

Horizon 2020 European Union funding for Research & Innovation

E-Infrastructures H2020-INFRAEDI-2018-1

INFRAEDI-02-2018: Centres of Excellence on HPC

EoCoE-II Energy Oriented Center of Excellence: toward exascale for energy

Grant Agreement Number: 824158

D6.6 Data Management Plan



Project and Deliverable Information Sheet

EoCoE-II	Project Ref:	EINFRA-824158
	Project Title:	Energy Oriented Center of Excellence:
		toward exascale for energy
	Project Website:	http://www.eocoe.eu
	Deliverable ID:	D6.6
	Deliverable Nature	Plan, report
	Dissemination Level*:	PU
	Contractual Date of delivery:	30/06/2021
	Actual Date of delivery	18/10/2022
	EC Project Officer	Matteo Mascagni

* - The dissemination levels are indicated as follows: PU – Public, CO – Confidential, only for members of the consortium (including the Commission Services) CL – Classified, as referred to in Commission Decision 2991/844/EC.

Document Control Sheet

Document	Title:	Data Management Plan
	ID:	D6.6
	Available at:	http://www.eocoe.eu
	Software Tool:	Microsoft Word
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	Reviewed by:	PEC, PSB

Document Keywords:

Data management; data accessibility, data security, FAIR data



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Executive Summary

This document defines the data management plan for digital contents generated from the EoCoE II project. We provide guidelines for preparation of DPMs with the examples for the energy-oriented communities supporting them in creation their own DMP for the scientific data. Different types of digital output are identified in the project, e.g deliverables, software and documentation and they are use to prepare example DPMs.

Acknowledgments

In case of PSNC the scientific/academic work is co-financed from financial resources for science in the years 2019 - 2022 granted for the realization of the international project co-financed by Polish Ministry of Science and Higher Education.(5057/H2020/19/2020/2)



1. Introduction

The Horizon Europe Model Grant Agreement requires that a data management plan (DMP) is established and regularly updated. EoCoE II project produce and maintain data that fall into the following categories

- 1. The data, including associated metadata, that is produced by simulation software and can be re-used by scientist to produce or validate knowledge.
- 2. Algorithms and tools that were developed during the project implementation
- 3. Deliverables, publications and another project documentation
- 4. The data, including associated metadata, needed to validate the results presented in scientific publications and information about tools and instruments at the disposal of the beneficiaries and necessary for validating the results

EoCoE-II does not provide a large and sustainable data infrastructure nor directly manage scientific data belonging to the first category, this is organized directly by the relevant scientific communities. However EoCoE-II has set up repositories for codes and publications that are accessible and will be continued after the project. This document provides the DMP for the above categories as well as guidelines with the example for the energy-oriented communities supporting them in creation their own DMP for the scientific data.

2. Data management plan

Data Management Plans (DMPs) are a key element of good data management. A DMP is a formal document that describes the data management life cycle, data preservation and metadata generation. As part of making research data findable, accessible, interoperable and re-usable (FAIR), a DMP should include information on:

- how research data is handled during and after the end of the project,
- what data will be collected, processed and/or generated,
- which methodology and standards will be applied,
- whether data will be shared/made open access,
- how data will be maintained and preserved.

It is highly recommended to prepare a data management plan before data are collected to ensure that data are in the correct format, organized well, and well annotated. DPM allows to increase research efficiency since consumers of the data might be able to easy understand and use well-annotated data.

Important component of a data management plan is data archiving and preservation to avoid loss of data and simplify reusage of data. The requirements for archiving and preservation can influence data formats used during collection and can simplify its future submission to a database. Preserved data are more relevant since they can be re-used and the data consumers can directly requests for data to the database, rather than address requests individually.



Following template has been proposed for the DMP. This template follows the format prescribed in the Horizon 2020 FAIR Data Management Plan (DMP) Template

3. FAIR Principle

The first formal proposal of the FAIR pinciples was published in [1].

The Four Basics of FAIR are :

- Findable i.e. discoverable with metadata, identifiable and locatable by means of a standard identification mechanism
- Accessible i.e. always available and obtainable; even if the data is restricted, the metadata is open
- Interoperable i.e. both syntactically parseable and semantically understandable, allowing data exchange and reuse between researchers, institutions, organisations or countries
- Reusable i.e. sufficiently described and shared with the least restrictive licences, allowing the widest reuse possible and the least cumbersome integration with other data sources.

The more detailed description of FAIR principles can be found in [2]

The FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals.

The FAIR Principles do not define readily implementable procedures, and the practicalities of their implementation and application can be different in different disciplines. However, by making their inclusion a main requirement of the Framework, better reusability across disciplines is encouraged. DMPs should take into consideration that data reuse will not be restricted to users from within a community or discipline; and that different interpretations and implementations of the FAIR Principles exist

4. ARGOS – DMP preparation and management tool

It is recommended to use ARGOS (argos.openaire.eu) for preparing Data Management Plan. The description below comes from ARGOS documentation [5].

Argos is an open and collaborative platform developed by OpenAIRE to facilitate activities concerning the implementation of Data Management Plans. It uses OpenAIRE guides created by the Research Data Managament Task Force to familiarize users with basic RDM concepts and guide them throughout the process of describing their data. By using Argos, researchers and students are able to create their DMPs in collaboration with other colleagues, learn basic RDM concepts throughout the process and publish DMPs as outputs in an open and FAIR manner, among other things by assigning DOIs and licenses and by maintaining DMPs as living documents through versioning.



Argos consists of two main functionalities: DMPs and Datasets. DMPs include vital information about the research project on behalf of which the DMP is created accompanied with more in depth information about the management, handling and curation of datasets collected, produced or reused during the research lifetime. Datasets hold answers to set up questions from templates that support the creation of descriptions of how data are / have been handled, managed and curated throughout the research data lifecycle. A DMP in Argos may consist of one or more datasets. That way datasets are provided with the flexibility to be described separately, following different templates per type of dataset or research community concerned each time, also possible to be copied and used in multiple DMPs. Datasets are then bundled up in a DMP and can be shared more broadly. Special attention is given to the handling of data that are being re-used.

Preparing DMP Dataset is just filling an online form that consists of questions defined in DMP template. One of the available templates is HORIZON 2020 and this template seems to be suitable for most research activities. It is also possible to user another template tailored to the specific funder or organisation requirements.

The Horizon 2020 Template consists of 7 section:

Data summary- the general information about dataset

Reused Data - if there are any reused data

FAIR Data - This section concerns the FAIR principles and how they are planned to be accomplished.

Allocation of resources - This section concerns the cost of data management. It can include for example potential use of proprietary services and tools or extra effort needed to perform specific tasks or even to develop tools from scratch.

Security – provides information about a security of data

Ethical aspects – concerns handling of sensitive and personal data

Other - If there are other used procedures for data management.

The complete template is included as Attachment 1

5. Data sets for EoCoE II projects

He goal of the task 6.4b was to prepare expertise and provide advises, guidelines and best practices to all its partners and to the energy community at large. Therefore it was not intended to prepare DMP for all data produced during the project, but rather to provide examples how the DMP should look like. Several DPMs were prepared conserning different data types wich different specific.



The DMP Datasets prepared are:

EoCoE-II Web Page

The EoCoE website (https://www.eocoe.eu/) stores little data per se, as it is used as a global advertisement page. It does point to external sources for additional, project-related materials. Publications are linked via OpenAire, videos and visual material are linked through the EoCoE YouTube channel, job offers via the institution publishing them, etc..

Individual contact details that appear on the website, through the "<u>People @ EoCoE</u>" page, were collected on a discretionary basis, using the project human resources listings. Partners who no longer wish to appear on the project's website can be removed with a simple email request to the project's management team.

EoCoE-II Training Materials

EoCoE training materials, whenever possible and upon written agreement of the training's provider, is recorded and made available on the EoCoE YouTube channel. Videos are public and under <u>Creative</u> <u>Common</u> license.

EoCoE-II Project Deliverables

EoCoE deliverables are stored on the European Commission's database. Public deliverables, as defined in the Grant Agreement, will also be made publicly available on the EoCoE website when the project is concluded and deliverables are approved by the European Commision's evaluation.

EoCoE-II WP4 Software

This dataset concerns is an example DPM for managing software codes. In this case it is result of WP4 workpackage and describes the I/O and data handling related software packages developed or extended by WP4 in the context of EoCoE II.

The dataset covers the work on:

- Additions and overall work on the PDI data interface (PDI)
- Additions to the Fault Tolerance Interface (FTI)
- The IME integration into SIONlib

EoCoE-II WP1 Materials simulations data

The simulation or engineering data are outside the scope of this project, for those there are mostly well-established mechanisms within the participating research centers and it is not proposed to change these procedures. However, the presented guidelines can improve the existing processes procedures or description. As an example we have prepared DMP for materials data. This approach should be followed by all researchers that uses EoCoE-II simulation software and manage the simulation output data.

This Dataset describes the output data from materials simulations.

Atomistic codes have been used to simulate electronic and tranport properties of silicon heterojunctions, molecular dynamics of solvents and electrodes in capacitive blue energy and



thermo-electrochemical devices, and the simulation of doped organic semiconductors and halide perovskites.

6. Practices of data management in EoCoE-II

As it was mentioned earlier there is no scientific data managed by the project. Nevertheless some data was produced during the project realisation and as any other data they should be treated according to FAIR principles. Standard services, tools and format are used to simplify information access and exchange. Below we present the means and tools used in EoCoE-II to fulfil FAIR requirements. Example DPM are attached to this deliverable with more detailed description.

Software codes

Software codes are stored in GIT repositories. Gitlab is the commonly used tool for maintaining and sharing of sources codes, especially in multideveloper projects. Each software module is stored in separate repository and the administrators of the repository are data managers for this dataset. Using gitlab ensures that data will be available after the project finished. Gitlab repositories configured with public access are widely accessible and can be reused by developers of derivative projects.

WebSite

The information is shared in the form of typical HTML pages divided into thematic blocks, e.g. project information, news, application descriptions. The manager of website is the leader of task WP6.1.

Access to the EoCoE-II webpages is public and unrestricted. Search mechanism is implemented. All pages are indexed by search engines, therefore information is easily findable by external services like Google or Bing.

Project documents

All internal project documents are stored in OnlyOfice service provided by ENEA

<u>https://eocoe.workplace.garr.it/.</u> According to grant agreements the repository will be maintained at least 5 year after the project finishes. Standard open document formats are used to store and share information. The manager of data is the EoCoE Project Office. Access to the data is limited to project consortium, unless the specific dataset is configured with public access.

Training materials

Training sessions are recorded as video materials and are published on youtube. This form of sharing training materials is chosen because youtu.be is the most popular service for sharing videos and has significant number of users. Access to EoCoE materials is public and free. The manager of the training material data is the Project Office, which is also the owner of youtube account.



Publications

As it was agreed in project grant agreement, all publications should be stored in OpenAIRE - a pan-European research information system, which provides services to find, store, link and analyse research output from all disciplines. Using OpenAIRE guarantees the wide distribution of EoCoE-II related publications. OpenAIRE publication database is searchable by authors, title, project and DOI.

The list of EoCoE-II related publications is not a typical dataset, it is just a subset of OpenAIRE publications database filtered by project. Therefore there is no typical data manager for it. Nevertheless the list of OpenAIRE publication is supervised but he Project Office and the reference to EoCoE-II related publications i included in the project webpage.

7. Recommendations for data management

There is a lot of guidelines about creation good Data Management Plan. E.g. [3][4] Below is the brief set of recommendation for Data Management Plan in EoCoE community.

- Everything produced in scientific research or in the course of project implementation should be treated as data. It includes software, sensor data, simulation results, documentation, web page etc.
- Always produce DMP for your data. Even if its management seems to be simple and straightforward
- Assign Data Manager for each dataset. In many case it is sensible and practical to define roles and responsibilities, e.g. quality assurance manager, backup managers, system administrator, etc.
- Prepare quality control procedures (e.g. who and when can modify data, update documentation or indexes when codes/data changed)
- Consider including considerable details in your DPM, e.g. about format description, file organization, naming convention, data processing instructions, etc. It could prevent knowledge loss when a key team member lefts and someone else had to take over their data management responsibilities.
- Think in advance about preservation and sharing of the data. It can influence the procedures and formats used for data creation. Take into account the size of data and the cost of storing and management of data, including security, backup and recovery plans.
- Plan how the data will be accessible after the research financing is finished.
- Use your Data Management Plan. Make sure that it is known the people involved in creating and processing data and to all potential data consumers
- Review the DMP periodically and check if data creation and management procedures comply with it.
- All data used to achieve results described in scientific paper must be preserved. It must be possible to reproduce the results using the same method, input data and software.

In some cases it is not possible to ensure open access to specific parts of research data or the research process could be jeopardised by making those specific parts of the research data openly accessible. In this case, the data management plan must contain the reasons for not giving access.



8. References:

[1] Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3**, 160018 (2016). <u>https://doi.org/10.1038/sdata.2016.18</u>

[2] GO FAIR Initiative, FAIR Principles, <u>https://www.go-fair.org/fair-principles/</u>

[3] William K. Michener, Ten Simple Rules for Creating a Good Data Management Plan, Published: October 22, 2015, <u>https://doi.org/10.1371/journal.pcbi.1004525</u>

[4] Guidance Document Presenting a Framework for Discipline-specific Research Data Management, DOI: 10.5281/zenodo.4925906

[5] ARGOS users guide: <u>https://argos.openaire.eu/user-guide</u>



Appendix 1 Horizon 2020 DMP template

1. DATA SUMMARY

WHAT IS THE PURPOSE OF THE DATA COLLECTION/GENERATION AND ITS RELATION TO THE OBJECTIVES OF THE PROJECT?

Data collection is usually at the beginning stages of research data management lifecycles to set the background of what is needed (data generation), what is already there (data reuse) and how to best use it to fulfill the project's objectives (why). Here you may add information about the scope and objectives of your data collection process.

WHAT ARE THE TYPES OF THE DESCRIBED GENERATED/COLLECTED DATA?

The main distinction between data types is between primary data and secondary data. Data collection may contain both primary and secondary data depending on the source where they have been derived from. Primary data is data that have been collected for the first time and have not undergone through data processing and/or analysis, yet. Secondary data is data that have been cleaned up, analysed and shared by others (published or unpublished) and they are those that are being typically reused. In addition, types of data unveil how they have been collected so they also depend on the process that led to their generation.

WHAT ARE THE FORMATS OF THE DESCRIBED GENERATED/COLLECTED DATA?

Data may be found in different formats. Usually, outputs of specific instruments/ services/ tools where data are generated and/ or processed have a default way of exposing their outputs following specific standards. Most common distinctions between formats are proprietary and non proprietary formats, because they may impact data access in the long-term.

WHAT IS THE ORIGIN OF THE DESCRIBED DATA?

WHAT IS THE EXPECTED SIZE OF THE DESCRIBED DATA?

Give measurable examples per type of output based on common practices in the field. These might be relevant to the volumes of data and how many bytes of storage they occupy, numbers of objects, files, rows, and columns.

TO WHOM MIGHT IT BE USEFUL ('DATA UTILITY')?

Data generated or reused in the project can be useful for a number of stakeholders and third parties. Think about the target audience of your research, but also about possible third parties who could further exploit this data even after the project ends.



2. REUSED DATA

ARE YOU RE-USING THE DESCRIBED DATA AND HOW?

Apart from data produced within your research, you might want to repurpose data that have been produced and shared by others, in different research context.

WHERE DO THE DESCRIBED DATA RESIDE?

WHICH DATA WILL BE RE-USED?

3. FAIR DATA

In general terms, your research data should be 'FAIR', that is findable, accessible, interoperable and re-usable. These principles precede implementation choices and do not necessarily suggest any specific technology, standard, or implementation-solution. This template is not intended as a strict technical implementation of the FAIR principles, it is rather inspired by FAIR as a general concept. Achieving FAIR data relies equally on the choices you make throughout a research process, but also on providers whose services enable FAIRness of data to be met.

Learn more about the FAIR principles: <u>https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4792175/</u>

Learn how you can comply with FAIR principles: <u>https://www.openaire.eu/how-to-make-your-data-fair</u>

MAKING DATA FINDABLE, INCLUDING PROVISIONS FOR METADATA

Data are findable when described with metadata and vocabularies in a standardized way, assigned a Persistent Identifiers (PIDs) and are registered or indexed in a searchable resource.

Will you use metadata to describe the data?

Metadata is data about data and is an essential set of information describing scientific outputs, in the form of either physical or digital objects, in a machine-readable format. According to the expected use, metadata can be given different attributes. Most common type which enables discovery and identification are descriptive metadata. Descriptive metadata contain information about key aspects needed to search for and successfully find a given scientific output, e.g. by its title, author/creator, abstract, keywords. Moreover, metadata may be used for describing a service or a scientific instrument.

Will your metadata use standardised vocabularies?

Standardised vocabularies enable greater interoperability across systems. There are generic and discipline specific metadata standards which have been compiled so as to contain vital information that enable exchange while taking into consideration specificities of work and demands in different disciplines, even in different areas of work within a discipline.

Will you make the metadata available free-of-charge?

You could offer your metadata records free of charge or assign them small fees. However, charging for metadata sharing would limit access and use. Please check your funder's policy before deciding how and when to share metadata.



Will your metadata be harvestable?

Usually, this is facilitated by services that apply standard protocols for information exchange. For example, in repositories, metadata exchange is supported by the OAI-PMH protocol.

Will you use naming conventions for your data?

Naming conventions used throughout the management process, such as file names or data entities, should be clearly described in order to make data understandable by other researchers who may reuse them after the project ends.

Will you provide clear version numbers for your data?

Versioning may be a built-in functionality, subject to an instrument/service/tool that has been used for data processing and analysis which automatically produces versioned data. In other occasions, you will need to keep track and adapt to a versioning mechanism for your data. Here you should state how versioning takes place.

Will you provide persistent identifiers for the described data?

Persistent and/or Permanent Identifiers (PIDs) uniquely identify objects, people, organisations and activities and can ensure that the scientific output is accessible even when the URL of the website has changed. PIDs can be assigned to research outputs including publications, data and software/code. PIDs can also be assigned to researchers, samples, organisations and projects. A PID may be connected to a metadata record describing an item rather than the item itself. PIDs are usually provided by data repositories and other deposit platforms. Re3data (https://www.re3data.org/) includes tags to show which platforms that it indexes assign PIDs to their content.

Persistent identifiers

A persistent identifier or PID is a long-lasting reference to a resource. Whatever resource it refers to, the primary purpose of the PID is to provide the information required to reliably identify, verify and locate it. A PID may be connected to a set of metadata describing an item rather than to the item itself.

Will you provide searchable metadata for the described data?

Searchable metadata are metadata indexed by search engines and are identifiable by web crawlers.

What services will you use to provide searchable metadata?

Will you use standardised formats for the described data?

Different types of data are acquired, processed and stored (preserved and/or archived) in different ways and can be discipline specific. Many proprietary file formats are "containers" for standard file formats. By packaging them into these containers, a software and/or hardware developer can provide additional functionality, usually by streamlining a process, to analyse data acquired on their platform. However, this has the negative consequence of making these data less interoperable.



Provide information about used standardised formats

Please describe the formats you plan to store the described data in, including any URLs to documentation.

Please describe the formats you plan to store the described data in, including any URLs to documentation.

Are the file formats you will use open?

Open file formats provide the software specifications to anyone for free and enable re-use. Examples: .png, .xml, .rtf, .wav

Please provide more details if data are not in an open format.

Closed file formats are intertwined with proprietary formats that either do not provide access to software specification as opposed to open or despite the fact that they do, they limit re-use by others. Examples: .doc, .jpeg, .mp3

Please provide more details if data are not in an open format.

Closed file formats are intertwined with proprietary formats that either do not provide access to software specification as opposed to open or despite the fact that they do, they limit re-use by others. Examples: .doc, .jpeg, .mp3

Do supported open-source tools exist for accessing the data?

Please provide the name and type of datasets that require the use of proprietary tools to be accessed.

Please describe if data require proprietary tools to access the data.

Will you provide metadata describing the quality of the data?

MAKING DATA OPENLY ACCESSIBLE

Not all data can be made publicly open, hence data can be FAIR but not open, or open but not FAIR or both FAIR and open. Data are accessible when uploaded in a data repository and retrieved by their PIDs. When data can not be shared openly, metadata should be provided (even when the data are no longer available). In the case of sensitive or personal data, anonymization or pseudonymization and specific access rights can be applied. Where accessing data requires the use of complementary methods or tools, such procedures should be documented.

Are there ethical or legal issues that can impact sharing the described data?

It is possible that data are sensitive, such as personal or confidential, and hence they can not be shared directly to others. For those types of data, specific processes need to be made in order to ensure their reliable exchange in the short and long-term.

Will the described data be openly accessible?

How will the data be made available?

A data repository, otherwise known as a data archive, is an online collection of datasets that are described and classified in a standard way that makes data discovery and retrieval easier to be performed by both humans and machines.



Is the storage sufficiently secure for the data and does the storage provide backup and recovery procedures?

To learn more about best practices for back up and data security, you may have a look https://www.openaire.eu/raw-data-backup-and-versioning and https://www.openaire.eu/raw-data-backup-and-versioning and https://www.openaire.eu/raw-data-backup-and-versioning and https://www.uu.nl/en/research-data-management/guides/storing-and-preserving-data

Are there any methods or tools required to access the described data?

Describe processes needed to query and access data. These might be relevant to SPARQL access points, visualizer software, download, etc. Data access controls, such as passwords or firewalls, should be used to limit access to confidential data and protect them from unauthorised changes.

Please provide information about the method(s) needed to access the data

Please provide information about the tools needed to access the data.

Will you also make auxiliary data that may be of interest to researchers available?

Auxiliary data are supplementary to the product generation data; data that come from an external source and not from direct instrument measures, but are used in the context of a study.

MAKING DATA INTEROPERABLE

Data are interoperable, meaning they can be easily understood and shared with other platforms and systems, when they are created using standard vocabularies and include references to other data and metadata.

Will you use a controlled vocabulary for the described data?

Controlled vocabularies provide standard terminology as opposed to keywords or tags used to classify information. Examples: taxonomies, ontologies, thesauri

Will you provide a mapping to more commonly used ontologies?

INCREASE DATA REUSE

Data can be reused when the conditions about how others can make use of the data are welldescribed following community-standards and are communicated as specified by the owners. Such information can be found in licenses attributed to data and in references about the data provenance.

When do you plan to make the described data available for reuse?

Please specify how long after the project has ended the data will be made available Please check with funders' or institutions's policies which might apply an embargo on data access.

What internationally recognised licence(s) will you use for the described data?

There are a number of licenses that can be assigned to your research outputs. There are different licenses for software and for publications and data. For the latter, a common practice is the use of Creative Commons licenses which are machine readable.

Do you have documented procedures for quality assurance of the described data?

Quality assurance procedures are closely related to RDM and are meant to validate that data are clean (no duplicates or inconsistencies), error-free, well structured and represented in analysis. Quality assurance checks can be facilitated by the use of tools or scripts.



Describe the data quality assurance processes

Will you provide any support for data reuse?

How long do you intend to support data reuse?

4. ALLOCATION OF RESOURCES

Data management can be costly, especially when its planning hasn't been sufficient from the very beginning of the research process. Costing of data management includes for example potential use of proprietary services and tools or extra effort needed to perform specific tasks or even to develop tools from scratch.

HOW WILL THE COST OF MAKING THE DESCRIBED DATA FINDABLE, ACCESSIBLE, INTEROPERABLE AND REUSABLE BE COVERED?

Research Data Management is not a costless procedure, so it is important that it is thought through at the planning stage of research.

WILL YOU IDENTIFY A DATA MANAGER TO MANAGE THE DESCRIBED DATA? IF NOT WHO WILL BE RESPONSIBLE FOR THE MANAGEMENT OF THE DATA?

Identify the people or roles that will be responsible for the management of the described data Provide names and responsibilities of researchers' or data managers' data management and stewardship activities that are performed throughout the project. Follow the research data management lifecycle to guide your steps in data capture, metadata production, data quality, storage and backup, data archiving, and data sharing.

HOW DO YOU INTEND TO ENSURE DATA REUSE AFTER YOUR PROJECT FINISHES?

Despite where data are stored for everyday activities during the project lifetime, there are certain options to choose from data storage that ensures reuse in the log run. Most popular are data archives, otherwise found as repositories. Depending of data volume, archiving might be subject to small fees.

5. DATA SECURITY

WHERE DO YOU PLAN TO KEEP THE DESCRIBED DATA?



6. ETHICAL ASPECTS

ARE THERE ANY ETHICAL OR LEGAL ISSUES THAT CAN HAVE AN IMPACT ON DATA SHARING?

ARE THE DESCRIBED DATA SENSITIVE?

ARE THE DESCRIBED DATA PERSONAL?

WHAT ARE THE METHODS USED FOR PROCESSING SENSITIVE/PERSONAL DATA?

7. OTHER

Do you make use of other procedures for data management?

Please check: <u>https://www.scienceeurope.org/our-resources/guidance-document-presenting-a-framework-for-discipline-specific-research-data-management , https://www.dtls.nl/fair-data/research-data-management-knowledge-tools/</u>