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Revision 1

WP6: Management



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Executive Summary

This document describes BioExcel's management organization and planning for the entire project. The current version is a revision based on the reviewers' comments.

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1 Introduction

This document should be read in conjunction with the BioExcel Grant Agreement, including the Description of Action and the Consortium Agreement. It contains information about partner contacts, email lists, project website, collaboration tools and reporting. Further procedures regarding the quality assurance processes, including documents rules, deliverables and approval procedures, and publications, and presentations will be defined in the upcoming deliverable D6.2 - *Quality Assurance and Risk Management Plan*

2 Partner List

The BioExcel Consortium includes 11 partners from 5 EU countries as listed in Table 1.

Beneficiary number	Beneficiary name	Beneficiary short name	Country
1	Kungliga Tekniska Högskolan	KTH	SE
2	Universiteit Utrecht	UU	NL
3	Fundacio Insitut de Recerca Biomedica (IRB Barcelona)	IRB	ES
4	Forschungszentrum Julich	JUELICH	DE
5	The University of Edinburgh	UEDIN	UK
6	The University of Manchester	UMAN	UK
7	European Molecular Biology Laboratory	EMBL	DE
8	Max Planck Gesellschaft zur Förderung der Wissenschaften e.V.	MPG	DE
9	Forward Technologies AB	FT	SE
10	BSC Barcelona – Centro Nacional de Supercomputacion	BSC	ES
11	Ian Harrow Consulting	IHC	UK

Table 1. Partner List

3 Contacts and Email lists

Contacts of the administrative personnel, partner representatives and workpackage leaders are presented in the following tables.

3.1 Contacts for Administrative, Legal and Financial Aspects

Partner	Name	Email
KTH	Anette Arling	an1@kth.se
UU	M. Vincent	M.Vincent@uu.nl
IRB	Raquel Furio	raquel.furio@irbbarcelona.org
JUELICH	J. Stier	j.stier@fz-juelich.de
UEDIN	A. McDonald, Mark Parsons	a.mcdonald@epcc.ed.ac.uk , m.parsons@epcc.ed.ac.uk
UMAN	Helen Taylor	helen.taylor@manchester.ac.uk
EMBL	Mark Green	grants@ebi.ac.uk
MPG	Manfred Messerschmidt	eu-finance@rzg.mpg.de , eu-goe@gwdg.de
FT	Holger Noack	holger@forwardtech.se
BSC	Ezequiel Masdelmolino	ezequiel.masdelmolino@bsc.es
IHC	Ian Harrow	ianharrowconsulting@gmail.com

3.2 Contacts for Partner Representatives

Partner	Name	Email
KTH	Erwin Laure	erwinl@pdc.kth.se
UU	Alexandre Bonvin	a.m.j.bonvin@uu.nl
IRB	Modesto Orozco	modesto.orozco@irbbarcelona.org
JUELICH	Paolo Carloni	p.carloni@fz-juelich.de
UEDIN	Mark Parsons	m.parsons@epcc.ed.ac.uk
UMAN	Carole Goble	carole.goble@manchester.ac.uk
EMBL	Steven Newhouse	steven.newhouse@ebi.ac.uk
MPG	Bert de Groot	bgroot@gwdg.de
FT	Holger Noack	holger@forwardtech.se
BSC	Losep Lluís Gelpi	josep.gelpi@bsc.es
IHC	Ian Harrow	ianharrowconsulting@gmail.com

3.3 Contacts for Work Package Leaders

Partner	Name	Email
WP1 leader	Mark Abraham (KTH)	mark.j.abraham@gmail.com
WP1 deputy	Adrien Melquiond (UU)	a.melquiond@gmail.com
WP2 leader	Adam Hospital (IRB)	adam.hospital@irbbarcelona.org
WP2 deputy	Stian Soiland-Reyes (UMAN)	soiland-reyes@cs.manchester.ac.uk
WP3 leader	Adam Carter (EPCC)	a.carter@epcc.ed.ac.uk
WP3 deputy	Ian Harrow (IHC)	ianharrowconsulting@gmail.com
WP4 leader	Rossen Apostolov (KTH)	rossen@kth.se
WP4 deputy	Vera Matser (EMBL)	matser@ebi.ac.uk
WP5 leader	Holger Noack (FT)	holger@forwardtech.se

WP5 deputy	Rosa M. Badia (BSC)	rosa.m.badia@bsc.es
WP6 leader	Rossen Apostolov (KTH)	rossen@kth.se
WP6 deputy	Erwin Laure (KTH)	erwinl@pdc.kth.se

3.4 Email lists

Communication within the consortium is organized along 4 email lists - *Bioexcel-all* includes all members of the project and is used for discussions concerning everyone involved; *Bioexcel-eb* is used by the executive board for coordination of the operations; *Bioexcel-pmb* for project management board communication; and *Bioexcel-finance* for financial topics.

List Name	Purpose
bioexcel-all@pdc.kth.se	All members of the Project
bioexcel-pmb@pdc.kth.se	PMB Members
bioexcel-eb@pdc.kth.se	EB Members (WP leaders)
bioexcel-finance@pdc.kth.se	Financial contacts

4 Project Organization and Management

Here we describe the organization and management of the project overall. As one of the main goals of BioExcel is to set up a sustainable center, this management structure is also responsible for the initial operations of the emerging center and dedicated management structures and procedures for the center are being developed during the course of the project (see Section 8 below).

Management structure

The management structure is designed to ensure the implementation of the overall project objectives in an efficient and secure way. The individuals selected for leading project positions are holding similar positions in ongoing projects and have extensive experience from international collaborative projects, and in delivering high-quality research and development, support, and training. Accurate quantitative and qualitative metrics for the project and its activities will be defined in the quality plan (D6.2 PM3).

Due to the size of the consortium and the complexity of the project, a lean management structure has been chosen to ensure successful technical and administrative execution of the project. Central to the management of the project is a set of roles and boards as described below.

Project Management Board

The ultimate authority of the project is the **Project Management Board (PMB)**, composed of one member per partner (see 3.2 Contacts for Partner Representatives), the Lead Scientist and the Project Manager. The PMB meets every 6 months, by telephone or in person, with at least one meeting per year

being in person. More frequent meetings will be called if necessary to deal with extraordinary issues. The PMB is chaired by the Project Coordinator (Erwin Laure, KTH). The PMB is responsible for approving major changes in project plans, including changing partner budgets as may be required to realise project plans and objectives. The majority rules for approval of such changes will be done in accordance with the guidelines in sections 6.2 and 6.3 of the Consortium Agreement. The PMB will monitor the project status based on regular progress reports provided by the Project Coordinator and approve project deliverables and reports. The PMB may request revised project plans from the Project Coordinator should a status review or external events warrant such a request. The intricacies of the consortium relations are governed by the Consortium Agreement, which also specifies clear conditions by which responsibility and corresponding EU funding will be re-assigned to other partners in case of persistent failure to meet delivery schedules.

The main tasks of the PMB are to:

- Set the strategic direction of the project and its roadmap and technical vision;
- Monitor on behalf of the partners the management of the project;
- Ensure that the work of the project is focused towards exploitable goals;
- Advise the Executive Board in the management of the project;
- Address external risks which may impair progress towards the project's objectives and propose strategies to address those risks;
- Delegate responsibility for the day-to-day running of the project to the Project Coordinator with support from the Executive Board;
- Give guidance to the work of the project through the Project Coordinator;
- Address and document all issues raised by external regulatory and other bodies relevant to the objectives of the project;
- Ensure proper implementation of the rights and obligations of all Partners in accordance with the Contract and the Consortium Agreement;
- Examine and approve any amendments to the Contract and Consortium Agreement;
- Address ethical, legal and gender issues relevant to the project;
- Decide upon the inclusion and exclusion of Partners;
- Approve project budgets;
- Assess the performance of the project and take appropriate measures if performance is found to be lacking;
- Address all relevant Intellectual Property issues raised by Participants;
- Resolve any conflict between the Executive Board and any Partner.

Conflict resolution

An important role of the Project Management Board is to arbitrate between partners should conflict arise. If the issue cannot be resolved within the project an external arbitrator will be appointed, as described in the Consortium Agreement. The provision in the Consortium Agreement in this regard is a customary mediation plus arbitration clause (ref. section 11.8 of the DESCA

Model Agreement). It is set out explicitly in the Consortium Agreement that, although one of the tasks of the Project Management Board is to arbitrate between the Parties, a Party may nonetheless opt to initiate mediation and arbitration in accordance with Section [11.8] of the Consortium Agreement at any time.

Executive Board

The executive management of the project is coordinated by the **Executive Board (EB)**, composed of the work package leaders and deputies:

- WP1: Mark Abraham (KTH, leader), Adrien Melquion (UU, deputy)
- WP2: Adam Hospital (IRB, leader), Stian Soiland-Reyes (UNIMAN, deputy)
- WP3: Adam Carter (EPCC, leader), Ian Harrow (IHC, deputy),
- WP4: Rossen Apostolov (KTH, leader), Vera Matser (EBI, deputy),
- WP5: Holger Noack (FT, leader), Rosa M. Badia (BSC, deputy)
- WP6: Rossen Apostolov (KTH, leader)

The EB also includes the Lead Scientist (Erik Lindahl (KTH)) and the project coordinator (Erwin Laure (KTH)), and is chaired by the Project Manager (Rossen Apostolov, (KTH, **WP6 leader**)). The EB ensures the progress of the project with respect to the Description of Work (including reporting, deliverables and milestones monitoring, key event coordination, and relations with collaborating projects) and will meet every second week (phone or in person). Issues not resolved in the EB will be forwarded by the Project Manager to the PMB. The main tasks of the EB are to:

- Direct the project according to the work plan taking corrective actions as needed;
- Ensure deliverables are of good quality and on time;
- Support the Project Manager in all reporting activities towards the Project Board and EC;
- Ensure that there is a shared technical vision across all activities;
- Monitor progress towards the technical objectives of the project;
- Ensure that the technical activities interact effectively;
- Ensure the free flow of information between the activities;
- Prepare and update quality-assurance procedures and guidelines;
- Ensure that the interdependencies of the technical activities are effectively addressed;
- Identify and address technical risks, which may impair progress towards the Project's technical objectives and propose strategies to address these risks.

To improve information flow between the partners and the collaborative spirit of the project, all-hands meetings will be organized every 6 months to assess the progress made and provide detailed planning of the next steps. See section 7 for a list of various meetings.

The EB is led by the **Project Manager** (Rossen Apostolov, KTH) supported by the relevant administrative and financial support team in the management activity WP1 (as described in Section 1.3), who will report directly to and liaise with the European Commission. The Project Manager reports to the PMB. More specifically, the Project Manager will:

- Set up the overall management structure according to the management plan
- Resolve issues
- Provide administrative support to partners via the WP1 support team
- Chair the Executive Board (EB) and ensure effective management is implemented at all levels of the project hierarchy
- Ensure effective operation of the project and ensure that all partners' efforts are focused towards achieving its objectives
- Act as primary point of contact between the project and the EC
- Ensure timely delivery of project deliverables to the EU
- Ensure documentation and dissemination of project results by responsible partners
- Provide Activity Report as requested by the EU
- Provide Management Report as requested by the EU.
- Act as primary point of management contact with other related National and European projects and initiatives

Other responsibilities as defined by the Contract and the Consortium Agreement.

The Executive Board is supported by the Project Office, which provides assistance with the financial and legal activities.

Workpackages

The technical and scientific management structure draws on the **Work Packages**, managed individually as described in section 1, with an overall management structure, particularly the EB, to ensure the coherence of the project. A dedicated Lead Scientist (Erik Lindahl, KTH) further ensures the scientific directions and coherence of the CoE. Each Work Package Leader is responsible for providing the Project Manager with detailed plans for the activities, and for the implementation of plans approved by the Project Manager. Work Package Leaders may request change of plans or staffing as warranted by project outcomes or insights gained. Work Package Leaders report to the Project Manager. This management structure permits on-going monitoring of the progress of the project against the work plan, with effective problem detection and resolution processes in place. All work package leaders are nominated by the Project Manager and approved by the Project Management Board. They are expected to set up regular meetings between participants within their work package.

Scientific Advisory Board

The project will also have a **Scientific Advisory Board (SAB)**, which will provide objective, external feedback on the strategic direction of the BioExcel project. The SAB will initially consist of four to five academic and industrial members with an appropriate background. The members of the SAB will be confirmed in the first months of the project (milestone M4) and suitable candidates have already been identified and contacted. Over the course of the project, representatives of user groups, as defined in WP3, will be added to the SAB to allow direct user input into the management structure. The SAB will also have a crucial role in defining the long-term governance structure and will be adapted to the emerging governance structure during the course of the project. Particularly, the SAB will be one potential basis for the future user council and board structure of the CoE.

The overall management structure is schematically represented in Figure 1 below.

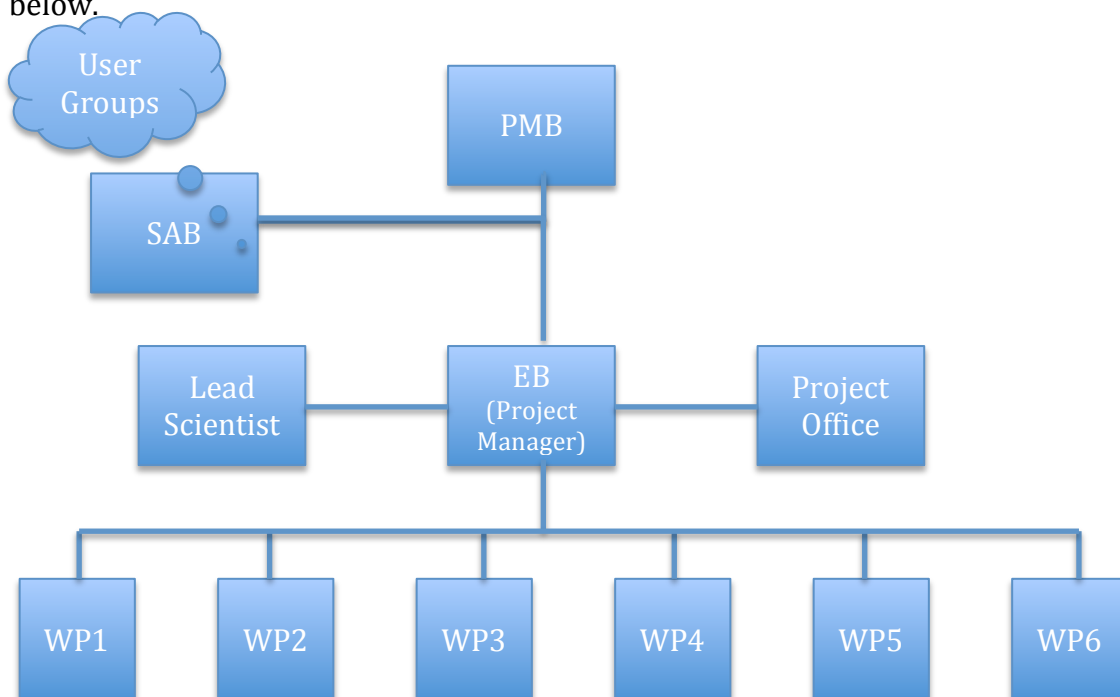


Figure 1. Project Management Structure

5 Operational management processes

5.1 Decision making

As mentioned above, initial center operations are run by the EB, which is responsible for making decisions regarding ongoing work. Those are discussed during the regular telecon meetings every two weeks. WP specific actions are made during separate telecon (or face-to-face) meetings of personnel involved in the corresponding WP. All decisions are shared with the rest of the board for recommendations.

Higher-level and strategic decisions are raised to the PMB for approval.

Each WP leader is responsible to ensure that a necessary progress is made along the planned WP activities. He oversees the work and communicates directly with

all the personnel (from different partners) who are part of that workpackage. Thus, day-to-day decisions are taken within the workpackage members and their outcome is reported to EB during the regular telecons.

5.2 Interactions with users and interest groups (IG)

In order to provide support along the available expertise, we have established a number of interest groups (IGs), as described in D3.1 “Selection and Establishment of User Groups”.

Each IG has an appointed leader who is in direct communication with the IG members. The groups have special support forums on <http://Ask.BioExcel.eu>. The IG leaders are monitoring the respective group’s discussion and either provide the help themselves or find an expert from the partners who can provide it.

The WP3 leader oversees the general progress of the IG interactions and has regular telecon meetings with the IG leaders. Higher-level strategic decision regarding user interactions are usually done either during EB or during the WP3 telecon meetings.

5.3 Conflict resolution

If conflict arises within a WP’s activities, the issue is first discussed at an EB meeting. If it cannot be resolved, then the issue is raised to the PMB. If the conflict cannot be resolved at that level, then an external arbitrator is appointed, as described above in section 4 with reference to the Consortium Agreement section 11.8.

5.4 Quality control

Workpackage leaders are overseeing the activities in the respective packages and progress is reported to EB. Results are discussed at the regular telecon and face-to-face meetings and KPI progress monitored.

All documents such as deliverables, reports, press releases as well as printed material (flyers, posters, roll-up etc.) are reviewed for acceptance by the PMB. Web content is curated by a designated member. Support forums are monitored by a number of administrators and IG group leaders.

More details are presented in D6.2 “Quality assurance and Risk Management”

5.5 Risk management

A number of potential risks and means for their mitigation are described in details in D6.2 “Quality Assurance and Risk Management”. The risks cover the

important aspects of work in each of the workpackages. Each risk has a person responsible for its monitoring and reporting to the board. As a rule, risk assessment is done during each reporting period.

5.6 Rules and procedures

Members of the consortium are requested to follow a number of rules and standards as agreed in the beginning of the project.

Operations

- Each partner organization has a representative in the PMB and they are expected to attend the PMB meetings. Minutes from the meetings are distributed to all partners as a notification of the taken decisions.
- Each partner appoints a designated person to lead the workpackage for which it is responsible. Some partners appoint a deputy WP leader. All WP leaders and their deputies are expected to attend all EB meetings.
- WP leaders are responsible for ensuring timely and quality execution of tasks within their WP. They are also responsible for curating the production of the respective deliverables, e.g. collecting contributions from partners and producing draft documents.
- All deliverables and associated reports are first reviewed by the EB. After that they are sent for approval to PMB. Documents are deposited in the EC portal and submitted to the commission by the Project Coordinator.

Documents

- All documents relevant to the project work should be stored in the shared platform (see section 6.1)
- Deliverables and reports should use the document template as described in D4.1
- Presentation slides should be made using the presentation template as described in D4.1. If BioExcel activities are included as part of a wider scope presentation, where the fully branded template is not suitable, then BioExcel's logo should be used in the acknowledgement sections.
- Center logo and EU flag/project number should be present on all promotional material such as posters and flyers.
- Publications by the partners should include in the acknowledgements sections a standardized paragraph describing the funding of the project.
- It is encouraged that all publications should be submitted to journal adhering to the Open Access policy and registered with OpenAire repositories.

Web content

- Every section of the website has a person responsible for gathering content for contribution from the partners. Before addition, the content is moderated by a website curator who ensures the quality and sufficiency of the material.

- All partners are expected to notify the curator of news and information that is of interest for the community such as upcoming events, recent publications, recent software releases, notable achievements in the area. Reminders are being sent once a month.
- The curator also manages the center's social outreach platforms such as Twitter channel and Google+/LinkedIn groups.

Webinars

- The webinar educational series are produced live and recordings are made available on the center's video channel. For that reason, we have three people who are responsible for smooth operation of the series with a requirement that each event is managed by two organizers for support. Organizers follow an extensive checklist for procedures before, during and after the completion of each webinar.

Interest groups

We have set guidelines to support the common purposes of IGs which include:

- to share scientific questions of interest to the group
- to consider potential solutions including BioExcel applications
- to understand and share the most common challenges for the IG
- to share new publications relevant to the IG
- to showcase success stories of the IG through BioExcel webinars
- to consider common questions arising through BioExcel webinars

The guidelines are as follows:

- Each BioExcel IG should have a named person to serve as leader. In this role he or she will build and maintain the group. They should have sufficient domain knowledge and connections to undertake this role. The IG leader is likely to be a partner of BioExcel.
- The IG is most likely to start by the leader inviting a few people to join as members. IG members are expected to come mostly from outside BioExcel, in the wider biomolecular community. We will also promote and encourage individuals from outside BioExcel to join particular IGs through appropriate mechanisms. (Do we have these yet?)
- It is expected that some of the IG members are likely to emerge as "core" because they show energy, enthusiasm and strong participation in IG communications.
- The IG is expected to communicate regularly with its members through activities of the IG leader and its core members. Each IG should decide on what means of communication works best for them and how regular this needs to be to achieve vibrancy and interest. A variety of communication channels are available to all IGs which includes ask.bioexcel.eu, GoToWebinars, Gitter, blog, wiki and email.

- It is recommended that each IG uses these common guidelines and connects with the BioExcel WP3 leadership (Adam, Ian and Rossen) who will be responsible for co-ordination between IGs.
- As each individual IG grows it would be natural for it to define its own additional guidelines to reflect group preferences and ownership. Also, they can be shared with the other IGs, by being appended to these common guidelines.
- Once an IG is established and we see a future potential for its operation, one of the members will be appointed as an “ambassador” to join the SAB. The details can be discussed later, e.g. ambassadors to be changed on rotating terms etc.

6 Project Management Tools

6.1 Document repositories

All documents needed or produced by the project are stored on a shared BSCW platform hosted by EPCC (<https://kth-bscw.epcc.ed.ac.uk/sec/bscw.cgi/264>). The platform is accessible by all consortium members.

In cases when collaborative editing of documents would be optimal, we are using a shared Google Drive folder. Google documents are also used for production of online surveys.

6.2 Task management

Keeping track of ongoing work is done using Trello (www.trello.com). It is a web application, which allows distributed teams to organize their tasks through an intuitive interface. It gives a good overview to WP leaders about ongoing work, upcoming deadlines etc.

Each task has an assigned person who is responsible for its completion, but it might involve several members in certain cases.

All tasks in Trello are part of lists (one for each of the tasks described in the DoA). Those lists in turn are part of separate “boards”, one for each WP. The WP leaders and deputies are responsible for monitoring the progress along the tasks in their boards, while all members can create new tasks with suggestions, ideas etc.

During EB meetings every WP leader (or deputy in his absence) reviews the progress on each of the tasks in the respective workpackage. New tasks are added as needed. Accomplished ones are archived.

6.3 Code repositories

Improvements and contributions to existing tools and projects, part of BioExcel, will go back into their existing source code repositories, if such are already in use. Newly developed code will be hosted on the GitHub platform

(<https://github.com/bioexcel>) under the GitHub organization. This will be a "holding station" for contributions that should be contributed upstream, but are not yet in such a state. Details of the software process adopted by BioExcel are described in D1.1.

7 Project meetings

Meetings will be held according to the following schedule:

- Executive Board (EB) – the main activity for project execution and coordination is run as telecon video meetings once every two weeks
- Work Package meetings – organized as needed by the WP leaders, typically also once every two weeks
- Project Management Board (PMB) – face-to-face meetings twice a year during the project all-hands meetings
- All-hands meetings – twice a year all project partners meet for typically a two day event

8 Center operations

As mentioned above, initial center operations are provided by the managerial structures of the project. As the tasks and services of the center become better defined during the course of the project, dedicated managerial and operational structures will be set up for the center to provide persistency and sustainability independent of the management of projects supporting the center. We will particularly explore the suitability of FitSM, <http://fitsm.itemo.org>, (or a subset of concepts defined therein) for the operations of the center. Details will be provided in the WP5 deliverables.