

# Project Management Protocol of the Netherlands eScience Center

Authors: Netherlands eScience Center Programme Managers

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1 December 2024	3.0 updates	Planning, Legal agreements, Project budget breakdown, change in the workshops and end report processes, open-access publications
1 October 2023	2.0 updates	DT and <b>PM</b> mandates, Roles of Directors, <b>PM</b> role in Ambition 2, SS, KD and external projects, Communications role, Editorial team, breakdown of hours, opportunities beyond project, Technology Status Report, End report
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# Contents

<b>1</b>	<b>Scope and definitions</b>	<b>3</b>
1.1	Scope . . . . .	3
1.2	Stakeholders . . . . .	3
1.3	Types of projects . . . . .	6
1.4	Project life cycle overview . . . . .	8
<b>2</b>	<b>Project Initiation</b>	<b>9</b>
2.1	<b>PM</b> assignment . . . . .	9
2.2	Administrative Setup . . . . .	9
2.3	<b>TL</b> assignment . . . . .	10
2.4	Preparation by <b>PM</b> . . . . .	10
2.5	Staffing . . . . .	11
2.6	Kick-off meetings . . . . .	12
2.7	Technology plan . . . . .	14
2.8	Legal agreements . . . . .	15
<b>3</b>	<b>Project execution</b>	<b>16</b>
3.1	Project logging . . . . .	16
3.2	Status update meetings . . . . .	16
3.3	Project team meetings . . . . .	17
3.4	Writing hours and managing project budget . . . . .	17
3.5	Workshops . . . . .	18
3.6	Data and Software Management Plans . . . . .	19
3.7	Knowledge transfer . . . . .	20
3.8	Code quality and sustainability checks . . . . .	23
3.9	Annual project review meeting . . . . .	23
3.10	Reporting . . . . .	26
3.11	Conflict resolution and complaint procedure . . . . .	27
3.12	Non-RSE Consultants . . . . .	27
3.13	Changes to the project . . . . .	27
3.14	Opportunities beyond the project . . . . .	30
<b>4</b>	<b>Project closing</b>	<b>31</b>
4.1	Handling end report . . . . .	31
4.2	Formally closing the project . . . . .	32
	<b>Appendices</b>	<b>35</b>

<b>A</b>	<b>Lead RSE role description</b>	<b>35</b>
<b>B</b>	<b>Role of PMs and others in external and Ambition 2 projects</b>	<b>36</b>
B.1	Fellowship projects . . . . .	36
B.2	External projects . . . . .	36
B.3	KD and SS projects . . . . .	37
B.4	D&C projects . . . . .	37
<b>C</b>	<b>Example of the project log</b>	<b>38</b>
<b>D</b>	<b>Examples of Technology Plan</b>	<b>39</b>
D.1	Technology plan for "Personalized cancer vaccine design through 3D modelling boosted geometric learning (3D-Vac)" . . . . .	39
D.2	Technology plan for "Exchange of CO2 in tropical ecosystems unravelled (EXCITED)" . . . . .	43
	<b>Index</b>	<b>45</b>

# 1 Scope and definitions

## 1.1 Scope

This document is the official project management protocol for the Netherlands eScience Center. It describes all phases of a project and the procedures required to successfully complete them.

The scope of this document is the execution of research projects awarded by the eScience Center through calls for proposals, though other types of projects are also briefly covered. This document gives a detailed description of all steps, both necessary and optional, that must or may be taken in the execution of projects, reflecting the so-called *project life cycle*. For each step, the document indicates the responsibilities of the project team members (RSEs) and other eScience Center employees (e.g. Programme Managers, **Finance**, Directors Team) involved in the process.

Call procedures follow a separate protocol [10] and are not covered by this document. The call procedure protocol ends with the formal awarding of projects by the eScience Center Governing Board or the Directors Team (DT), the notification of Lead Applicants and the formalization of the awarding by means of a *toekenningsbrief* ('Awarding letter'). The current document describes all activities that (need to) take place from that moment onwards, until the formal closing of the project. An independent evaluation of projects, including impact, output, process and collaboration with project partners is outside of the scope of the current document, and will be published as a separate document or a subsequent version of this document in the future.

This document has been approved by the DT and will be subject to evaluation and possible adaptation annually.

The structure of this document largely follows the project life cycle (see Section 1.4); the protocol describes activities in chronological order.

## 1.2 Stakeholders

An eScience project is a project involving the eScience Center, where responsibility is shared between different stakeholders who each have their own roles and responsibilities during specific phases of the project.

Stakeholder	Abbreviation	Assignment	Role	More info
Lead Applicant	LA	main applicant and recipient of the grant	primary contact for the eScience Center project, accountable for the (quality of the) scientific contribution to the project	responsibilities defined in the call text, the Terms and Conditions document, and potentially a Consortium/Collaboration agreement.
Programme Manager	<b>PM</b>	assigned by the <b>PM</b> team <sup>1</sup>	accountable for the eScience contribution to a project, responsible for realization of project results given predetermined resources and timelines, project budget holder	Full text of responsibilities available in the <b>PM</b> job profile document and <b>PM</b> mandate (see [15])
Lead Research Software Engineer	<b>Lead RSE</b>	appointed by accountable <b>PM</b>	responsible for the timely execution of the project, main contact person for the project with other stakeholders	More details on responsibilities, see the formal role description of <b>Lead RSE</b> (Appendix A).

Stakeholder	Abbreviation	Assignment	Role	More info
Research Software Engineer (assigned to a project)	RSE	assigned by the accountable <b>PM</b>	responsible for the timely completion of the project	All RSE activities coordinated by <b>Lead RSE</b> in agreement with <b>PM</b> .
Consulting Research Software Engineer	Consulting RSE	involved at request of <b>Lead RSE</b> or accountable <b>PM</b>	responsible for contributing expertise to a project for a limited but predetermined time, can be involved in some of the key meetings, in addition to an expertise contribution	All activities coordinated by <b>Lead RSE</b> in agreement with <b>PM</b> in case the project team needs additional expertise.
Technology Lead.	<b>TL</b>	assigned by the <b>TL</b> team <sup>2</sup>	acts as point of contact for <b>Lead RSE</b> to the <b>TL</b> team. Safeguards the technological aspects of a project; accountable for the quality, reuse and sustainability of the research software developed.	The <b>TLs</b> team is responsible for internal training programme of RSEs.
Section Head	SH	assigned by the <b>PM/SH</b> team <sup>3</sup>	line manager of RSEs, responsible for monitoring the overall effectiveness of RSEs in bringing projects to completion; maintain overview of a research domain.	The SH team assigns one SH to each RSE team, and the SH ensures that team keeps its capacity and planning up to date.
Communications			advise and facilitate internal and external communications of projects, including but not limited to showcasing projects through news items, website, newsletters, social media, interviews and videos.	
Community Manager	CM		advise on developing outreach activities and promoting community engagement, responsible for external training programme	
Secretary			organizes formal meetings, provide with agenda and slide template, invitation text, list of participants (with emails), and timeline.	

Stakeholder	Abbreviation	Assignment	Role	More info
Programme Director	PD		the escalation point for <b>PMs</b> , the contact point of <b>PMs</b> to DT for project related changes that need the DT decision, approves the workshops plans (in the agreement with <b>Finance</b> on the financial part). The budget holder of Acquisition.	
Director of Technology	DoT		The escalation point for <b>TLs</b> , the contact point of <b>TLs</b> to DT, accountable (and responsible) for licences and Intellectual Property (IP), software sustainability budgets holder	
Director of Operations	<b>DoO</b>		handles legal questions (e.g., contracts, Collaborative Agreements and guest agreements)	
<b>Finance</b> & Control	<b>Finance</b>	part of Operations, includes Controller, and led by <b>DoO</b>	responsible for maintaining finances and project administration	
Directors Team	DT	comprised of DoT, <b>DoO</b> , General Director and PD	approves formal decisions regarding projects (e.g., budget changes)	
GDPR contact person		appointed by the DT, see the Intranet for contact information	consults on GDPR [5] or privacy-related issues in the project	The eScience Center has not appointed a Data Protection Officer. GDPR aspects must be discussed with the contact person.
eScience Center project team	eScience project team	comprises RSEs, <b>PM</b> and <b>TL</b> working on the project	responsible for the timely completion of the project	

Stakeholder	Abbreviation	Assignment	Role	More info
Project team		comprises the eScience project team, LA and their team (including team members indicated in the project proposal)	responsible for the timely completion of the project	
Editorial Team			provides support with outreach	The eScience Center maintains a blog, and has presence in major social networks

## 1.3 Types of projects

The eScience Center receives an annual budget from NWO and SURF, the larger part of which is allocated to projects submitted by researchers working at eligible research performing organizations in the Netherlands in the form of the in-kind provision of RSEs. Projects may also be funded from external sources (henceforth referred to as *an external project*) or funded from the annual budget but carried out internally.

By awarding subsidy to a project or by pledging a contribution to an external project, the eScience Center takes on the obligation to deliver high-quality work in a timely manner.

### 1.3.1 Call projects

The eScience Center publishes a range of calls. Each project is a part of a specific call (regular calls such as OEC, SS, SSI, or calls in collaboration with other funders such as Big Data & Health, JCER, ESI-FAR). Projects from the regular calls before 2021 are partly in-cash, while projects awarded later are fully in-kind (plus a reserved budget for workshops).

Calls can reserve part of the project or the call budget to serve the eScience Center agenda to increase the impact of software beyond the project itself. Henceforth this will be referred to as the software sustainability budget, formerly known as generalization budget). The budget is intended for software generalization, reuse and sustainability, and community building. The DoT is the holder of this budget. Details concerning this budget are included in the Awarding letter. See Section 3.14.1 for more information.

Project teams (mainly **Lead RSE**, **PM** and **TL**) are expected to consult legal documents such as the specific call text, Awarding letter ('Toekenningsbrief'), Terms and Conditions document ('Bijzondere voorwaarden', 'Subsidieregeling', etc.), Consortium/Collaboration Agreement (CA), and/or contracts for grant terms and conditions. The LA is responsible for adhering to the conditions of the project, while the **PM**, with the help of the **Lead RSE**, monitors this.

In our call projects, most of the total requested budget is dedicated to project work and project-related activities. The remaining part (referred to as "general activities") covers activities that benefit our ability to contribute to high-quality research, such as the professional development of RSEs through training, work meetings, conferences, etc, as well as the administrative coordination and project management within the eScience Center. It is up to the **PMs** and RSEs in consultation with the SHs to fairly distribute hours for general activities across all the projects they contribute to (cf.

<sup>1</sup> All **PMs**, led by the Programme Director, constitute the **PM** team.

<sup>2</sup> All **TLs**, led by Director of Technology, constitute the **TL** team.

<sup>3</sup> All SHs, led by Executive Director, constitute the SH team.

Section 3.4). The exact percentage set aside for general activities is defined in the call within which a project has been awarded.

### 1.3.2 External projects

Projects funded externally by e.g. NWO or the EU, or via private-public partnerships, are governed by external funding conditions specified in a contract or agreement that may supersede our own rules. The LA is responsible for adherence to these rules and conditions, while the **Lead RSE** monitors this. Again, the project team (mostly, **Lead RSE**, **PM**, **TL**) must consult the specific call text and other formal documents (Awarding letter, Terms and Conditions document, Consortium/Collaboration Agreements, contracts for the conditions and rules). Projects under external funding are covered partially by this protocol. The formalities around the acquisition process follow the workflow described in “External funding” (see Section 3.14.3 for more information).

### 1.3.3 Other projects

This document only briefly covers other types of projects such as those funded through Ambition 2 [16], namely Dissemination & Community (D&C), Knowledge & Development (KD) and Fellowship projects in Section 3.14.4 and Appendix B.



## 1.4 Project life cycle overview

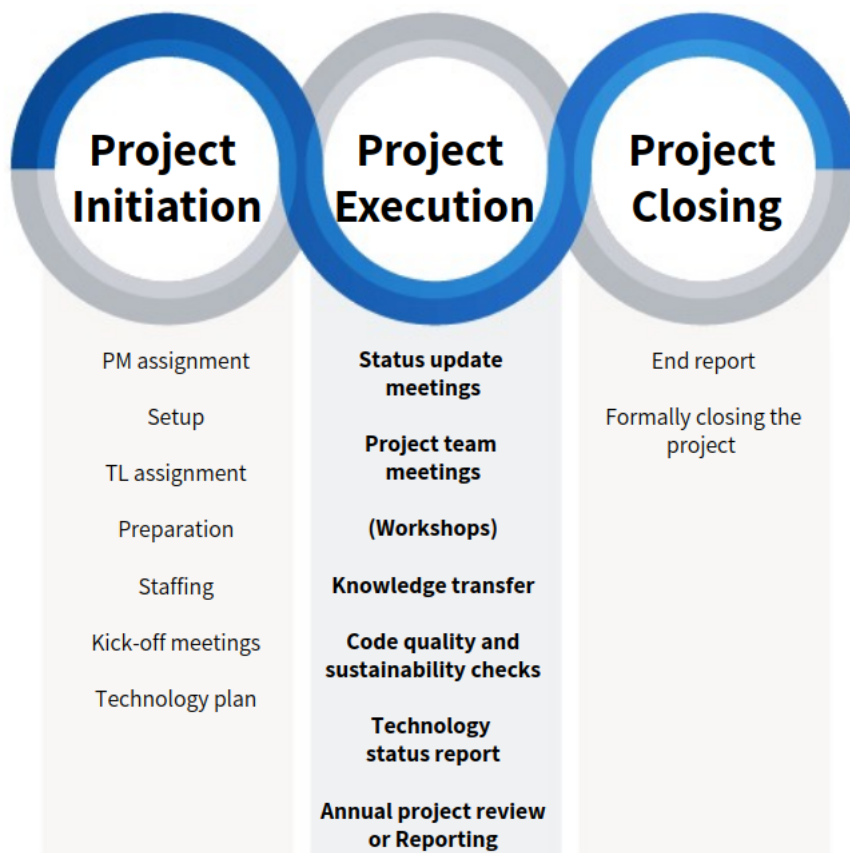


Figure 1: Project lifecycle stages

At the eScience Center, a standard project life cycle is a three-phase process (see Figure 1). First, project stakeholders initiate the project. Next, the project team executes the project and monitors its progress. Finally, once the project reaches its end, it is formally closed.

These three phases are covered in detail in the next sections.

## 2 Project Initiation

The project initiation phase starts immediately after the project has been granted. Its goal is to set up the project within the eScience Center, including a planning in terms of staffing and a work plan.

For **external projects** and projects from specific calls (e.g., collaborative calls), **Finance** ensures that all paperwork is in place (e.g., contracts, Consortium/Collaborative Agreements, Memorandum of Understanding) before making a project active in Exact, allowing RSEs to write hours spent on the project. The PD regularly keeps **PMs** up to date on outstanding applications for external funding, signals to **PMs** and **Finance** whenever a project has been granted, and hands over relevant documents (such as proposal, agreements made, preliminary budget, etc) to **PMs**.

**PMs** are accountable for call projects. For the **external projects**, **PMs** assign a **PM** and **Lead RSE** to the project (i.e., the RSE involved in the submission procedure). The **Lead RSE** with the help of **DoO**, PD and the **PM** works with the project partners to get all paperwork in order (such as a subcontract), see Section 2.8.

### 2.1 PM assignment

Each project has one accountable **PM**. The **PM** team assigns **PMs** to new projects at the first **PM** meeting following the granting decision, records the assignation and asks **Finance** to update Exact with new budget holder information (the newly assigned **PM**). If agreement over an assignment is not reached, the PD makes the final decision in their capacity as **PM** team chair.

**Responsible: PM team.**

### 2.2 Administrative Setup

The table offers an overview of the responsibilities of the different stakeholders in setting up a project:

**Table 2:**

What	By	Responsible for
Exact	<b>Finance</b>	<ul style="list-style-type: none"><li>• Creating project code</li><li>• Entering and uploading granting package documents <sup>5 a</sup>. If the signed start form (Meldingsformulier start) is not received, <b>Finance</b> requests the LA.</li><li>• Making <b>PM</b> a budget holder</li></ul>
Project portfolio in the relevant folder [17]	<b>Finance</b>	<ul style="list-style-type: none"><li>• Creating folder in project portfolio (with template subfolder &amp; documents)</li><li>• Uploading granting package documents <sup>5</sup>, signed start form, and CA if applicable</li></ul>
Research Software Directory (RSD), project page and software pages	<b>PM</b>	<ul style="list-style-type: none"><li>• Creating an RSD project page [18], putting placeholder image with the eScience logo <sup>4</sup>.</li><li>• Signalling requirements for corporate website to Communications</li><li>• Copying website summary from the proposal (if applicable) or writing a summary and obtaining approval from LA for edited versions</li><li>• Finding appropriate image (e.g., royalty-free images offered by shutterstock.com and unsplash.com)</li><li>• Ensuring <b>Lead RSE</b> has a maintainer access to the RSD page</li></ul>

Continued on next page

Table 2: (Continued)

What	By	Responsible for
	Communications	<ul style="list-style-type: none"> <li>Advising and reviewing content for the pages, including editing summaries, supporting with images</li> </ul>
Corporate website	Communications	<ul style="list-style-type: none"> <li>Ensuring content is displayed on the corporate web page with information supplied by <b>PM</b></li> <li>Promoting projects to target stakeholders, when relevant. Promotion may include but is not limited to news items, inclusion in newsletters and social media</li> </ul>
Gantt	<b>PM</b>	<ul style="list-style-type: none"> <li>Checking if import project information from Exact is correct</li> <li>Adding labels</li> <li>Adding respective project portfolio URLs</li> <li>Planning RSEs, if applicable (e.g., for external projects)</li> </ul>

4 5

For **external projects**, in particular, EU projects, PD and **DoO** make sure that the **Finance** and the **PM** have access to the project via the EU portal.

**General status and progress are monitored by the accountable PM.**

## 2.3 TL assignment

The **PM** asks the **TL** team to assign a **TL** to the project, providing all project information. The **TL** team does so at the **TL** meeting and informs the **PM** of their decision (by assigning **TL** to the project in Gantt as well as a confirmation by email).

**Responsible: TL team (at request of the PM).**

## 2.4 Preparation by PM

**PM** provides an overview of project requirements based on the project proposal, covering the following topics:

- What technology/eScience expertise is requested from the eScience Center, and at what level (novice, expert)? **Action:** In collaboration with the **TL**, the **PM** checks the skills survey for technological expertise required by the project.
- What are the research questions and goals? **Action:** **PM** asks senior members of the Center with relevant domain expertise for their opinion and prepares relevant tags for the project information.
- What is the proposed workplan and timeline? Is the work feasible? **Action:** Together with the **TL**, the **PM** assesses if a workplan is feasible or needs to be adjusted in the context of the Technology plan (Section 2.7).
- What type of support other than RSE expertise is requested and needed? (e.g., training workshops, time and help of CMs, use of SURF or other infrastructure) **Action:** **PM** notes this information for discussion with the LA and **Lead RSE**. **PM** consults **TL** about management plans (see Section 3.6) and CMs about training workshops (see Section 3.7.2).

**PM** flags issues such as:

<sup>4</sup>The image is provided by the Communications.

<sup>5</sup>In this case, the proposal and all supporting documents submitted by the LA, Awarding letter.

- GDPR – is there any personally identifiable information involved in the data required by the project?
- IP and licensing – does the project team ask for an exception to the Apache 2.0 and the CC by 4.0 default?
- Long term sustainability of the software – does the project have a sustainability plan?
- Anything else potentially problematic – for example, military application, animal or human tests, etc. (see also the final statements in the application form).

Depending on the issue, **PM** contacts relevant consultants (see Section 3.12).

**PM** records all relevant information in the project log (Section 3.1).

**Responsible: accountable PM**

## 2.5 Staffing

**PM** assigns the project to a team [6] and appoints a **Lead RSE** in agreement with SHs and budget holders relevant to the team activities. The **PM** can adjust staffing at any point during the project life cycle whenever necessary. The **PM** informs the LA on staffing changes concerning **Lead RSE** and **PM**. Otherwise, the **Lead RSE** is the primary contact for the project.

### 2.5.1 Project vacancy announcement

Project vacancies are announced internally at the discretion of the **accountable PM** in a timely manner. RSEs can express their interest (also on behalf of their team) within the allocated time and provide a motivational text including expertise and skills relevant to the project work. **PM** informs RSEs on staffing results.

### 2.5.2 Assignment of RSEs

The **PM** assigns RSEs in consultation with the relevant SH, based on RSEs' expressions of interest, availability, technological skills, disciplinary match, and seniority and/or potential. If a team of RSEs is assigned to a project, the **PM** and the team agree as to which member(s) and in which capacity they work on the project, as described in 2.5.4.

The **Lead RSE** plays a leading role in the project execution phase. The **PM** consults the relevant SH regarding the professional and/or personal development needs of the **Lead RSE**.

### 2.5.3 Key stakeholders availability

If the project cannot be staffed, the **PM** signals the vacancy to the respective SH and the **PM** representative in the hiring committee following rules described in the hiring process [15].

**PM/TL availability** If the **PM** or the **TL** becomes unavailable, their team appoints new one for the project. The **PM/TL** plans with **Lead RSE** any pending important milestone on the project (review meeting, code release, paper publication). The former **PM** informs LA of the changes and planning, and introduces the new **PM** in the email. The former **TL** informs the **PM** and the **Lead RSE** of the change.

**Lead RSE availability** If the **Lead RSE** has limited availability during the project for an extended period, this is signalled to the **PM** and the SH by the **Lead RSE**. The **PM** discusses with the SH whether the **Lead RSE** should be temporarily or permanently replaced. The eScience project team puts forward a candidate to take up the role of **Lead RSE**. The **PM** approves replacement of a **Lead RSE**, communicates the change to the LA (or Consortium for external projects) and includes both the former **Lead RSE** and the new **Lead RSE** in the correspondence.

The former **Lead RSE** ensures a proper knowledge transfer with the new **Lead RSE** and the **PM**, reporting and recording on the status of the project (current workplan, tasks, responsibilities of all project RSEs and the next steps in the project execution), ensures proper RSD pages handover.

**LA availability** For the case of the LA change, Section 3.13 describes overall procedure.

## 2.5.4 Project Planning

Project planning in Ganttlic is used as an agreement between the **PMs** and the RSEs. RSEs are expected to adhere to the planning as agreed; if required, they can discuss and renegotiate the planning with the **PMs**. The **Lead RSE** is responsible for the planning of the project, following the rules described in "Project planning" [15].

## 2.6 Kick-off meetings

Once administration and staffing are finalized, the **PM** organizes two kick-off meetings: an administrative start meeting introducing the eScience Center and our way of working and a project kick-off, which is focused on the project research and workplan. The secretary can assist with organizing the meetings.

The **PM** archives the material used during the meeting and the meeting notes (from LA, **PM** or others) internally in the project portfolio folder.

The **PM** can combine the two meetings, if necessary, into a single workshop-style meeting. This applies in particular to specific categories of projects (e.g., based on a collaborative call, or an OpenSSI call). This is held at the eScience Center office, and a suitable room is arranged by the **PM**.

For **external projects**, the way kick-off meetings are arranged depends on the nature of the project. The **Lead RSE** attends all formal meetings of external projects. The **PM** joins these meetings if they deem this necessary. It is the responsibility of the **Lead RSE** to keep the **PM** in the loop.

### 2.6.1 Administrative start meeting

<b>Scheduled:</b>	Soon after awarding, but not before the Awarding letters have been sent and <b>Finance</b> has collected all the paperwork and put it in Exact and Project Portfolio).
<b>Stakeholders:</b>	<b>PM</b> (organizer, chair), LA, <b>Lead RSE</b> (optional). The <b>PM</b> can involve others at their discretion.
<b>Purpose:</b>	A procedural meeting to discuss how the cooperation on this project will be organized, administrative questions the LA may have, current availability of software and data, staffing, etc., so that problems can be caught early (e.g., licensing issues, no data, etc.).
<b>Duration:</b>	1.5 hours
<b>Location:</b>	At the eScience Center (preferably), but can be also online.

For this meeting, the **PM** uses the administrative (PowerPoint) presentation [17], ensuring that information is in the line with the call text, and current Terms, IP policies, etc.

The meeting covers the following topics:

- The eScience Center Introduction (mission, structure)
- Working with the eScience Center (calls, different eScience stakeholders, guest status)
- Project life cycle and SURF support
- Community and impact (RSD, digital skills programme)
- Intellectual Property, Software Licenses as well as publication protocol
- Project needs and expertise.

The **PM** logs the agreements reached in the slides or the project log (Section 3.1). The **PM** updates the project log with the meeting date, stakeholders present and (link to) the agreements. The **PM** and LA share slides with each other and the **PM** stores both slide decks (from **PM** and LA) and agreements in the project portfolio.

### 2.6.2 Project Kick-off

<b>Scheduled:</b>	Around the date indicated by LA in the start form, after the administrative start meeting.
<b>Stakeholders:</b>	<b>PM</b> (organizer, chair), the entire project team, <b>TL</b> , and other relevant stakeholders (e.g., SH)
<b>Purpose:</b>	The project kick-off focuses on the execution of the project, on the technological requirements, scientific challenges, relevant communities, project goals and outputs.
<b>Duration:</b>	Max. 1.5 hours
<b>Location:</b>	At the eScience Center office or at the institute of the LA <sup>6</sup>

<sup>6</sup>

For this meeting the standard agenda is:

- Round of introductions (the entire project team) (10 min)
- Project introduction and goals by LA (20 min)
- Discussion on the workplan and any updates needed by the project team (30 min)
  - eScience team explains the purpose of the technology plan
  - Project team in agreement with the **PM** and **TL**, decides when the technology plan should be submitted
- Roles of the project team members in carrying out the project workplan (10 min)
- (Updates to) Software Management Plan (SMP) and Data Management Plan (DMP) (5 min)
- Agreements on initial project planning and deliverables (with concrete action points) (10 min)
- Agreements on collaboration (e.g. frequency and location of project team meetings, planning days to work together and location)
- Any other business (5 min).

A workplan should always include a clear set of steps, divided into work packages, a detailed and realistic schedule, a list of deliverables and management plans (see details in Section 3.6).

The licensing of software is discussed at the project admin meeting and if needed, the project kickoff. If the proposed plan for a project does not fully match the IP policy, the **PM** must ensure a document is written (ideally by the LA or **Lead RSE**) with the proposed exceptions. **TL** reviews the exception document and provides input. The **PM** formally

<sup>6</sup> Mandatory participants of a meeting be present in-person at the office, while all optional participants can also participate via video conferencing if they prefer.

approve the IP exceptions document taking the input of the **TL** into account. The IP exceptions document is archived in the project portfolio folder along with other formal documents. The **PM** notifies all RSEs working on a project of the exception such that they can take this into account while working on the project.

In agreement with the project team, the **Lead RSE** prepares the project for the code development (see details in Section 3.8.1). **PM** logs the agreements, asks LA for the slides, and archives all of it in the project portfolio.

## 2.7 Technology plan

Every research project starts with a review of existing literature and technologies, and an eScience project is no exception. To that end, the **Lead RSE** should write down a technology plan for the project before executing it. The starting point of a technology plan is the eScience section, the workplan and the timeline of the project proposal as well as agreements from the kick-off meeting.

The project team submits a technology plan by the date agreed during the project kick-off, describing

- possible choices of the available technologies and which of them will be used for the project, and for which reason
- the technological outcomes of the project (software and data)
- steps to be taken regarding reusability and adoptability, etc.

The technology plan covers the choice of programming language(s), expected quality levels, etc. The plan should be seen as an evolving record of the considerations and choices regarding the technology employed; it ensures that RSEs make good use of the expertise present in the Center and that optimal choices are made throughout the project. An example of project technology plan is included in the Appendix D.

<b>Written by:</b>	<b>Lead RSE</b> , in collaboration with project team (including LA, <b>TL</b> ), CMs, and others RSEs or colleagues (e.g. with relevant expertise on the subject), or relevant SIG.
<b>Target audience:</b>	Project team, <b>TLs</b> , <b>PMs</b>
<b>Schedule:</b>	<ul style="list-style-type: none"> <li>• written at the start of the project work, before any software development starts,</li> <li>• submitted to PM/TL by email before the deadline agreed during the project kick-off,</li> <li>• as a part of the project log (either full document in the log or a URL to it).</li> </ul>
<b>Approved by:</b>	<b>PM</b> after due consultation of <b>TL</b> .

The **Lead RSE** is encouraged to reach out to RSEs or other colleagues who have the relevant expertise in the process of developing the technology plan. CMs can advise on engaging the target audience with regard to software reusability and adoptability. Since **TLs** are accountable for safeguarding the suitable technology in the project, the involvement of the **TL** in writing the technology plan is important. Therefore, the **PM** must consult the **TL** on the technology plan, submitted by the **Lead RSE** before any technological decisions are made in the project.

Upon approval of the technology plan (via email), the project team updates the management plans, if necessary. The **Lead RSE** logs the decisions in the project log (see Section 3.1) and archives emails in the project portfolio, if necessary. The **Lead RSE** keeps the technology plan up to date: if it changes during the project, this should be simply appended to the original technology plan (e.g., in a separate document or in the project log). The **Lead RSE** explains why adaptations to the plan were required. The aim is to obtain a record of the lessons learned from beginning to end of the project, to facilitate collaboration and to document decisions in case a project must be transferred to other RSEs due to unforeseen circumstances. The **Lead RSE** discusses any changes made to the technology plan during the status update meetings (Section 3.2).

## 2.8 Legal agreements

The eScience Center champions and supports open and reproducible science and open-source development. LAs get their projects awarded under the eScience Center's Terms and Conditions [11]. The default agreement forms offered by universities often contain IP related provisions that contradict our Terms and conditions.

Regardless of the type of the project, RSEs must not sign any formal agreement document prior to consulting the **PM**. Such documents include but are not limited to:

- Guest agreement (to get guest status at the project partner organization)
- Data sharing agreement
- IP related document
- Consortium agreement
- Collaborative agreement
- Non-disclosure agreement

**PM** checks the draft agreement document and decides whether it can be signed and informs the RSE. If needed, the **PM** can consult PD. The RSE archives the final signed version of the agreement in the project portfolio.

**PM** and PD signal to the **DoO** if legal advice is required. In that case, any proposed contracts are sent to the **DoO** by the **PM** for final approval. The **DoO** shares the information within **Finance**.

The procedure for agreements regarding software licenses is described in Section 2.6.2.



## 3 Project execution

Projects at the eScience Center vary in duration from 3 months to 5 years, depending on the call through which they were granted. In all call projects, the **PM** (with the help of **Lead RSE**) monitors progress of the project and involves relevant stakeholders whenever necessary. The **Lead RSE** takes on a leading role during the execution phase of the project life cycle. The **Lead RSE** ensures that the Project team meetings take place on a regular basis: the frequency may vary with the size of the team, e.g. full team meetings once per month and meeting with only with the LA and/or LA team once in two weeks.

In terms of technical project management, an eScience project is a research process that does not have a one-size-fits-all plan for execution. Rather the project team has to adapt to unforeseen challenges and deviations from the initial research and technology plan, if needed. Therefore, during execution phase of the project, it is recommended that **Lead RSE** (and RSEs) utilize a variety of methods and tools related to project management and communication strategies, for example in [2, 8, 9].

### 3.1 Project logging

eScience project team members routinely log important project events and agreements. The project log is placed in the Project portfolio. The **Lead RSE** keeps the log up to date (see example in Appendix C). The project log facilitates the information flow between different stakeholders about project activities.

The following should be included in the project log:

- RSD project page URL
- important meetings, including dates, links to slides and fully written agreements/decisions
- infrastructure used and decisions regarding infrastructure
- output/deliverables (their URLs, or this is registered as an output in RSD)
- participation in workshops, external events, conferences related to the project (or this is registered as an output in RSD)
- changes to the project team
- records on management plan updates
- technology plan decisions and updates
- results of (code) reviews of the project.

Links pointing to other documents (e.g., files in the Project portfolio, project output, repositories) should be used in the project log to improve readability of the log and avoid duplicate information.

### 3.2 Status update meetings

The **PM** stays informed about the status of the project and communicates with the **Lead RSE** on a regular basis.

<b>Scheduled:</b>	Once every 4-6 weeks
<b>Stakeholders:</b>	<b>PM</b> (organizer), <b>Lead RSE</b> , optionally: <b>TL</b> <sup>7</sup> , other RSEs.
<b>Purpose:</b>	Status update on the project and discussion around project management.
<b>Duration:</b>	30 min -- 1 hour
<b>Location:</b>	In-person meeting is default.

**PM** and **Lead RSE** discuss:

- project status (including any changes in a project workplan)
- technological issues, with due consultation of **TL**, respective SIG, or other RSEs, if necessary
- changes in technology plan, technological choices (Section 2.7), management plans (Section 3.6). For any of these changes, **TL** presence is required
- synergies with other projects in the Center
- issues related to the budget, communication, staffing, etc.
- knowledge development and transfer, potential for software reuse, software sustainability.

The frequency and duration of these meetings are at the discretion of the **PM** and depend on factors such as the experience of the **Lead RSE** and the size of the team and/or the project.

In projects that have a stronger focus on technology (such as the eTEC, CIT projects), the **TL** is involved in these meetings more frequently. For some projects, update meetings can be combined (e.g., for projects within the same Call) or organized in the context of a larger meeting (such as a SIG on a relevant topic). Together with the **Lead RSE**, the **PM** decides on the format of the status update meeting.

### 3.3 Project team meetings

To keep the entire project team informed on project progress, the **Lead RSE** together with the LA organizes a periodical project meeting. The frequency and format depend on the complexity of the project and size of the project team.

<b>Scheduled:</b>	Once every 2-6 weeks
<b>Stakeholders:</b>	<b>Lead RSE</b> or LA (organizer), LA (chair), RSEs and other project team members from the LA side.
<b>Purpose:</b>	Progress update on the project by all team members.
<b>Duration:</b>	30 min -- 1 hour
<b>Location:</b>	In-person meeting is default.

The agenda of this meeting should include:

- status update from all stakeholders
- discussion of scientific progress
- discussion of technological progress, issues and choices
- alignment of project progress with the project workplan, and adjustment of the latter, if necessary.

### 3.4 Writing hours and managing project budget

The **PM** and **Lead RSE** must have a firm grasp of the project budget and the project duration. This information is in the Awarding letter, the proposal and Exact.

The project execution phase roughly consists of three parts: exploration, development, sustaining. For the call projects, the rough breakdown of work vs budget is as follows: 25% of the budget goes to exploration (including learning), 50%

<sup>7</sup>The **TL** participation is mandatory for the technology-oriented projects.

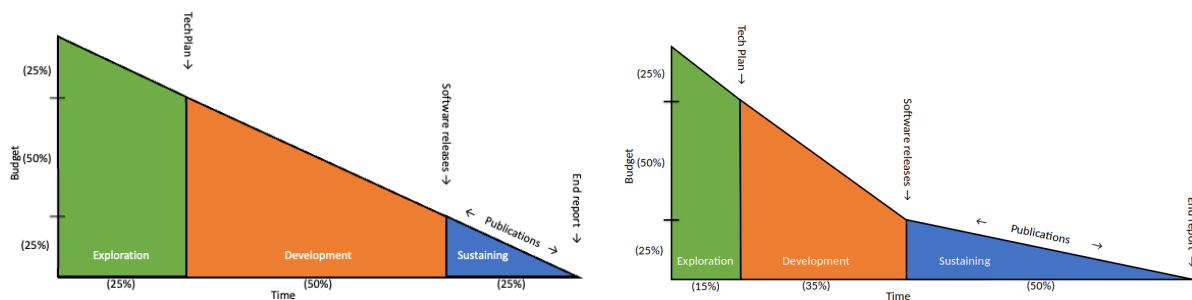


Figure 2: Project's budget breakdown: standard (left) and fast (right)

of the budget is to be spend on development, and 25% is for sustaining (including research and dissemination activities). **Lead RSE** must discuss with the **PM** if project execution deviates from this plan.

The left figure in Figure 2 assumes a constant rate of budget spending during the runtime of the project. If possible, RSEs are encouraged to do the first two phases of a project faster. The end date of the project remains the same, leaving more time for the sustaining phase (cf. Figure 2), which can be beneficial for output such as publications. This also helps to spend most of the budget of a project quicker, and in the eScience Center current financial system yields to better results.

The LA and RSEs are free to spend the awarded hours ahead of the project end date. However, the **Lead RSE** is responsible for results being delivered on time for the project and not exceeding the budget, and timely informing the **PM** and the LA about any changes to the agreed planning. If a project budget is fully spent ahead of its schedule, the **PM** asks **Finance** to restrict writing on the project budget only to the **PM**.

The eScience project team (including **PM** and RSEs) must submit their project hours in Exact by the end of each month. All data must be entered no later than one working week following the end of the month. For regular call projects, RSEs can write hours on awarded projects as soon as they are active in Exact, which in general happens within a month of the project being granted. The **PM** writes management hours on the project budget.

Project hours are managed by different parties with different responsibilities:

It is possible to travel for a project, however RSEs must ask approval of their line managers (a respective SH) before committing to an event requiring travel and fill out a travel form. See the Intranet for more information.

For **external projects**, the rules on writing hours differ from regular call projects. Only RSEs and the **PM** working on the project are allowed to write hours on the project budget. Moreover, for some projects (e.g., Horizon Europe projects) only direct contributions to the project are allowed; other non-project related activities such as time spent on a SIG cannot be declared on these projects. The **Lead RSE** and **PM** are aware of restrictions related to their project (otherwise, consult **Finance**).

### 3.5 Workshops

Some call projects require the LA to organize workshops. These workshops aim at fostering research communities around the software we develop on projects. A focus of a workshop could be, for instance, the early adoption of software requirements suggested by potential users, the addition and expansion of new features, or the linking of the exiting tool to a wider or more mature community. Based on the call text, the **PM** and **Lead RSE** determine whether one or more workshops must be organized. **Finance** provides a financial status of the project workshop budget. There are two types of workshops, namely, (a) organised by the LA, and (b) organized by the Lorentz Center.

**For workshops organized by the LA:** the LA writes and submits the workshop plan(s) to the **Finance** (cf. [17] for the templates) in a timely manner. The plans need to be approved by the **Finance** in consultation with PD and the **PM**. The **Lead RSE** is expected to contribute to the workshop and its organization. A CM can advise the LA (via the **Lead**

Stakeholder	Responsibilities	More info
<b>PM</b>	<ul style="list-style-type: none"> <li>checks and approves the hours submitted in Exact for the projects they are accountable for before the 5th workday of the next month</li> <li>provide monthly hour status to RSEs via Gantt</li> <li>checks and signals to <b>Finance</b> if there is an issue (for example, if project budget is incorrect)</li> <li>informs <b>Finance</b> of project budget changes</li> </ul>	
<b>Lead RSE</b>	<ul style="list-style-type: none"> <li>monitors project hour expenditure</li> <li>signals deviation from the workplan to the <b>PM</b></li> </ul>	Asks <b>PM</b> for hours status in Exact or via Gantt
<b>Finance</b>	<ul style="list-style-type: none"> <li>maintains accurate budget information</li> <li>monitors and processes approved project hours</li> <li>makes financial information available to the budget holders (including <b>PMs</b>) each month</li> <li>recalculates project budget if extension is granted over the year threshold</li> <li>automatically puts read-only status on the project when project hours are depleted/exceeded early</li> </ul>	All budget changes require a <b>PM</b> and DT decision.
DoT	<ul style="list-style-type: none"> <li>monitors and approves software sustainability hours</li> </ul>	There is a separate protocol on handling software sustainability.

**RSE**) on supporting the engagement and growth of relevant communities around the software; a CM is involved in the introductory part of the workshop, including an opportunity to address participants. **Finance** requests feedback on the scientific part of the workshop proposal of the **PM** team and handles the administrative and financial part of the request.

**For workshops organised by the Lorentz Center:** the LA must apply through the Lorentz Center webpage<sup>8</sup>. The LA has the leading role in the application. The **Lead RSE** takes an advisory role in the writing and design of the workshop proposal and is expected to actively participate during the workshop event. The **PM** must ensure enough hours are allocated for the **Lead RSE** (or RSE from the project team) to help the LA with the proposal and attend the workshop, if they want to take an active role.

These workshops differ from the eScience-Lorentz Center Competition workshops that are funded by both the eScience and the Lorentz Center. Besides co-funding workshop expenses, the eScience Center supports such a workshop with an additional in-kind contribution. The role of the eScience RSEs is described in the awarded proposals. The project initiation and assignment of the eScience project team proceeds similar to other type of project. The eScience team clarifies with the organizers the planning and outcome of the workshop (e.g. research paper, white paper, software release, consortium creation for a grant application, etc.). The **Lead RSE** has a pivotal role in the preparation and delivery of the workshop, and, possibly, in post-workshop stage to publish any outcome drafted during the event.

### 3.6 Data and Software Management Plans

For some projects, Data and Software Management plans (DMP [3] and SMP [7], respectively) provide details regarding the maintenance of the data and software output of the project.

Depending on the call, the LA must provide a fully worked out SMP and DMP within the first 6 months of the project. The **Lead RSE** can assist the LA and their team in drafting the DMP. The LA submits the DMP to the **PM**, who asks a **TL** for review and approval. For call projects since 2021, an SMP is a part of the proposal itself.

<sup>8</sup>The procedure is described in the eScience - Lorentz Center Agreement and Annexes (add the link when signed).

The LA maintains these plans and communicates any changes to the **PM** and **TL** via the **Lead RSE**. If needed, the **PM** requests an update. The **Lead RSE** can help the LA to update the plans.

## 3.7 Knowledge transfer

To increase visibility of the project and its results, the project team (including RSEs, **PM**, **TL**), Communications, CMs, share knowledge and outcomes both inside and outside of the organization. The **Lead RSE** ensures that

- information on project results is properly shared with Communications, CMs and relevant SH in a timely manner;
- project and software pages on the RSD are properly updated; and
- specific requests to facilitate project visibility are sent to Communications by RSEs.

Moreover, **PMs**, Lead RSEs and **TLs** work together to spot opportunities for cross project collaboration (e.g., by reusing software or knowledge in these projects or as a new reusability project, read more in Section 3.14.1).

### 3.7.1 Output management

Projects deliverables include output such as research articles, presentations, invited talks, posters, tutorials, datasets, blog posts, white papers and workshops but also more software-oriented output types such as software or code releases, dedicated software publications, software demonstrators, software videos, tutorials and training material around software.

RSEs strive to apply FAIR principles [20, 1] to all project deliverables. Therefore, all project deliverables should have

- concept DOIs (obtained from the publisher or created by uploading to Zenodo, arXiv, DANS or similar open-access archives);
- acknowledge the eScience Center project grant<sup>9</sup>; and
- listed RSEs working on the project as (co-)authors.

To formally record results and facilitate knowledge transfer, RSEs must make all project output available in the relevant systems, online locations and databases, see Table 3. In terms of project output, the **PM** expects the project team to follow the plan on deliverables; project deliverables are described in the proposal and workplan. RSEs contribute to the publications and software/data releases.

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<sup>9</sup>By adding the following sentence into the publication: "<full project title> is a project of the Netherlands eScience Center, funded under grant number <grantid>."

**Table 3: Output management**

What	Responsibility of	Responsible for	URL	Additional info
<b>Zenodo (NLeSC community)</b>	PM/CMs	curating and approving new publications	<a href="#">Zenodo link</a>	<ul style="list-style-type: none"> <li>Publications uploaded to Zenodo, are added to this community</li> <li><b>PMs</b> and CMs are curators of this community and approve new publications</li> </ul>
	RSEs	getting a concept DOI for a data or software release, or a document (e.g., non-peer-reviewed publications)		
<b>RSD, software and project pages</b>	<b>Lead RSE</b>	<ul style="list-style-type: none"> <li>creating RSD project page, if needed</li> <li>maintaining RSD pages and ensuring the meta data is complete and up to date</li> <li>ensuring <b>PM</b> has maintainer access to the page</li> </ul>	See <a href="#">RSD intro</a> and <a href="#">Adding RSD project</a>	Each project has its RSD project page. The <b>Lead RSE</b> in agreement with the <b>PM</b> can use the same RSD project if a direct continuation of the project is granted from another funding source. In this case, the funding source and respective text should be added.
	RSEs	<ul style="list-style-type: none"> <li>creating RSD software pages</li> <li>a timely and accurate registration and maintenance of the output</li> <li>keeping the (meta) data stored such as description, GitHub organization(s), concept DOI, mentions (via DOI or URL), related software and projects complete and up to date</li> </ul>		
<b>Project portfolio</b>	<b>PM</b>	adding direct link to the project portfolio folder to Ganttlic	cf. <a href="#">[17]</a> for structure explanation.	<ul style="list-style-type: none"> <li>An internal archive, which is periodically and automatically backed up</li> <li>Direct link to the project portfolio folder is available in Ganttlic</li> </ul>
	<b>Lead RSE</b>	ensuring that the output is uploaded		
	RSE	<ul style="list-style-type: none"> <li>uploading the output such as papers, reports, and presentations</li> <li>adding links to the source material to the project log</li> </ul>		
<b>The eScience Center blog</b>	RSEs	<ul style="list-style-type: none"> <li>Creating blog entry regarding project, its progress or project output</li> </ul>	Indexed at <a href="#">eScience Blog</a> , instructions on blogging are posted on the Intranet <a href="#">[15]</a> .	<ul style="list-style-type: none"> <li>URL of final blog entry added to project RSD page</li> </ul>
	Editorial Team	<ul style="list-style-type: none"> <li>Reviewing blog post entry of project team</li> <li>Helping at any stage with writing and publishing process</li> </ul>		

Open access publications and open software are a requirement for all call projects; **PM** and **Lead RSE** keep the LA informed on this matter, if necessary. The funds for open access publication fees are internally budgeted in the call

budget by **Finance** (with the approval of the PD every year). If no budget is available, the following option could be explored:

- publishing through the LA's institution (either open access funds are available or the LA organization is connected to publish open access in a lot of journals through the library without a fee)
- choosing the best option for open-access publishing (is it a diamond or gold open-access journal)
- publishing closed access but self-publishing preprint or after six months (as allowed by the Taverne agreement in Dutch copyright law, see for example [19]).

The **Lead RSE** and **PM** consult **Finance** regarding payments for an open access publication.

For **external projects** the expected deliverables are also part of the formal project documents (proposal, contract, etc. The **Lead RSE** is expected to keep the **PM** informed of the status of deliverables throughout the project.

### 3.7.2 Outreach

The **Lead RSE** stimulates and promotes the visibility of the project through project demonstrators, presentations, and other means. All RSEs are expected to communicate about the project and its deliverables externally, as described in Section 3.7.1. Communications advises and supports the project team to highlight projects through various communications channels, including but not limited to news items, social media posts, videos and interviewing team members about relevant scientific output and impact obtained as a result of the research software applied or developed in the project). The **Lead RSE** (or in rare occasion the **PM**) contacts Communications with relevant information.

Blog posts are an optional but highly recommended output of the projects. They can be authored by any member of the project team, from LA to RSE. Topics for a project's blog post can vary greatly. Examples include, but are not limited to,

- a simplified version of (parts of) the research, or
- a tutorial about a skill or technology a member of the team has learned during the project
- a communication about workshops, publications, releases or other type of project output.

RSEs engage in activities to inform colleagues about the project and the results (e.g., technology plan, milestones, code releases), including presentations at SIGs. For internal and external events, each RSE should prepare a three-slide presentation or a pitch [17] regularly update it. The **Lead RSE** is responsible for ensuring a presentation in the form of a demonstrator (e.g., of the software developed in the project) is available after the first major release of the software.

The LA and their team are encouraged to participate in relevant Digital Skills Workshops [13] from the eScience Center. Furthermore, if the LA and their team require a project-specific training workshop, the **Lead RSE** involves

- workshop coordination (via CMs) who can advise the eScience project team with workshop organization and the development of new training material. If applicable, the payment for the overall organization (either through or on top of the project budget) is handled by **Finance**; and
- the **PM** to discuss the RSE hours spent on organizing the training. If necessary, the **PM** contacts **Finance** for a consult.

Again, for **external projects** separate agreements may exist with the project consortium on how to communicate results of the project (for example, Non-Disclosure Agreement or NDA). The **Lead RSE** and **PM** consult these agreements at the start of project to know what can be communicated and what not.

## 3.8 Code quality and sustainability checks

Taking care of software quality and sustainability is integral to the code development process cycle at the eScience Center. All RSEs must follow our guide and best practices [4] for software development. Code should be made as generic and reusable as possible from the start.

### 3.8.1 Code development

At the initial stage of code development in the project, the **Lead RSE** together with RSEs:

- set up a GitHub organization for the project, following the eScience Center Guide and the Turing Way [2]
- add the URL of this organization to the RSD project page.

RSEs must always ask at least one project team member, relevant SIG member or other RSE at the eScience Center to review, comment and approve pull requests in the project codebase.

### 3.8.2 Code review

As part of the annual review (see Section 3.9), a code review is organized by the **Lead RSE**. Depending on the project it could take the form of a reusabilithon<sup>10</sup>, a review of code on GitHub, or something else entirely (format to be approved by **TL**). The reviewers for this process are typically other RSEs at the eScience Center.

The goal is to review software of the project for:

- its usability (reproducing steps of installations, and running it on a machine/laptop)
- overall software quality and suitability
- whenever appropriate, correctness of code
- adherence to the technology plan (Section 2.7)
- adherence to eScience Center best practices
- opportunities for reuse of software in other projects
- correct inclusion in output systems (Section 3.7.1).

Reviewers make written suggestions for improvements, and flag major issues encountered. These issues serve as input for the **TL** for the formal annual review meeting (see Section 3.9). These notes are stored in the project log.

## 3.9 Annual project review meeting

For all call projects lasting longer than one year, the **PM** organizes annual reviews. The details are described in the terms and conditions document [11]. For the projects with the duration of exactly one year, organizing a review meeting is at the discretion of the **PM** (in consultation with **TL** and **Lead RSE**).

A standard part of every review is a discussion and list of actions on how the results of the project will be made reusable and sustainable (as described in the DMP and SMP), how the collaboration is going and possibilities for follow-ups to projects.

The agenda of this meeting is:

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<sup>10</sup>The term coined by the Software Sustainability SIG. It refers to the 2-3 hours session with a group of RSEs to check usability of a software, give feedback to the developers and to come up with recommendations to improve the software (re-)usability.



<b>Scheduled:</b>	Yearly
<b>Stakeholders:</b>	<b>PM</b> (organizer, chair), <b>Lead RSE</b> , LA, <b>TL</b> , optional: other project team members, SH
<b>Purpose:</b>	<ul style="list-style-type: none"> <li>• to ensure that the project is still on track</li> <li>• to discuss any persistent issues to ensure optimal collaboration between project team</li> <li>• to explore opportunities beyond the project</li> </ul>
<b>Outcomes/Actions:</b>	List of agreements, action points, advises (from the <b>PM</b> and the <b>TL</b> ) for project team members on future steps.
<b>Duration:</b>	Max 1.5 hours
<b>Location:</b>	At the eScience Center or the project location <sup>6</sup>

- Introduction by eScience Center (round of introductions and purpose of meeting)
- project overview and deliverables so far
  - status of the scientific goal(s) by the LA and their team
  - status of the output (e.g., publications, software, datasets, methods, documentation) by the project team
- status of the collaboration (including admin status of hours, bottlenecks)
- use of digital infrastructure and support of SURF (if applicable)
- next steps
- opportunities beyond the project.

The goals of the meeting are to:

- review the progress of the project in comparison to the original workplan (are we on track?)
- discuss research results and their novelty and current deliverables of the project
- discuss status and update the management plans, if necessary
- discuss strategies to expose project results to a broader community
- discuss strategies and actions to ensure the reuse and sustainability of the software
- identify bottlenecks and areas for improvement to ensure efficient work of the project team
- report financial status of the project (RSE hours left)
- brainstorm on further collaboration and funding options, if relevant
- brainstorm on the potential for cross project collaboration.

For **external projects**, review meetings are usually organized as part of the project process. Whether or not (a lightweight version of) our internal review procedure is needed for a project is determined by the **PM**, in consultation with the **Lead RSE**.

### 3.9.1 Review meeting preparation

The **PM** sends the LA team the standard review meeting presentation template [17], updating the slide on RSE hour status. This template provides a list of the important points to be discussed. LA and **Lead RSE** collaboratively prepare the slides. In particular,

	Stakeholder
<b>Prepared by:</b>	LA and <b>Lead RSE</b> of the project. Other stakeholders of the project can contribute.
<b>Reviewed by:</b>	<b>PM</b> accountable for project, <b>TL</b> accountable for technology.
<b>Target audience:</b>	<b>PMs, TLs</b> , SHs and RSEs.

- the LA adds 3-5 slides (can be separate from the template) to report concisely on the extent to which the research objectives of the project have been met. The LA is not expected to present the content of published papers or the original workplan or proposal;
- the **Lead RSE** prepares 1-2 slides on a status of the current technology plan and software, datasets, methods or/and documentation, and remarks on reusability, adoptability and sustainability of the software;
- the LA and **Lead RSE** compile the list of project deliverables. If applicable, the LA reports on the workshops;
- the **Lead RSE** compiles the technology status report (see Section 3.9.2) based on the input from LA and the rest of the project team, and provides it to the **TL**;
- the LA and **Lead RSE** point out any scientific or technological bottlenecks, e.g., approaches that did not work, data that was not collected, or any other reasons for delays in the workplan. To this end, the LA and **Lead RSE** comment if the project is on track or whether the planning needs to be revised;
- the **PM** reports on the financial status of the project (the number of hours already spent); and
- the entire project team is invited to comment on how the collaboration is going, in terms of interaction between the team members and suggestion for improvements, if there are any issues.

The **Lead RSE**:

- requests other project team members to contribute to the slides, wherever appropriate, and technology status report;
- meets with CM before the review meeting to draft the technology status report, and together with **TLs** to draft the rest of the report.
- coordinates with the entire project team to finish the preparation of the presentation at least 2 working days before the review meeting;
- ensures that output is correctly registered in systems described in the output management (Section 3.7.1) and all missing URLs and DOIs are added to the slides;
- uploads the slides to the project portfolio; and
- informs **PM** and **TL** that slides are ready and are in the project portfolio.

### 3.9.2 Technology status report

Prior to the annual review meeting, the **PM** asks **Lead RSE** to fill in the technology status report. This is a document containing an overview of the technical development of the project such as project RSD page with its deliverables, URLs to project plans, and information on quality and community involvement. The information provided by the **Lead RSE** (in collaboration with the project team) in this report serves as input for the **TL** at the project review meeting.

Two weeks prior to the review meeting, the **TL** should receive from the **Lead RSE** the filled-out form. Based on the final report the **TL** performs a code review or software health check, and ensures that the review results are shared with the eScience project team before the annual meeting. The **Lead RSE**, the **TL** and the **PM** can meet additionally to discuss the status report and/or the results prior to the annual review meeting.

The report and the review are archived by the **TL** in the project portfolio folder.

### 3.9.3 At the review meeting

The time breakdown of the meeting agenda is follows:

- presentation by the LA (max. 20 min)
- presentation by the **Lead RSE** (max. 20 min), including a description of RSE roles and project deliverables.
- discussion (max. 40 min)
- summary, action points and conclusions.

The **PM** chairs the meeting, acting as a reviewer together with the **TL**. The **TL** raises possible issues related to technology and software. Other invited stakeholders can comment and contribute to the discussions. The **PM** and **TL** comment on the status of the deliverables:

- have the objectives outlined in the proposal been sufficiently addressed? (**PM**)
- does the project follow the workplan in terms of deliverables? (**PM**)
- has the output been registered according to the rules of output management (Section 3.7.1)? (**PM, TL**)
- does all project output have publications (including software and data papers)? (**PM**)
- are there any issues flagged during the code review that needs to be discussed with the project team? (**TL**)
- does the project team sufficiently engage and align with relevant communities (e.g., via the workshops)? (**PM**)
- does the project adhere to the technology plan, SMP and DMP? (**TL**)

The eScience project team comments on any further possibilities for reusability, adoptability and sustainability of the software, and the project team comments on possible collaborations beyond the project.

The **PM** updates the slides with action points, agreements and plans (with the project partners agreement). The **PM** logs the meeting in the project log.

### 3.9.4 After the review meeting

**PM** shares the updated slide deck with the project team members to check the agreements written down. **PM** ensures that the final version of the presentation(s) uploaded to the project portfolio is correct.

## 3.10 Reporting

For call projects the annual review meeting and end report serve as formal progress reports.

**External projects** may require periodic reporting to the consortium on progress according to the workplan, including deliverables. The **PM** and **Lead RSE** consult the Consortium/Collaboration Agreement, the contract and the proposed workplan and involve **Finance** for the financial part of the report. Normally, the external project coordinator (e.g., EU project coordinator, NWO programme officer) signals the deadline of a deliverable or report. The **Lead RSE** contributes to the report on project activities required to be done by the eScience Center, and the **PM** checks the document. The **PM** asks **Finance** to check or fill in the financial part of the report, signed by the **DoO** if necessary. Once the final version is ready, the **PM** sends it to the external project coordinator (via EU portal done by **Finance**) and archives this report in the project portfolio.

### 3.11 Conflict resolution and complaint procedure

The eScience Center follows the Code of Conduct as outlined in the Personnel Policy (cf. [12] for the details).

All conflicts on projects involving the eScience Center RSEs and the LA and their team should be resolved using the following four-step process:

1. When problems arise in a project, the **Lead RSE** is expected to resolve problems in consultation with the LA. If needed, the **PM** can be asked to join in discussions on finding the best course of action;
2. Both RSEs and LA can escalate issues related to the project to the **PM** (preferably, via the **Lead RSE**). The **PM** organizes a meeting to discuss the problem and tries to resolve it;
3. If the problem remains unsolved, the RSEs or the LA can escalate it to the PD by sending a letter summarizing the situation to the accountable **PM**, who will forward it to the PD; and
4. The PD can escalate the problem to the DT.

If the problem is with the **PM**, RSEs can escalate to their manager (SH).

The eScience Center also has an external confidential advisor ('Vertrouwenspersoon') who can be contacted anonymously. See the Personnel Policy for details.

Resolving conflicts may result in changes to the project, such as changes in staffing or changes described in Section 2.5.

### 3.12 Non-RSE Consultants

Certain issues will require that the project team consults with other persons inside the eScience Center. The following situations require the team member to notify the **PM**, any actions may be delegated to any eScience team member:

- For project related GDPR issues, or personal identifiable data, consultation with the GDPR contact person is obligatory. For contacts, cf. GDPR section on the Intranet [15].
- For issues related to software or data accessibility and quality, contact the **TL**.
- For issues related to scientific integrity, contact the scientific integrity officer (cf. the Intranet page [15]).
- For issues related to SURF (use of their infrastructure or need of advisor), contact SURF liaisons. For contacts, see the intranet page [15].
- For issues around sustainability, contact the **TL** and CMs.
- For IP and licensing issues, contact **TLs** and the DoT (cf. Section 2.6.2).
- For legal matters, contact the **DoO** (cf. Section 2.8).
- For external opportunities, contact PD (cf. Section 3.14.3).

### 3.13 Changes to the project

During the project life cycle, the workplan may change substantially:

- New deliverables because of additional funding
- New workplan because of changes in the research goal and/or in the technology used
- Timeline, leading to a different end date.

Type of request	Decided by:
Budget requests within the <b>PM</b> mandate [15]	<b>PM</b> team
All requests regarding budget changes outside the <b>PM</b> mandate	DT (via PD)
Early termination	DT (and DT informs the Board)

Any of these changes needs explicit approval from the **PM** team or the DT.

For **external projects** changes to a project must be handled as described in the formal documents for this project (e.g., grant agreement, consortium agreement). If it is within the **PM** mandate, the **PM** discusses with the **PM** team any extensions required for the project. Otherwise, the decision is made by the DT. The **PM** informs the external funder or consortium of the decision.

### 3.13.1 Proposal changes request

The LA must submit a formal request to the **PM** team (by email via the **PM**, in PDF format, signed) containing:

- project title and project number
- requested change (e.g., time/dates, RSE hours, scientific goal) and motivation for this change
- conditions such as deliverables:
  - If there are new deliverables, what are those and what is the new planning?
  - If there are no new deliverables, that should be stated explicitly.
- any motivated budget change, such as
  - LA wants to increase their involvement
  - change in research personnel (if applicable in the case of older projects)
  - transfer from hardware costs to RSE contribution or PYR for research personnel on the LA side (or vice versa) (if applicable in the case of older projects)
  - any in-kind to cash change, or vice versa (including requests with the extra cash budget from the LA).
- any prior or planned inactivity on the project, such as
  - shortage of personnel on the LA side due to e.g. maternity leave, sick leave, hiring delays (for example, a PhD student or a postdoc needs to be hired but there is a concise timeline on the hiring procedure)
  - unavailability of RSEs
  - additional data that needs to be collected.
- any delay with the start date.

### 3.13.2 Processing the changes request and decision

Upon receipt of the request, the **PM** assesses if the request should be granted based on considerations such as

- whether the new objective is scientifically promising or technologically interesting? (if applicable)
- collaboration status with the LA;
- prior problems regarding the project;

- the benefit of continuing the project for the eScience Center (e.g., good wrap up of the collaboration, this leads to another funding opportunity together); and/ or
- availability of RSEs with relevant expertise to work on it.

The **PM** can consult with RSEs and the **TL** on whether the new planning is feasible, and with **Finance** for a budget remaining after necessary recalculation. In case of additional funding, the DT (via the PD) will decide, after a budget calculation by the **Finance** and approval by the **DoO**. Otherwise, the **PM** puts the request on the agenda for the next **PM** meeting, containing:

- the motivated request (uploaded to the project portfolio)
- the recommended action
- the prepared decision on the **PM** meeting agenda.

The **PM** team may request more information from the LA via the **PM** (and thus postpone the decision on the request). The LA can provide the new information via an additional PDF signed letter or as amendment to the original letter.

After the final decision, the **PM** notes the official decision in the decision document. If the request is not approved, the **PM** communicates this to the LA. If the request is approved, the **PM**

- communicates with **Finance**, which finalizes the extension (recalculation of project hour budget, changes in Exact, the extension letter for the LA, communication to the LA);
- double checks if budget and hours in Exact are still correct;
- communicates the extension to the **Lead RSE**.

The **Lead RSE** then

- communicates the extension to the project team;
- updates planning and adjusts staffing, if necessary;
- ensures website and RSD are updated (e.g., if dates or affiliation changed); and

If the request involves a DT decision, the **PM** submits a request formally through the PD.

### 3.13.3 Early project termination

Early project termination can be

- agreed on by mutual consent;
- initiated by the LA; and/ or
- initiated by the eScience Center.

In the first and the second case, the **PM** submits a letter (written together with and signed by the LA) explaining the situation to the DT. The letter should contain (a proposal for) an agreement on how to handle all the remaining resources of the project (RSE hours, cash contribution, FTE commitment for LA, workshops, software sustainability budget, etc.).

The **PM** can request the termination of a project if the conditions and agreements in the Awarding letter and Bijzondere voorwaarden have been violated by the LA or the project partners. The **PM** submits the letter to the DT (via the PD explaining the situation). If the DT approves the termination, the **PM** communicates this decision to **Finance**, which finalizes the process (by making changes in Exact and preparing a termination letter).

## 3.14 Opportunities beyond the project

A project team can explore different opportunities for ideas that stem from the project that go beyond its scope and/or budget. Appendix B summarizes the role of **PM** in such projects. The **PM** discusses these opportunities with the project team during the review meeting.

### 3.14.1 Increasing reusability (in this document called software sustainability)

For some projects, or entire calls, specific budget is available for software sustainability. Until 2020, each individual project was assigned a so-called Generalization budget (“Generalisatie”), for generalization and reuse of project results. Since 2020, however, this budget is no longer assigned per project, but for the entire programme/call. The **PM** and the **Lead RSE** check the corresponding call text and the awarding letter of the project to determine if the software sustainability budget is available.

The **PM** signals potential for reusability to the **TL**. The **TL** discusses this opportunity with the **Lead RSE** and if necessary, the **TL** team. If RSEs have an idea and are interested to work on a project funded by this budget, they may contact **TLs** or DoT for more information. The process follows the SS protocol [15].

### 3.14.2 Knowledge and Development

For the development of broad and deep knowledge on digital technologies and their application, RSEs can apply for so-called Knowledge and Development (KD) project. The process is described by the KD protocol [15].

### 3.14.3 External funding

The project team may decide to pursue other funding opportunities. The eScience Center encourages RSEs to pursue external funding opportunities to promote the organization profile as research organization. PD oversees the Acquisition activities and the process. The relevant information is available via Intranet [15].

### 3.14.4 Fellowship

To stimulate community engagement lasting longer than project lifetime, the eScience Center funds annual Fellowship Program [14]. The eScience project team is not eligible for this program, however, the LA and their team are.

## 4 Project closing

Project closing is the final phase of a project. In this phase the **Lead RSE** requests and previews the end report, the **PM** (with the help of **Finance**) processes the end report and accepts the project deliverables. Once the project is formally closed, RSEs can no longer write hours or work on this project.

### 4.1 Handling end report

All completed call projects at the eScience Center must have an end project report.

<b>Written by:</b>	the LA, assisted by the <b>Lead RSE</b> .
<b>Target audience:</b>	<b>PMs</b> , RSEs, Communications (layman summary), <b>Finance</b> (accountants), <b>TLs</b>
<b>Schedule:</b>	<ul style="list-style-type: none"><li>• written in last months of the project,</li><li>• submitted 3 months after the project end at latest,</li><li>• archived in the project portfolio.</li></ul>
<b>Approved by:</b>	The <b>PM</b> team and <b>Finance</b> .

For call projects, one month before the project end, the **Lead RSE** requests the LA to submit the scientific and financial end report ('Financieel en wetenschappelijk eindverslag'), providing the eScience Center template [17].

The RSEs provide necessary information to the LA to write the end report (deliverables via the RSD project page, other relevant information as a follow-up to the project, lessons learned, etc.). A complete end report contains:

- Public summary (written in English) with clearly stated objectives/results
- Challenges (the team encountered during the project)
- Opportunities (the work of the project led to)
- remarks on sustainability of project results and the latest version of the management plans
- a list of deliverables and project outcomes missing from the RSD project page (e.g., software, papers, presentations, pitch), including list of workshops (if applicable)
- information on the project workshops
- financial overview (if applicable)
- signature of the LA and date of signing (in case the **PM** cannot get the LA signature, a signature of financial or project manager would also be acceptable).

For collaborative call projects, the end report written by the LA and the **Lead RSE** for the other funding organization (e.g., NWO) is sufficient, if it contains all necessary information, covered by the bullet list above.

Before the formal closing of the project, the **Lead RSE**

- receives the signed end report from the LA (preferably, in PDF format)
- verifies the scientific part of the end report against the end report checklist. If needed, the **Lead RSE** asks the LA for additional information or corrections to the end report, before submitting it to the **PM**.
- ensures all missing project output is registered in the appropriate systems (see Section 3.7.1)
- archives the end report, the latest DMP and SMP, checklist in the respective project portfolio.



If the end report is satisfactory and all the aforementioned steps are completed, the **Lead RSE** submits it to the **PM** to get the project formally closed. The **PM** requests **Finance** to review the financial part of the report and either approve it or request corrections to it.

Projects that are funded by software sustainability budgets have their own procedure for end reports (see Appendix B.). The end report of these projects consists of output registered on the RSD project page and updated summary of the project.

For **external projects** the way a project is formally closed depends on the formal documentation for a project and requirements from the external funding organization. If an end report is required, the **Lead RSE** contributes to it (**PMs** can assist when needed), and care should be taken to reserve some time (and budget) during the project for this effort. **Finance** prepares the financial part of the report. The **Lead RSE** shares the final version of the end report written for the external party or funding organization (e.g., EU, NWO) with the **PM** and **Finance**, and archives it in the project portfolio. In any case, the **Lead RSE** ensures that the RSD project page is up-to-date (with complete deliverables and layman summary of the completed project).

**Finance** periodically sends a list of missing end reports to the **PM** team. If the end report is not submitted yet, the **PM** sends a reminder to the LA.

## 4.2 Formally closing the project

If both scientific and financial part of the end report is satisfactory, the **PM** puts decision to formally close project on the **PM** meeting agenda. After the formal decision<sup>11</sup>, the **PM** notifies the **TLs**, **Finance** and Communications (with the links to the documents). **Finance** handles the approved reports and formalities related to closing the project. This includes getting the final signature by **DoO** or Executive Director on the official letter for the LA about the project closing ('Afsluitingsbrief'), communicating it to the LA, and archiving the letter in the project portfolio.

The **PM** ensures that the project is marked as complete on the

- RSD: The **Lead RSE** updates the project page with the lay summary (from the end report), any missing meta-data (e-Infra use, keywords, deliverables, etc.) and sets the project status to 'Closed'.
- Corporate page: Communications may also request more information to promote the completion of the project through various channels, including but not limited to a news item, social media post, video and interview.
- Exact/Project portfolio: **Finance** closes the Exact project budget, uploads the official closing letter to the LA, as well as all appropriated documents.
- Gantt: The **PM** ensures that no one is assigned to the project in the future.

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<sup>11</sup> Formally recorded by the **PM** team, and thereafter ratified by the DT team (see more in [15]).

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# Appendices

## A Lead RSE role description

*This role description includes guidelines that need to be followed by RSEs fulfilling the role; they will be complemented by protocols.*

1. Role	<b>Lead RSE</b>
2. Place in the organization	Project
3. Contacts	<b>PMs</b> , project team RSEs, external project partners, <b>TLs</b> ,
4. Purpose	To carry responsibility for the day-to-day running of a research project at the eScience Center and act as main contact point for the project. Each project has one <b>Lead RSE</b> .
5. Main tasks & responsibilities	<ul style="list-style-type: none"> <li>• Coordinating day-to-day activities with other RSEs working on the project;</li> <li>• Carrying responsibility for agreements with the accountable <b>PM</b> on the division of tasks and the allocation of time within the project;</li> <li>• Making sure that activities, procedures and targets agreed upon are carried out and met on time;</li> <li>• Monitoring project progress, including project hour expenditure, and regularly reporting progress to the accountable <b>PM</b>;</li> <li>• Ensuring the presence of the accountable <b>PM</b> at all formal meetings;</li> <li>• Ensuring that general technological solutions are approved by the <b>PM</b> after due consultation of <b>TL</b>, and monitoring their implementation;</li> <li>• Ensuring that generalization and re-usability opportunities are implemented from the start of the project, after due consultation of <b>TL</b> and on approval of the accountable <b>PM</b>;</li> <li>• Solving everyday technical and managerial problems, and, if needed, communicating these to the <b>PM</b>;</li> <li>• Ensuring the visibility of the project through project demonstrators, slide decks and other means; and/or</li> <li>• Making sure all project output is properly released, documented and archived in the designated systems.</li> </ul>
6. Competencies	<ul style="list-style-type: none"> <li>• Negotiating</li> <li>• Communicating</li> <li>• Cooperating</li> <li>• Leading</li> <li>• Result orientation</li> <li>• Planning and organizing</li> </ul>
7. Available resources (budget, hours, training)	In project budget
8. How to get this role	<b>PM</b> assigns <b>Lead RSE</b> based on skills, experience, knowledge, interest and availability, after prior consultation of SH.

## B Role of PMs and others in external and Ambition 2 projects

This section focuses specifically on the role and involvement of the **PM** team in Fellowship, External, KD, SS and D&C projects.

### B.1 Fellowship projects

Funded by the Calls budget, the purpose and the organization of these projects are different from call projects. CMs are responsible for Fellowship projects, and a **PM** assigned by the **PM** team is advising them.

### B.2 External projects

#### 1. Acquisition

- The eScience Center employees signal an acquisition opportunity and must follow the policy for external funding and the process to ask for permission. The **PMs** must be consulted as part of this process.
- During this consultation, the **PM** needs to know about:
  - (estimate of) the work involved in person hours:
  - composition of the project team and whether the person submitting the proposal wants to be the **Lead RSE** themselves
  - timeline of the proposal/project
- The **PM** can advise the **Lead RSE** on the proposal. If this advice is negative or critical, the **PM** contacts the PD. If the **PM** thinks that additional (temporary) capacity is needed in case the project is granted, the **PM** contacts the relevant SH. Note: the planning cannot be made definitive at this stage.

#### 2. Preparation of project – call/subsidy projects

- The **Lead RSE** informs the PD, **Finance**, **PM**, SH and other relevant persons as soon as a granting confirmation has been received
- The PD, **Finance** and **Lead RSE** are involved in the preparation stage of the project such as grant and/or consortium agreements, starting documents, etc.
- The **PM** discusses the planning with the **Lead RSE** and other project team members and provides a planning in Gantic.

#### 3. Preparation of project – contract projects

- The **Lead RSE** and **Finance** are in charge of arranging the contract. The **Lead RSE** keeps the **PM** in the loop about starting dates
- The **PM** discusses the planning with the **Lead RSE** and other project team members and provides a planning in Gantic.

#### 4. During the project

- See project protocol for the relevant parts. The **PM** acts in consulting role and **Lead RSE** is accountable.

#### 5. Reporting

- See project protocol for the relevant parts. As described in Section 3.9, the **PM** must see/check the end report, the **Lead RSE** or the person who asked for the grant to be in charge of getting the financial report from **Finance** and to send it to the external coordinator.

#### 6. Closing of project

- **Lead RSE** informs **PM** of closing of project for funder or end of contract
- **PM** follows formal closing steps as described by Section 4.

### B.3 KD and SS projects

The process for KD and SS projects is fully described by the KD and SS protocols [15], respectively.

1. Call and selection
  - Follows the protocol
  - Upon granting, DoT (or **TLs**) gives **Finance** instructions (cc'ed to **PMs**) which projects are granted and need to be created in Exact.
2. Preparation of the project
  - The **PM** formally assigns **Lead RSE** and discusses the planning with the **Lead RSE** and other project team members and provides a planning in Gantt.
3. During the project
  - The **PM** is not directly involved in the project unless requested by **Lead RSE**.
4. Reporting
  - The extent of reporting is decided upon by DoT and **TLs**.
5. Closing of project
  - **Lead RSE** informs **PM** of closing of project
  - **PM** follows formal closing steps, as described in Section 4.

### B.4 D&C projects

D&C projects for external funding follow the same process as other external projects.

The process for the D&C projects for training and workshops is as follows:

- 1) Each year in October the training lead from the D&C team provides the SHs and **PMs** with an overview of the hours needed for training purposes including an estimate of the hours needed for externally funded trainings
- 2) SHs discuss a planning with RSEs that will be involved in training in the coming year. The total training hours should add up to the total number of hours needed for D&C projects. SHs communicate the planning to the **PMs** and to the training lead. **PMs** take the training planning into account in the projects planning.
  - a. If the progress on projects that RSE is planned on seems to be at risk by training activities, the **PM** signals this to the SH. Together they decide to either transfer the training hours to another RSE or to transfer the project to another RSE.
- 3) During the year
  - a. If an RSE exceeds their agreed upon training hours, the SH is responsible for discussing this issue with the RSE and taking appropriate measures.
  - b. If a project is (unexpectedly) progressing unsatisfactory due to the RSE involved in training, the **PM** discusses this with the SH and the RSE and takes appropriate measures.
  - c. If the request for externally funded trainings exceeds the estimate given for that year, the training lead contacts the **PMs** to discuss planning possibilities before agreeing to give this external training.

## C Example of the project log

### Running log for Project XXX

2022-03-12 Output: submitted paper

2022-02-02 Mr. X assigned as **Lead RSE**

2021-01-01 Kick-off meeting

Present – NLesC: AB (**PM**), AA (**Lead RSE**), AC (**TL**), AD (RSE)

Present – Team: FA (LA, TU Delft), PA (PhD student, TU Delft), RA (TU Delft)

Agreements:

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- sed do eiusmod tempor incididunt ut labore et dolore magna aliqua.
- Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris.

2021-02-10 SURF proposal granted

We received a grant (link) to infrastructure. We did not get Snellius access but were sent to Lisa as that also has enough harddrives.

2021-02-02 SURF infrastructure proposal

We submitted a proposal to SURF (talked to Henk). We decided to use Snellius as the harddrive in my laptop is too small.

### Project Start

	Date	Slides/Meeting notes/URLs?	Notes
Administrative Start meeting	2021-01-01		
Project Kick-off	2021-01-01		
Review1	2022-06-01		To plan final date
Review2			
Tech plan v1	2022-06-20	github.com/shico/techplan.rst	<b>TL</b> comments...
Paper			TODO: Add to RSD
Presentation		URL (to the project portfolio)	Uploaded to RSD and Zenodo

## D Examples of Technology Plan

### D.1 Technology plan for "Personalized cancer vaccine design through 3D modelling boosted geometric learning (3D-Vac)"

- 3D-Vac proposal

#### ❖ Task 0: Refactorization of `deeprankcore`

- **DONE (March-May 2022)**
- Such repository was initially a cloned version of [Deeprank-GNN](#), called `deeprank-gnn-2`.
- Partially rewrite `Deeprank-GNN`, making it:
  - A more object-oriented package.
  - Usable for unifying it with the original [deeprank](#).
  - Class diagram they used to implement such edits.

#### ❖ Task 1: Construction of databases for protein complexes and features on HDFS

- One eScience Research Engineer (0.2 FTE) with expertise in big data, HDFS and database (e.g., MySQL) will be responsible building a database hosting these data. LA and the PhD students at RU will be responsible generating 3D pMHC models and calculating various interface features. We together apply for the national computation resources at SURF-Sara. We will build on and extend `DeepRank(-GNN)`'s data generation module. Therefore, a small FTE from EG is likely needed.
- (EG): Evaluate and implement the use of the best HDFS filesystem to host our heterogenous data (making use of the national infrastructure at SURFSara).
  - **Expected: Q1 2022**
  - **DONE (March 2022)**
  - We decided to save the generated grids/graphs data (inputs for the neural networks) in `hdf5` files, being HDF Hierarchical Data Format. This was already implemented in the original code-base.
    - ★ Main pros
      - Designed to store large amounts of data in an organized manner (folder-like architecture)
      - Consist of *Datasets* that can store arrays of data, *Groups* which can store datasets or other groups, and *metadata* consisting of mapped key-value pairs for attributes of the data
      - Fastness: writing to HDF5 is 16 times faster than to a simple CSV file
      - Open-source
      - Pythonic interface: [h5py](#)

#### ❖ Task 2: Training, tuning and testing GNN on GPUs.

- One eScience Research Engineer (1.0 FTE) with expertise in deep learning will implement efficient scheme for generating graph and training of our designed graph network for 3D atom clouds. EG and RU together define UML (object relationship diagram) and determine the optimal graph aggregation steps for proteins. LA, the PhD students and postdocs will define optimal graphs, mapping the interface features to graphs, working with EG on deep learning implementation. RU team will conduct cross-validation over MHC allele types and benchmark 3D-Vac against state-of-the-arts.



- (EG & RU): Build DB4 - Generate interface graphs for DB2, map features in DB3 to graph nodes and edges.
  - **Expected: Q2-Q3 2022**
  - **ONGOING (July 2022 - ongoing)**
  - pMHCI
    - \* We generated DB4 (in the form of hdf5 files) for a small subset of data, the only one available at the time of writing (~7000 data points). We're waiting for the new data from RU side. Giulia is testing the data that the master student put on Snellius (~140000 data points).
- (EG & RU): Implement, train and optimize GNN for MHC epitope predictions.
  - **Expected: Q3-Q4 2022, Q1 2023**
  - **ONGOING (August 2022 - ongoing)**
  - pMHCI
    - \* We're waiting for the new data to be generated, but the scripts for training and saving/plotting results are ready and working ([link](#)). We already trained a small subset of the data, mentioned in the bullet point above.

### ❖ Task 3: Implementation and dissemination.

- *One eScience Research Engineer (0.8 FTE) with expertise in software development will integrate the resulting GNN into DeepRank. Our IT engineer (RU) will work together with EG to implement the web server and publish neoantigen database as part of the web service. The PhD students at RU will use 3D-Vac to scan human cancer proteomes and create neoantigen database. All members will work together in organizing workshops and write publications.*
- (EG): Integrate resulting GNNs into DeepRank.
  - **Expected: Q2-Q3 2023**
  - **TODO**
- (EG & RU): Develop the web server for epitope predictions.
  - **Expected: Q3-Q4 2023**
  - **TODO**
  - **Unrealistic, I would cut this out**
- (EG & RU): Use 3D-Vac to scan human cancer proteomes and build predicted neo-antigens into a database (DB6).
  - **Expected: Q3-Q4 2023, Q1 2024**
  - **TODO**
- (EG & RU): Organize workshops and work on publications.
  - **Expected: Q3-Q4 2023, Q1-Q2-Q3-Q4 2024**
  - **TODO**

### ❖ Deliverables

#### ➤ D1. Publications

- **Expected: 2023, 2024**
- **TODO**
- Publish our technology advances and discoveries in open-access journals and conference proceedings.
  - \* Two publications focusing on the science part led by our research group and targeting the user community

- \* Two focusing on the eScience technology part led by the e-science engineers and targeting the eScience communities.
- D2. Software and web server
  - Software for GNN-based data mining on 3D atom clouds with GPUs and MPI supports
    - \* **Expected: 2023**
    - \* **TODO**
  - DeepRank v2, a general GDL framework for data mining protein interfaces
    - \* **Expected: 2024**
    - \* **TODO**
  - 3D-Vac software for MHC epitope predictions (GitHub)
    - \* **Expected: 2024**
    - \* **TODO**
  - A web server for MHC epitope predictions (hosted at CMBI)
    - \* **Expected: 2024**
    - \* **TODO**
    - \* **Unrealistic, I would cut this out**
- D3. Databases
  - **Expected: 2024**
  - **TODO**
  - Neoantigen database (DB5)
- D4. Tutorials and documentation
  - **Expected: 2024**
  - **TODO**
  - Online tutorial describing the use of 3D-Vac to epitope predictions on the web server
  - Online documentation for DeepRank v2 (GitHub)
  - Online tutorial blogs on [Towards Data Science](#)
- D5. Workshops and conferences
  - **Expected: 2023, 2024**
  - **TODO**
    - a. Geometric deep learning for protein structures workshop
    - b. DeepRank v2 tutorial workshop (co-organize with the human genetics department at Radboudumc)
    - c. 3D-Vac tutorial workshop (co-organize with the cancer immunotherapy group at Radboudumc and Immuno company)

## Generalization budget

- **Generalization plan**
- **Task 1:** make the interface more flexible to attract new users (240 hours).
  - o The code was not suitable for users, the API functionality was limited and the documentation was extremely lacking.
  - o **ONGOING (November 2022 – ongoing)**
  - o [Generalization](#) kanban board
- **Task 2:** Integrate DeepRank classes and functions into [DeepRank-core](#) (160 h).

- Their API should be very similar and coherent and should give the user the possibility to choose among CNNs and GNNs with no difficulty, only changing the classes called.
  - i. Uniform DeepRank and DeepRank-core APIs, according to the modifications done in DeepRank-core during task 1. (100 h)
  - ii. Integrate DeepRank functions and classes in DeepRank-core. (60 h)
- **Task 3: Update documentation** accordingly. (100 h)
  - o Release to Read the Docs including automatic API reference. (20 h)
  - o Outward-facing classes and functions documentation in the codebase. (80 h)
- **Task 4: DeepRank-core package deployment.** (20 h)
  - o PyPI. (10 h)
  - o Anaconda. (10 h)
- **Task 5: Publish material for dissemination and outreach.**(140 h)
  - o A software paper (either SoftwareX or JOSS) on DeepRank-core. (80 h)
  - o Basic and advanced tutorials. (60 h)

## D.2 Technology plan for "Exchange of CO2 in tropical ecosystems unravelled (EXCITED)"

- **EXCITED proposal**

The goal of the EXCITED project is to create a dataset of temporally and spatially consistent CO2 emissions by natural ecosystems (i.e., the Net Ecosystem Exchange).

This dataset will be created from site-scale measurement data (Fluxnet), inverse model results (CarbonTracker), and the 'ERA5' global weather reanalysis product.

Besides the resulting dataset(s), we will also provide the trained model(s) and code.

### 1. Used technologies

The project will make extensive use of Python, due to its broad ecosystem of (netCDF) data processing and machine learning packages.

More specifically, we will make use of the following packages:

*Data intake/processing:*

- xarray
- dask
- flox (xarray+dask extension for fast groupby operation).

See <https://flox.readthedocs.io/en/latest/>.

With these packages, we will be able to efficiently load and process the data and use all computing cores, both on a local PC and HPC.

*Machine learning:*

- sklearn
- pycaret (for comparing performance of different ML models)
- Possibly LightGBM ("Light Gradient Boosting Machine" a decision tree model like XGBoost, but much faster). Mostly for performance reasons.

Additionally, we will make use of ONNX to be able to save and share the trained models in an open format.

Analysis and cooperation with the LA will be through Surf Research Cloud.

### 2. Technological outcomes

In the project we will develop an efficient and reproducible workflow to generate the following outcomes:

- A python workflow
  - which preprocesses input data, trains the ML model, as well as provide some useful plotting utilities to analyze the trained model
  - hosted on Github, Zenodo, and the RSD. If the workflow proves to be sufficiently reusable and generic, we can publish it as a package on pypi.
  - To ensure code quality, we will make use of testing, (static) code analysis and typing (i.e., pytest, black, ruff, mypy). Workflows will be added to Github Actions. We will guide the LA on these aspects as well, so they can maintain the code once the project is finished.

- The trained models in ONNX format, on Zenodo.
- The output datasets, where the model is applied on (global) ERA5 data. To be hosted on Zenodo.

### **3. Reusability and adoptability**

To allow others to (re)use the results, access to the datasets and models will be provided, and documentation will be created to guide the users.

If others want to reproduce the results, or train similar models, the methods will be available and documented as well.

The software and resulting models will be used by the Lead Applicant as a focus of their research in the coming years and will be used by their (MSc) students as well. To create a larger community of users a Lorenz workshop will be held, which will focus mostly on (potential) users of the resulting models/dataset.

## Index

**DoO**, 5, 9, 10, 15, 26, 27, 29, 32

**Finance**, 3, 5, 9, 10, 12, 15, 18, 19, 22, 26, 29, 31, 32, 36, 37

**Lead RSE**, 2–4, 6, 7, 9–14, 16–27, 29–32, 35–38

**PM**, 1–7, 9–32, 35–38

**TL**, 1, 4–7, 10, 11, 13, 14, 16, 17, 19, 20, 23–27, 29–32, 35, 37,  
38