

DOKU User Guide

(Version 1.4)

Long Term Archive (LTA) group

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Contents

1	Introduction	2
1.1	Submission Steps	2
2	Check Permission and Quota	2
3	Initial Contact	3
4	Data Preparation	3
4.1	Data Format	3
4.2	File Size	3
4.3	Directory and Dataset Structure	4
4.4	Labeling of Files and Directories	4
5	Submission of Metadata – MetaXA Guide	5
5.1	Person	5
5.2	DOKU-Dataset Group	6
5.3	DOKU-Dataset	6
5.4	Additional Info	7
5.5	Citation / Reference	7
5.6	Finalize Entries	7
6	Final Check	8
7	How to cite your data	8
7.1	PIDs for DOKU-Datasets	8
	Appendix A: Description of MetaXA fields	9
	Appendix B: License	15
B.1	Creative Commons Licenses	15
	Appendix C: Hierarchy Structure Description	16
C.1	Nomenclature	17

1 Introduction

DOKU offers long-term archiving for Earth System data and climate-related products. It is hosted by the German Climate Computing Center (DKRZ) in Hamburg and is maintained by its Data Management (DM) department.

DOKU is a service that is only available for DKRZ HPC (high performance computing) projects with a quota for long-term archiving. In comparison to WDCC, DOKU is the simpler solution to preserve your research data while still meeting the requirements of good scientific practice.

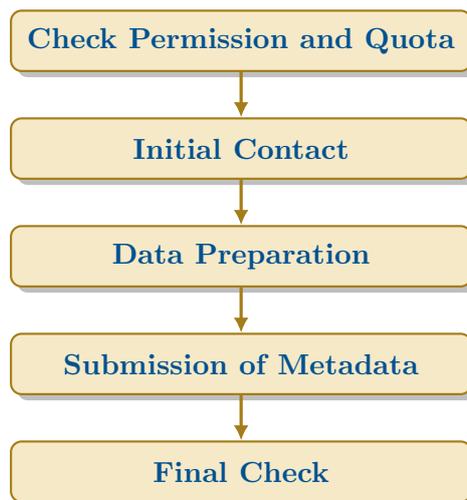
This document supports the DOKU Step-by-Step Guide (https://www.wdc-climate.de/WDCC/ui/ceraresearch/info?site=guide_doku) and aims at guiding users through the process of archiving data in DOKU.

1.1 Submission Steps

DKRZ's Data Management (DM) will support you, starting from your initial intent to long-term archive data until they are completely archived in DOKU.

Before you start the submission process in DOKU, please make sure that you have the authorization to publish the data.

In DOKU the submission process includes the following steps, which are described in detail in the remainder of this document:



2 Check Permission and Quota

Only data that is part of a DKRZ project can be archived in DOKU. Before the archiving process is started, you therefore need to make sure that your data belongs to a project that requested and was granted quota for DOKU.

For that log in to <https://luv.dkrz.de> with your DKRZ username and password. Under “Projects” all projects that you are a member of are listed. By clicking on the correct project all current allocations are listed. For DOKU the quota for “Archive long term” is of importance.

If you find on luv that you have quota for DOKU in your project remaining (and have discussed in your group/with your PI that you may use it), you can start the archiving process.

General information about resource allocation and how to apply for it (including DOKU quota) at DKRZ can be found here: https://docs.dkrz.de/doc/getting_started/resource-allocation.html#resource-allocation.

Please be aware that the data archival process might take some time and quota is accounted for the allocation period when the data is actually archived – not when you send the first request. Especially at the end of the allocation periods (e.g. at the end of the year) many DOKU archival requests come at the same time and thus data archival might take even longer. Please plan enough time for your DOKU request to get processed, so that quota from the current allocation period can still be used. Also please keep in mind that larger requests take longer time.

3 Initial Contact

Whenever you wish to archive data in the DOKU, please get in contact with DKRZ Data Management (DM) by writing an email to data@wdc-climate.de. In this email state the project (DKRZ account number) you would like to archive data under and the amount of data (approximate number of files and size).

Your first email to data@wdc-climate.de will open a ticket in a request tracker. DM will contact you shortly with further instructions. Please do not write a new email, but only answer to this thread. Otherwise a new ticket would be opened.

4 Data Preparation

Please prepare your data files for submission. In the following, you can check what to take into consideration.

Most importantly you need to structure and document your data in a way that reusability is ensured even in years' time.

4.1 Data Format

Only open source data formats are accepted in DOKU. The preferred file format for archiving is NetCDF (Network Common Data Format). More information on NetCDF can be found at <https://www.unidata.ucar.edu/software/netcdf/>.

Other supported data formats are for example GRIB (GRIdded Binary), CSV, and ASCII. However, in many cases it might be sensible to create tar-bundles from your files.

4.2 File Size

The preferred file size is 10 GB to 100 GB. There is no lower limit, but small files are not optimal for tape storage and each file smaller than 1 GB will be charged 1 GB of quota. It also takes longer to archive many small files than a few larger files. Therefore, it is recommended to pack small files into tar-bundles. Files larger than 100 GB are possible. Even a file of a size of a few TB could be possible, but it is highly recommended not to exceed 200 GB. (If you have files larger than 200 GB, please note that your DOKU request might take much longer to process.)

4.3 Directory and Dataset Structure

While preparing your data, please keep the following limits in mind:

- The upper limit of files per DOKU-Dataset is 500 (but fewer files are preferred).
- The total size of all files per DOKU-Dataset should not exceed 5TB (but smaller total sizes are preferred).

In case of questions about these limits, please contact DM.

For each DOKU-Dataset please create a subdirectory in your project space on Levante or in the tape archive (see sections 4.3.1 and 4.3.2 for further details). These subdirectories should contain all files to be archived, but nothing else (everything in these subdirectories will be archived!). Except for the first part of the path (`/<arch or work>/<your DKRZ project account number>/<your DKRZ user number>...`) you may choose any path. But please be aware that the entire path will be kept in `/doku`. For example

```
/arch/bm0000/path/to/your/data/<name_of_first_dataset>/ will become  
/doku/bm0000/DKRZ_LTA_0000_ds00001/path/to/your/data/<name_of_first_dataset>/.
```

Your data may be archived directly from Levante disk (`/work`) or from the tape archive (`/arch`). If your data is not already archived on tape, we recommend archiving from Levante disk.

4.3.1 Data located directly on Levante

If your data is located on Levante, please make sure it is in the correct DKRZ project directory. The paths will look like this:

```
/work/bm0000/x123456/path/to/your/data/<name_of_first_dataset>/,  
/work/bm0000/x123456/path/to/your/data/<name_of_second_dataset>/, ...
```

Please note that during your archival request (until your data is completely archived) the files must not be touched anymore (if necessary contact DM first) and the files need to be globally readable. Once your data is completely archived, you may change permissions again or even delete them from Levante.

4.3.2 Data located in the tape archive (`/arch`)

If your data is already archived in `/arch`, you do not need to transfer it to Levante. We can archive it in `/doku` directly from `/arch`. However, please note that it still needs to be sorted according to the DOKU-Dataset structure and needs to be located in `/arch` under the correct DKRZ project directory. The paths will look like this:

```
/arch/bm0000/x123456/path/to/your/data/<name_of_first_dataset>/,  
/arch/bm0000/x123456/path/to/your/data/<name_of_second_dataset>/, ...
```

Please note that once you have provided DM with the location of the data, the files must not be touched anymore (if necessary contact DM first). After the data is completely archived, the files will only be located on `/doku` and will be removed from `/arch`.

Further documentation on how to use the tape archive is provided here: https://docs.dkrz.de/doc/datastorage/hsm/man_pages.html

4.4 Labeling of Files and Directories

Files should be labeled in a consistent manner. Special characters and spaces in directory and file names should be avoided. The file names have to be unique (even if spread over multiple

directories). Please also take care that the file names describe the content, so that others are able to “read” the names.

Once your data is located in /work or /arch in the correct subdirectories, please write to DM with the following information:

- the data path for each DOKU-Dataset
- the number of files for each DOKU-Dataset
- the approximate size for each DOKU-Dataset

With this information, DM can start the process of data filling.

5 Submission of Metadata – MetaXA Guide

The metadata belonging to your data can be entered via the graphical user interface, MetaXA (<https://www.wdc-climate.de/metaXA>). Before you can use this application, you need an WDCC account. If you do not have one already, please apply for an account here: <https://www.wdc-climate.de/WDCC/ui/ceraresearch/register>.

Alternatively, DKRZ users can also login with their DKRZ credentials (DKRZ username and password). Please press “Switch to DKRZ login”, if you want to do this.

In MetaXA you can enter metadata for DOKU-Datasets. Furthermore, you can add (or edit) a Person, add a DOKU-Dataset Group, an Additional Info, or a Citation/Reference. These elements will be explained in the following paragraphs in the order in which they appear in MetaXA.

Only marked fields are required, but try to fill out as many details as possible. Help texts are available directly in MetaXA (via the little ?) and more details for each field are given here in Appendix A in the respective tables.

5.1 Person

Please start with the Person entry. Here you should enter all persons relevant to your data (e.g. all authors who should be listed in the citation). Via the search form you can check if the person in question is already listed. Please do so to avoid duplicate entries. If you find the person in the database, check if all information is still correct. Make corrections, if necessary.

If you cannot find the person, click the button “Add new person”. Please enter the personal details here.

External Identifier: We would like to get the ORCID from all users (even though it is not a required field). If you do not have an ORCID, you can get it here: <https://orcid.org>. Additionally (or alternatively) you can also add the ID for ResearchGate or ResearcherID.

Please enter it in the “External Identifier” field. For that you need to choose the correct identifier type in the first row and enter the corresponding ID in the second row.

Institute: When entering information for a person, please choose an institute from the list. If you do not find the correct institute, click on “Other (new) Institute” and enter the details for the institute here.

5.2 DOKU-Dataset Group

DOKU-Dataset Groups may be used to group DOKU-Datasets that belong together. In many cases they will not be necessary and can be omitted. If you would like to use this option, please discuss it with DM first.

The following elements are important for DOKU-Dataset Groups. The tables in Appendix A will help you to enter metadata into MetaXA.

Once you have finished editing your metadata and want to inform DM that you have completed all entries for the DOKU-Dataset Group, click on “Finalize Entries”. If, later on, changes need to be made, this is still possible.

Metadata Entry: Please refer to table A1 for a detailed description.

Citation Information: Please refer to table A2 for a detailed description.

Temporal Coverage: This block is only available if the box “Data has no temporal information” has NOT been checked. Please refer to table A5 for a detailed description.

Spatial Coverage: This block is only available if the box “Data has no spatial information” has NOT been checked. Please refer to table A6 for a detailed description.

5.3 DOKU-Dataset

There are different methods to enter metadata for Datasets. If you have only a few DOKU-Datasets you will use MetaXA. Otherwise (only for a large number of DOKU-Datasets), you can discuss with DM whether submission via CSV-lists might be better.

5.3.1 MetaXA

The following elements are important for DOKU-Datasets. The tables in Appendix A will help you to enter metadata into MetaXA.

Once you have finished editing your metadata and want to inform DM that you have completed all entries for the DOKU-Dataset, click on “Finalize Entries”. If, later on, changes need to be made, this is still possible.

Metadata Entry: Please refer to table A3 for a detailed description.

Data Citation: Please refer to table A4 for a detailed description.

Temporal Coverage: This block is only available if the box “Data has no temporal information” has NOT been checked. Please refer to table A5 for a detailed description.

Spatial Coverage: This block is only available if the box “Data has no spatial information” has NOT been checked. Please refer to table A6 for a detailed description.

5.3.2 CSV-Lists

In case you have many DOKU-Datasets that do not differ strongly from each other, it might be more convenient to create a CSV-list containing all relevant metadata. DM will assist you with this and will give you further instructions in case this applies to your data.

5.4 Additional Info

Fewer fields are needed for the Additional Info (please refer to Appendix C for an explanation of the different hierarchical elements). Please do not forget to go to “Finalize Entries” once you are finished.

Metadata Entry: Please refer to table A7 for a detailed description.

Citation Information: Please refer to table A8 for a detailed description.

File upload: The Additional Info can consist of one or more files. You can upload the file(s) directly in MetaXA. The preferred file format for Additional Infos is PDF. If you cannot upload your file, this is most probably caused by an unsupported file format. Please convert it to PDF or contact DM to discuss if it possible to upload your preferred file format.

5.5 Citation / Reference

You can add references to your entries. Use the upper left field to search for existing citations and update them if necessary.

If you want to add new citations, use the button in the upper right corner “Create Reference Template”. This opens the form to enter metadata for a new Citation/Reference. If a DOI is available, please enter it in the respective field in the format `doi:10.1045/january2015-brase` and click on “Insert from CrossRef”. Otherwise, fill in the fields below (required fields are marked with a red asterisk).

If you edit or add a reference via MetaXA, you can also connect it with your entry. If you have already entered the DOKU-Dataset or DOKU-Dataset Group in MetaXA you will find it in a list and can choose one or more of the entries. Otherwise contact DM and they will assist you in connecting the reference to your entries.

5.6 Finalize Entries

Once you have completed entering all relevant metadata for an entry and want to finalize your entries (which notifies DM that they can further process your entries and continue with your request), please do not forget to go to “Finalize Entries”. This needs to be done for DOKU-Dataset Groups, DOKU-Datasets, and Additional Infos. Persons and Citations can be added without “Finalize Entries”.

Check all appropriate entries and click on “Finalize Selected Entries”. After you have finished your work with “Finalize Entries”, DM will further process your entries.

Even at this stage changes to your metadata are still possible. Please contact DM, if you find that amendments are needed.

6 Final Check

Once your data has been filled and is set to completely archived, DM will inform you and ask you to make final checks. Please check the metadata one last time. Also check if all your files are ready for download. It might be also advisable to try to download one or two sample files to see if everything works well.

7 How to cite your data

All DOKU-Datasets (and DOKU-Dataset Groups) are assigned a persistent URL once the metadata is online. So even before the data filling process has been completed, the URL is final and can, for example, be used for publications. For journals it is often sufficient to provide a persistent URL with the metadata when submitting a paper – of course, the data needs to follow.

7.1 PIDs for DOKU-Datasets

Once the data is available for download the DOKU-Dataset Groups and DOKU-Datasets are assigned a PID (persistent identifier). This is a unique code of digits and letters that makes your data better citable. A PID is even more suitable for referencing your data in a journal publication than a persistent URL.

Appendix A: Description of MetaXA fields

List of Tables

A1	Description of MetaXA fields for DOKU-Dataset Groups – Metadata Entry . . .	9
A2	Description of MetaXA fields for DOKU-Dataset Groups – Citation Information	10
A3	Description of MetaXA fields for DOKU-Datasets – Metadata Entry	11
A4	Description of MetaXA fields for DOKU-Datasets – Data Citation	12
A5	Description of MetaXA fields for DOKU-Datasets – Temporal Coverage	12
A6	Description of MetaXA fields for DOKU-Datasets – Spatial Coverage	13
A7	Description of MetaXA fields for Additional Infos – Metadata Entry	14
A8	Description of MetaXA fields for Additional Infos – Citation Information	14

Table A1: DOKU-Dataset Groups – Metadata Entry

Field	Required	Comment
DKRZ Project Number	✓	The internal DKRZ Project Number, eg. “bm0000”
Name	✓	<p>The entry name uniquely identifies the metadata entry (DOKU-Dataset Group). Maximum length: 200 characters. The name should meet the following criteria:</p> <ul style="list-style-type: none"> • The first letter should be in upper-case • Do not use underscores if not necessary • Whitespaces are the preferred word delimiters • It should provide proper information about the Entry • Give non-scientists an idea about the content • Avoid constant change of letters and numbers as well as constant change of upper and lower case letters. This will worsen the searchability. • If a version number needs to be provided, use the following format: Title of the entry (Version 2.1)
Summary	✓	It should be described here what is covered by the DOKU-Dataset Group. Give information on the entry that has not been entered into any other fields. The summary may contain links to further information. Maximum length: 4000 characters.
Data has no temporal/spatial information		Check these boxes (or one of these) if the data has no temporal and/or no spatial information.

Table A2: **DOKU-Dataset Groups – Citation Information**

Field	Required	Comment
Citation Title		The title of the citation. Please follow the same rules as for the entry names. The entry name can also be used here. If left empty, the entry name will be used.
Authors List	✓	The authors of this data for the citation.

Table A3: DOKU-Datasets – Metadata Entry

Field	Required	Comment
DKRZ Project Number	✓	The internal DKRZ Project Number, eg. “bm0000”
Parent		If a DOKU-Dataset Group is a parent element for this DOKU-Dataset Group, select it from the list.
Name	✓	The entry name uniquely identifies the metadata entry (DOKU-Dataset). Maximum length: 200 characters. The name should meet the following criteria: <ul style="list-style-type: none"> • The first letter should be in upper-case • Do not use underscores if not necessary • Whitespaces are the preferred word delimiters • It should provide proper information about the Entry • Give non-scientists an idea about the content • Avoid constant change of letters and numbers as well as constant change of upper and lower case letters. This will worsen the searchability. • If a version number needs to be provided, use the following format: Title of the entry (Version 2.1)
Summary has been provided with parent metadata		Check this box, if the summary has already been provided with the parent element (DOKU-Dataset Group)
Summary	✓	It should be described here what is covered by the DOKU-Dataset. Give information on the entry that has not been entered into any other fields. The summary may contain links to further information. Maximum length: 4000 characters.
Responsible Person	✓	The person selected here will be responsible for the metadata published for the DOKU entry.
Use Constraint (License)		“Use Constraint” reflects constraints regarding the use of the data. Refer to Appendix B for further details.
Format	✓	Select format of data from the list. For details see section about Data Format.
Data has no temporal/spatial information		Check these boxes (or one of these) if the data has no temporal and/or no spatial information.

Table A4: DOKU-Datasets – Data Citation

Field	Required	Comment
Authors have been provided with Dataset Group metadata		Check this box, if you want to take the citation information from the parent DOKU-Dataset Group (if available).
Citation Title		The title of the citation. Please follow the same rules as for the entry names. The entry name can also be used here. If left empty, the entry name will be used.
Authors List	✓	The authors of this data for the citation.

Table A5: DOKU-Datasets – Temporal Coverage

Field	Required	Comment
Start Year	✓	The first year of the considered time period.
Month	✓	The first month of the considered time period.
Day	✓	The first day of the considered time period.
Stop Year	✓	The last day of the considered time period.
Month	✓	The last day of the considered time period.
Day	✓	The last day of the considered time period.
Currentness Reference		Currentness Reference reflects the construction of the time axis. Choose the correct calendar from the list. Use “not filled” if no entry matches.

Table A6: **DOKU-Datasets – Spatial Coverage**

Field	Required	Comment
Min Lon	✓	The minimum longitude of the considered domain [0.0, 360.0].
Max Lon	✓	The maximum longitude of the considered domain [0.0, 360.0].
Min Lat	✓	The minimum latitude of the considered domain [-90.0, 90.0].
Max Lat	✓	The maximum latitude of the considered domain [-90.0, 90.0].
Min Altitude		Minimum altitude. Example for ocean/atmosphere data: -6200m (ocean) to 10hPa (atmosphere)
Min Alt Unit		Unit for minimum altitude.
Max Altitude		Maximum altitude. Example for ocean/atmosphere data: -6200m (ocean) to 10hPa (atmosphere)
Max Alt Unit		Unit for maximum altitude.

Table A7: **Additional Infos – Metadata Entry**

Field	Required	Comment
Name	✓	<p>The entry name uniquely identifies the metadata entry (Additional Info). Maximum length: 200 characters. The name should meet the following criteria:</p> <ul style="list-style-type: none"> • The first letter should be in upper-case • Do not use underscores if not necessary • Whitespaces are the preferred word delimiters • It should provide proper information about the Entry • Give non-scientists an idea about the content • Avoid constant change of letters and numbers as well as constant change of upper and lower case letters. This will worsen the searchability. • If a version number needs to be provided, use the following format: Title of the entry (Version 2.1)
Summary	✓	<p>It should be described here what is covered by the Additional Info. Give information on the entry that has not been entered into any other fields. The summary may contain links to further information. Maximum length: 4000 characters.</p>
Parent	✓	<p>If a DOKU-Dataset Group is a parent element for this DOKU-Dataset Group, select it from the list.</p>
Publication Type		<p>If your publication is well described by an “additional info”, but something from this list fits better, you can specify that here.</p>
Use Constraint (License)		<p>“Use Constraint” reflects constraints regarding the use of the data. Refer to Appendix B for further details.</p>

Table A8: **Additional Infos – Citation Information**

Field	Required	Comment
Citation Title		<p>The title of the citation. Please follow the same rules as for the entry names. The entry name can also be used here. If left empty, the entry name will be used.</p>
Authors		<p>The authors of this additional info for the citation. Please select from the list.</p>

Appendix B: License

You need to decide under which license to publish your data. We suggest CC-BY 4.0 for data submissions. The Creative Commons Licenses are commonly used for sharing research data by academics and offered as a choice by WDCC. A short overview over is given here.

B.1 Creative Commons Licenses

- <https://creativecommons.org/licenses/by/4.0/>
- <https://creativecommons.org/licenses/by-nd/4.0/>
- <https://creativecommons.org/licenses/by-nc/4.0/>
- <https://creativecommons.org/licenses/by-nc-nd/4.0/>
- <https://creativecommons.org/licenses/by-nc-sa/4.0/>
- <https://creativecommons.org/licenses/by-sa/4.0/>

Summary (human readable): To see which terms apply to which Creative Common license in detail, please refer to table B1.

You are free to (green in table B1):

- *Share* – copy and redistribute the material in any medium or format
- *Adapt* – remix, transform, and build upon the material.

The licensor cannot revoke these freedoms as long as you follow the license terms.

Under the following terms (blue in table B1):

- *Attribution* – You must give appropriate credit, provide a link to the license, and indicate if changes were made. You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.
- *NoDerivatives* – If you remix, transform, or build upon the material, you may not distribute the modified material.
- *NonCommercial* – You may not use the material for commercial purposes.
- *ShareAlike* – If you remix, transform, or build upon the material, you must distribute your contributions under the same license as the original.

No additional restrictions: You may not apply legal terms or technological measures that legally restrict others from doing anything the license permits.

Notices: You do not have to comply with the license for elements of the material in the public domain or where your use is permitted by an applicable exception or limitation.

No warranties are given. The license may not give you all of the permissions necessary for your intended use. For example, other rights such as publicity, privacy, or moral rights may limit how you use the material.

License	Share	Adapt	Attribution	NoDerivatives	NonCommercial	ShareAlike
CC BY 4.0	█	█	█			
CC BY-ND 4.0	█		█	█		
CC BY-NC 4.0	█	█	█		█	
CC BY-NC-ND 4.0	█		█	█	█	
CC BY-NC-SA 4.0	█	█	█		█	█
CC BY-SA 4.0	█	█	█			█

Table B1: Summary of Creative Commons Licenses

Appendix C: Hierarchy Structure Description

Data in DOKU is organized in multiple layers with a hierarchical structure. These layers are named: *Projects*, *Experiments*, *Dataset Groups* and *Datasets*. The relationships between them can be described with a tree structure as in figure 1. For the top-level elements only single-parent (mono-hierarchical) relationships are supported. That means that only one parent is allowed for each Experiment and Dataset Group, but a parent can have multiple children-elements. Datasets and *Additional Infos* (which are a bit of an exception and will be described later in this section) need to have at least one parent, but it is possible that they have more than one.

The Project, Experiment and Dataset Groups contain the overall description of the data, i.e. the metadata. Metadata is the description of the data itself. Detailed metadata is essential for later reuse of the data and therefore for long-term archiving. These elements (Project, Experiment and Dataset Groups) are be used to structure the data. The data itself is located in the Datasets (which also contain description of the data).

Each DOKU-Dataset is part of a hierarchical tree with an Experiment and a Project. DOKU-Dataset Groups are optional elements in between. The most minimalistic data to be archived needs to contain at least one Project, one Experiment and one DOKU-Dataset in the hierarchical structure.

Project: A Project is the top hierarchical element. All data that is archived under DOKU belongs to the same Project: “Long-term Archiving of Climate Model Data at WDC Climate and DKRZ (DOKU)” (https://www.wdc-climate.de/ui/project?acronym=DKRZ_lta).

Experiment: An Experiment is the hierarchical child element of a Project and a compilation of Datasets. In DOKU each DKRZ project (e.g. bm0000) becomes an Experiment and will compile all DOKU-Datasets that are archived under the project account bm0000. (It has to be noted that “Experiment” is just a name for a hierarchical element and should not be confused with a model run for example.)

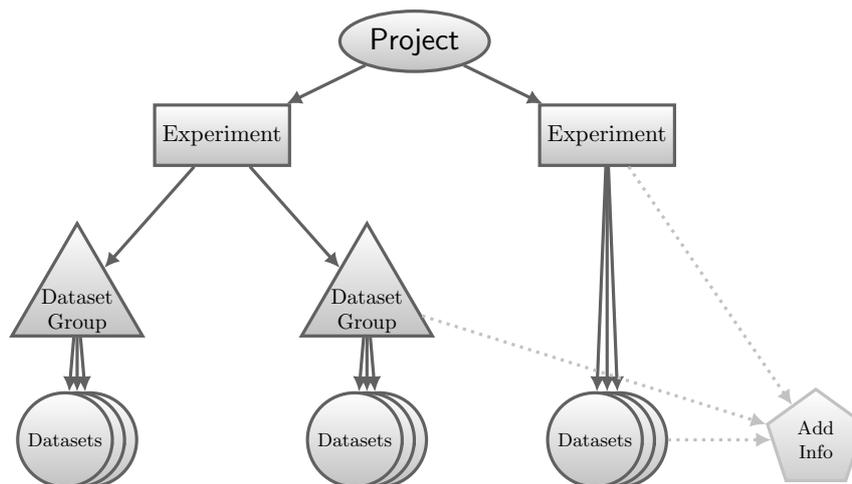


Figure 1: Hierarchical structure elements

Dataset Group: A Dataset Group is a compilation of Datasets or Dataset Groups. This is an optional element that does not need to be used for smaller projects, but can be helpful for bigger or more complex projects to sort them into finer structures. A Dataset Group is a child of an Experiment or another Dataset Group. In DOKU usually Datasets are direct children of Experiments without the further need of DOKU-Dataset Groups. However, for bigger projects or in some special cases it can be useful to group several DOKU-Datasets in a DOKU-Dataset Group.

Dataset: A Dataset consists of the data itself and its description (the metadata) needed to make the data understandable. A DOKU-Dataset is a child of an Experiment or a DOKU-Dataset Group.

Additional Info: There is another element a bit outside of the hierarchical tree in figure 1. An Additional Info is an optional element that is located in the same layer as a Dataset, i.e. is the child of an Experiment or Dataset Group (but can also be the child of a Dataset) and can have more than one parent. It is defined as a compilation of documents or plots enhancing further understanding of the data.

C.1 Nomenclature

DM will help you to organize your data into the hierarchical structure described above. In this context the nomenclature of the elements will also be discussed. You have to give each element a name which is the title for this entry and will also be used in the WDCC search interface. Hints for good entry names will be given in the section “Submission of Metadata”.

You can decide together with DM which structure and nomenclature makes sense for your data.