits and remotely using collaborative communication tools.

Examples

Scientific support services are offered by knowledge management and text analytics vendors, for example Promocell¹⁶ and Linguamatics¹⁷.

A more academic-focused (but still for-fee) example here would be the short and medium user-support offered by NBIS. This takes the form of short projects focused on a well-defined bioinformatics problem. Project applications are reviewed every second week; projects are selected based on available expertise and feasibility. Time and outcome estimations are done individually for each project before contracting. Charging a fee helps to define projects, and this works well. (Previously projects often were open-ended, whereas a fee helps to maintain focus and verify user interest). The only disadvantage is the administrative burden of charging fees.

3.3 Training support service

This service will deliver bespoke training to users and administrators in customer organisations. This could be delivered by a training expert to small groups during on-site visits. It would complement the on-line training materials available to the wider community. Application workshops could be organised for customers to foster sharing across the user community within and between companies in a precompetitive manner.

Example

Training support services are provided by numerous IT training vendors. One of many examples is Learning Tree¹⁸ which offers access to multiple courses and to bespoke training.

3.4 Matchmaking consortia

This service modality would seek big challenges in high performance computing infrastructure and biomolecular research. BioExcel would be a partner along with other organisations in academia and industry who would bring relevant resources to create a consortium which can attract public or public-private funding.

Example

An example of matchmaking consortia is the Innovative Medicines Initiative (IMI)¹⁹ which is Europe's largest public-private initiative aiming to speed up the development of better and safer medicines for patients. IMI supports collaborative research projects and builds networks of industrial and academic experts in order to boost pharmaceutical innovation in Europe. IMI is a joint undertaking between the European Union and the pharmaceutical industry association EFPIA.

¹⁶ <http://www.promocell.com/scientific-support>

¹⁷ <https://www.linguamatics.com/products-services/professional-services>

¹⁸ <https://www.learningtree.co.uk>

¹⁹ <https://www.imi.europa.eu>

4 Other relevant modalities

4.1 An Industry Partner Programme

This kind of modality establishes a longer-term relationship with a number of partners in industry as a pre-competitive group and who also contribute financially with an annual fee to the running of the programme. The programme acts as an umbrella for a number of different activities, including expert scientific advice and enhanced access to resource (tools and data) services and infrastructure.

Example

A good example of this kind of this is given by the EMBL-EBI Industry Partners Programme²⁰. This programme includes quarterly meetings with partners (22 members) and regular training workshops. The priorities for the programme are set by the members, and membership provides privileged access to scientists at EMBL-EBI and the Sanger Institute and opportunities to engage with the ELIXIR infrastructure hub. It supports small-scale collaborations with industry members and provides access and support for EMBL-EBI's databases and services. EMBL-EBI's programme has been running successfully for around two decades.

4.2 A software management collective

This modality is collective of relative small software projects which are managed by a host not-for profit organisation.

Example

The Sustainable Software Institute (SSI) obtains most its funding from research funders. SSI then takes on the administrative burden of funding smaller projects which positions it to undertake a number of related initiatives. This is a modality that a CoE could adopt, and it could collect its funding, for example, from multiple funding streams, which could include the Commission but could also include, for example, national funding bodies.

One thing that SSI tries to do is to evaluate modalities and ideas for activities that will support its target communities. In the longer term, for those that are successful, it aims to *hand these back* to the communities, having demonstrated their value. This allows SSI to have growing impact in the community without needing to constantly grow in terms of the number of people that it employs.

4.3 A pre-competitive, collaborative alliance

This is usually a not-for-profit organisation which supports member companies to collaborate on pre-competitive projects using a legally safe vehicle. This is particularly important for those sectors where there is significant risk of collusion to manipulate market prices e.g. pharmaceutical companies.

²⁰ <http://www.ebi.ac.uk/industry>

Example

The Pistoia Alliance Inc²¹. is an example of this modality. It is a global, not-for-profit alliance of life science companies, vendors, publishers, and academic groups that work together to lower barriers to innovation in R&D. It hires professionals to manage projects which transform R&D innovation through pre-competitive collaboration. It brings together the key constituents to identify the root causes that lead to R&D inefficiencies. It develops best practices and technology pilots to overcome common obstacles. Our members collaborate as equals on open projects that generate significant value for the worldwide life sciences community.

5 Future Plans

Work on Task 3.5 continues until the end of the project. In the next 18 months, we will explore the modalities described above in more depth, look for further examples of where they are used successfully and explore possible funding options. We will feed this information to WP5 to ensure that these consultancy modalities are considered as part of the Centre's business plan and future service offering and we will be responsive to the needs of WP5 in terms of evaluating these options through discussions with the user communities.

5.1 Next steps

- Members of Interest Groups, particularly the Industry Interest Group will be invited to comment on the modalities, in particular with reference to those modalities that they would find most useful.
- We will consider opening an online questionnaire asking people their views on which modalities are of most interest in the context of the CoE.
- In conjunction with WP5, we will create a prioritised short list from this of modalities and undertake a more in-depth analysis of the likely costs of running such a service and seek to identify appropriate funding sources.

²¹ <http://www.pistoiaalliance.org/>

6 Appendix 1: Partnership Agreements

6.1 Agreement with ELIXIR



Framework for collaboration Between BioExcel Center of Excellence and ELIXIR

Background information

BioExcel CoE provides the necessary solutions for long-term support of the biomolecular research communities in academia and industry: fast and scalable software, user-friendly automation workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code, personalized consultancy support and community outreach activities.

ELIXIR unites Europe's leading life science organisations in managing and safeguarding the increasing volume of data being generated by publicly funded research. It coordinates, integrates and sustains bioinformatics resources across its member states and enables users in academia and industry to access services that are vital for their research

Purpose

The purpose of this document is to define a framework for collaboration between **BioExcel CoE** and **ELIXIR**. This document outlines the main activities through which the two parties will be collaborating along with timelines, where applicable.

Joint Workplan



Below are outlined the main planned activities and timelines, where applicable. The workplan is included in the Project Plan for the 2017 [Tool and Workflow Discovery & Interoperability](#) (ELIXIR Interoperability Platform), and included curation activities related to the improvement of bio.tools registry and EDAM annotations of biomolecular simulation tools (ELIXIR Tools Platform).

Milestone	Activity	Date
M1	Define list of tools to be included in the roadmap	Apr 2017
M2	Registration and complete annotation of BioExcel tools in bio.tools/EDAM	Jun 2017
M3	Adoption of API specification for BioExcel libraries	Oct 2017
M4	Adoption of WF specification for BioExcel workflows	Oct 2017
M5	Joint co-webinars - one each for the BioExcel and ELIXIR's series (after M3 and M4)	Nov 2017
M6	CWL specification of selected BioExcel WFs	Dec 2017
M7	Benchmark of BioExcel WFs under CWL Control	Feb 2018

Rights and Responsibilities

This document does not prevent either party from cooperating with other projects performing similar activities to those described herein. When considered of mutual benefit, both parties are encouraged to involve third parties in similar activities towards achieving the objectives of this collaboration framework.

6.2 Agreement with Open PHACTS

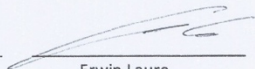



Memorandum of Understanding
Strategic Partnership Agreement

between BioExcel Center of Excellence and OpenPHACTS Foundation

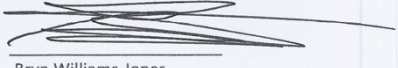
1. This Memorandum of Understanding (MoU) signifies a statement of intent to collaborate between the BioExcel Center of Excellence (hereafter "BioExcel CoE") and << Organisation >>, but is **not a legally binding document**. This MoU does not restrict the rights of either party to enter into collaborative agreements, contracts or working relationships with other parties.
2. This MoU recognizes the intention of BioExcel CoE and << Organisation >> to establish a relationship to co-operate in a range of areas in the scope of BioExcel and to work together for their mutual benefit.
3. The period covered by this MoU is from the date of signing to 31 October 2018 and will be reviewed thereafter. Each party has the right to discontinue the arrangements subject to a period of 3 months' notice being given. The MoU may also be terminated at any time by mutual consent of both parties. In any cases of discontinuance, the parties will honour agreed commitments either via accepted arrangements or suitable alternatives negotiated at that point.
4. **Separate agreements will be required for any and all collaborative projects that the parties wish to enter into. The parties understand that any financial considerations associated with any form of collaborative project will be dealt with separately via a legal contract. As part of this, the parties agree to cooperate on resolution of contractual and IPR issues.**
5. The parties recognize the importance and value of this MoU in promoting their individual and joint activities. However, each party understands that any activity which includes reference to the other party (such as grant applications) must be sent to and be approved by this party before use. Each party will use reasonable efforts to provide a response within 7 working days.
6. The parties agree to cooperate in establishing the BioExcel CoE, including, but not limited to i) joint projects involving scientists on both sides, ii) sharing of expertise and/or biomolecular software, iii) exchange of students and or teaching material and iv) exchange of expertise, materials, documents or information at the organizational level.
7. The parties agree to encourage collaborative research in the areas of biomolecular research within their respective programmes and with mutual collaborators.
8. The parties agree to encourage the development, publishing and sharing of services that can be used in their mutual support activities, with a view to enabling public access to more of these resources, including within the BioExcel activities.
9. The parties agree, wherever appropriate, to pursue possibilities for bilateral and multilateral collaborations aiming at the development of an interoperable pan-European and global infrastructure for biomolecular research.

2017-01-31
Date



Erwin Laure
on behalf of BioExcel CoE

12/2/17
Date



Bryn Williams-Jones
on behalf of OpenPHACTS Foundation

6.3 (Draft) Agreement with MolSSI



Letter of Intent to Collaborate

between the Molecular Science Software Institute (MolSSI) and
BioExcel Center of Excellence

1. This Letter of Intent (LOI) signifies a statement of collaboration between the BioExcel Center of Excellence (hereafter "BioExcel CoE") and the MolSSI, but is not considered to be a legally binding document. This Letter does not restrict the rights of either party to enter into collaborative or joint agreements, contracts or working relationships with other parties.
2. This LOI recognizes the intention of BioExcel CoE and MolSSI to establish a relationship to cooperate in a range of areas in the scope of computational biomolecular modelling and to work together for their mutual benefit.
3. Separate agreements will be required for any and all joint projects that the parties wish to enter into. The parties understand that any financial considerations associated with any form of joint project will be dealt with separately via a legal contract. As part of this, the parties agree to cooperate on resolution of contractual and IPR (Intellectual Property Rights) issues.
4. The parties recognize the importance and value of this LOI in promoting their individual and joint activities. However, each party understands that any activity that includes reference to the other party (such as grant applications) must be sent to and be approved by that party before use. Each party will use reasonable efforts to provide a prompt response.
5. The parties agree to cooperate in developing the area of computational biomolecular modelling, perhaps including, but not limited to i) joint projects involving scientists on both sides, ii) sharing of expertise and/or biomolecular software, iii) exchange of students and or teaching material, iv) exchange of expertise, materials, documents or information at the organizational level and v) organizing joint training events and promotion of other ongoing activities. The specific activities chosen will depend on the available resources for each party.
6. The parties agree to encourage collaborative research in the areas of biomolecular research within their respective programmes and with mutual collaborators.
7. The parties agree to encourage the development, publishing and sharing of services that can be used in their mutual support activities, with a view to enabling public access to more of these resources.
8. The parties agree, wherever appropriate, to pursue possibilities for bilateral and multilateral collaborations aiming at the development of an interoperable pan-European and global infrastructure for biomolecular research.

Date

Erwin Laure
on behalf of BioExcel CoE

Date

T. Daniel Crawford
on behalf of MolSSI