

Data Management at the FIBEr Lab

ManGO User Day 2024
Heleen Fehervary & Ronny Moreas

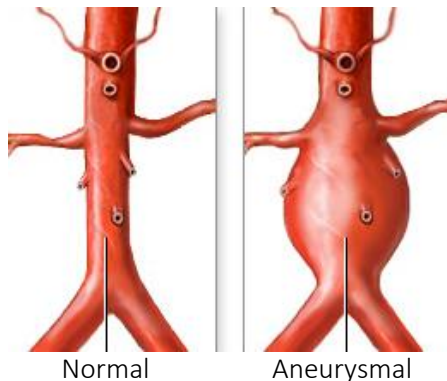
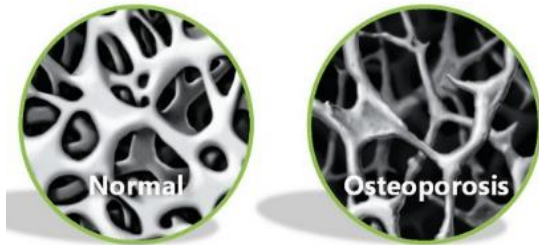


We test what's vital for you

WHY

do we need biomechanical experiments?

Understanding
mechanics-related
pathologies



Development of treatments, medical
products, diagnostic tools



WHAT are biomechanical experiments?

Material characterization



Aorta

Medical device testing



Fracture plate

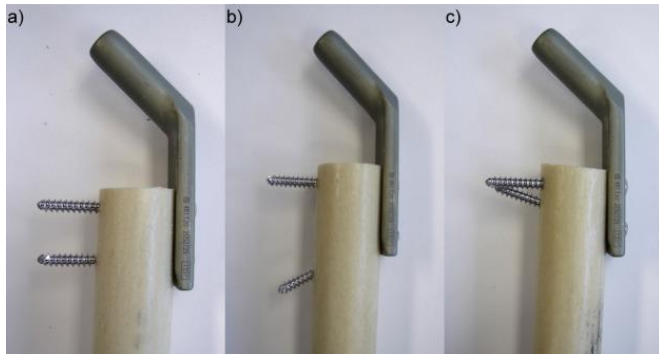
Non-exhaustive list of the **mechanical properties** we can measure:

- compliance or **stiffness** (e.g. Young's modulus),
- **strength** (tensile, compressive, flexural, peel, tear) and elongation,
- energy to **failure** and fracture toughness,
- Poisson's ratio,
- crack growth velocity,
- **fatigue** & fatigue life,
- visco-elastic properties (creep, stress relaxation)
- ...

WHEN are biomechanical experiments useful?

at multiple stages of product development

R&D stage



Regulatory

INTERNATIONAL
STANDARD

ISO
7198

Cardiovascular implants and
extracorporeal systems — Vascular
prostheses — Tubular vascular grafts
and vascular patches



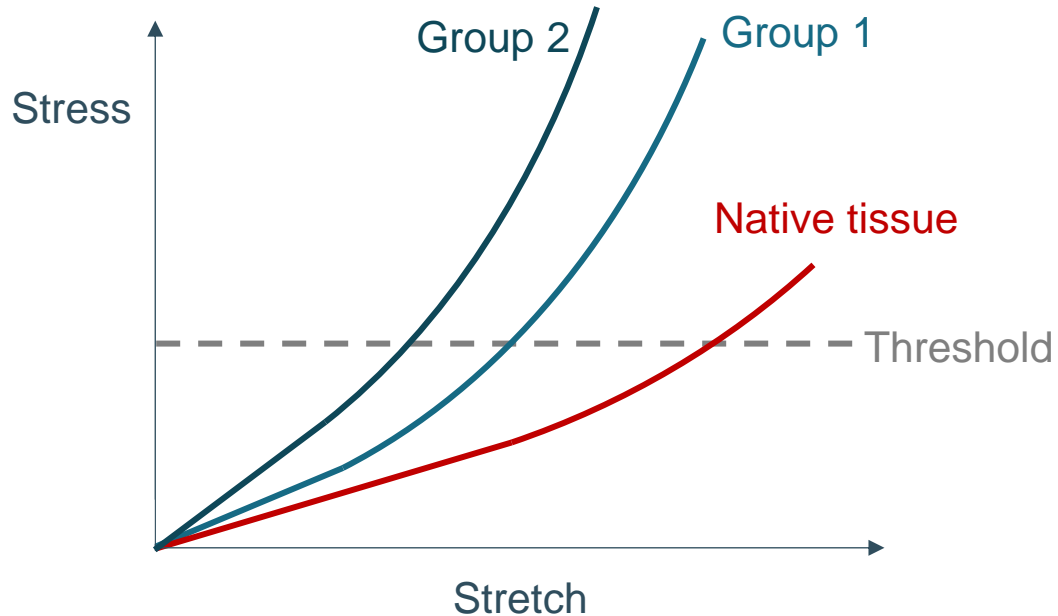
Quality
control

HOW

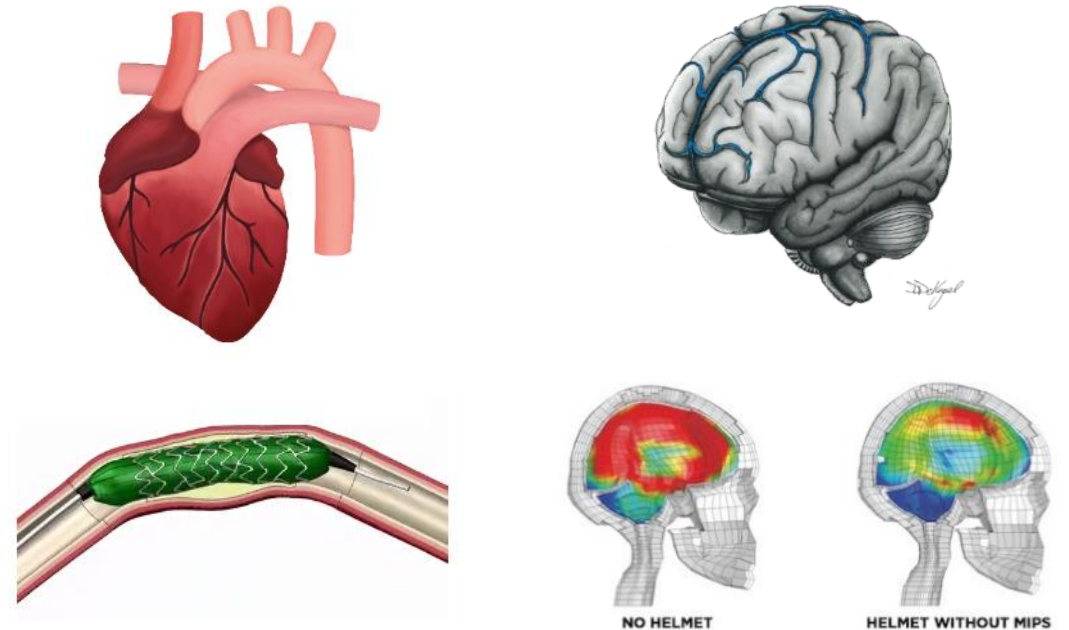
can data from biomechanical experiments be used?

Direct comparison

- Strength
- Stiffness/Elasticity
- Visco-elasticity
- Permeability
- Fracture behavior
- ...



Input for in silico models

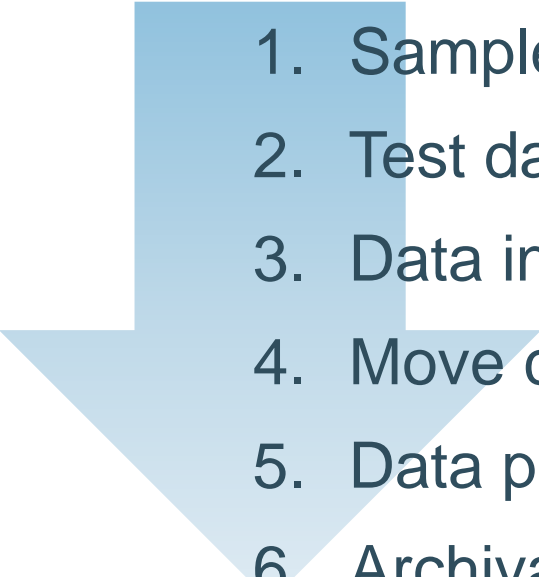


Grogan et al. 2015, Kleiven et al. 2006

What is important for good data management at FIBEr?

- Different types of clients
 - Lab users (internal, external)
 - FIBEr team running service projects
- Samples (storage, traceability, linked data, ...)
- Large portfolio of testing equipment
 - Almost all measurements are digitalized
 - Some data is combined in post processing
 - Different data sizes (few KB to a few hundreds of GB)
- Sharing raw/processed data within/outside KU Leuven
- QMS: back-up, confidentiality, data integrity

Overview Data Management at FIBEr

- 
1. Sample, project and experiment (meta)data
 2. Test data acquisition
 3. Data ingestion into ManGO
 4. Move completed data ingests to project collection
 5. Data processing
 6. Archival of completed projects



Sample, project and experiment (meta)data

- **FIBEr Sample Manager:**
Webapp for management of samples, projects and experiments



Welcome

Log out

+ Store new sample

📄 Copy data to new samples

🔧 Add/modify sample data

✂ Divide sample

🔥 Thaw in fridge E

🏷 Take over sample

📊 Inspect sample

👤 Show all my samples

📋 Show all stored samples

📦 Take out sample

📦 Bring back sample

🗑 Dispose of sample

🔗 Link a new publication

📄 Show my experiments

📄 Show linked publications

🗑 Cleanup Management

+ New experiment

📄 Experiment management

👤 User management

📋 Project management



Test Data Acquisition

- **FIBEr DAQ Manager App**
 - Installed on instrument computers
 - Collect data and metadata to be added to dataset for upload
- After a test run the operator:
 - Selects files to be added to dataset
 - Adds metadata (from FIBEr Dashboard)
 - Instrument
 - Sample
 - Project
 - Experiment
 - Test Operator
- Dataset moved to drop location for upload to ManGO



1105210056-2410041417

MainWindow

Sample Selection

Project

fiber_oef

Search All

Project ID	Project	Sample ID	Storage Date	Name	Origin	Type	Remarks
b85cf558-f560-4d15...	FIBEr_oefenstaal	2510230001	2023-10-25	Balb/c mice femurs ...	Mouse	Bone	spare femurs from ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	1105210056	2023-01-19	Human brain 8/23 ...	Human	brain	Tryout brain without...
b85cf558-f560-4d15...	FIBEr_oefenstaal	1105210055	2023-01-19	Human brain 8/23 ...	Human	brain	Tryout brain sample ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	3011230001	2023-01-19	Human brain 8/23 ...	Human	brain	Tryout brain sample ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	3011230002	2023-01-19	Human brain 8/23 ...	Human	brain	Tryout brain sample ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	1105210064	2022-08-09	Crux-Project Minipig...	Human	Adipose tissue + skin	
b85cf558-f560-4d15...	FIBEr_oefenstaal	0402220083	2022-02-09	aorta practice material	Pig	Aorta	
b85cf558-f560-4d15...	FIBEr_oefenstaal	1612200001	2020-12-16	OEFENSTAAL FIBEr - ...	Pig	Aorta	Meerdere stalen ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	0903200036	2020-03-09	OEFENSTAAL FIBEr - ...	Pig	Aorta	Left over material ...
b85cf558-f560-4d15...	FIBEr_oefenstaal	0903200037	2020-03-09	OEFENSTAAL FIBEr - ...	Pig	Aorta	Left over material ...

F I B E R

Log Out

Select Device:
BIAx-01

Data Collected

Name	Size	Type	Date Modified
sample rat...		File Folder	04/10/2024 13:19
test20...		File Folder	04/10/2024 13:19
du...	794 bytes	CSV document	24/04/2024 16:15
du...	993,85 KiB	TIFF image	24/04/2024 16:15
du...	993,85 KiB	TIFF image	24/04/2024 16:15
du...	993,85 KiB	TIFF image	24/04/2024 16:15
input_...	327 bytes	plain text document	24/04/2024 16:15
input_...	683 bytes	plain text document	24/04/2024 16:15
chang...	43,94 KiB	PNG image	24/04/2024 16:15
PB_pro...	2,99 MiB	Gzip archive	24/04/2024 16:15
PB_pro...	213,00 KiB	Gzip archive	24/04/2024 16:15
Outpu...		File Folder	04/10/2024 13:18
PB_protoc...	213,00 KiB	Gzip archive	24/04/2024 16:15

Selected Data to Upload

Name	Size	Type	Date Modified
PB_protoc...	2,99 MiB	Gzip archive	24/04/2024 16:15

Notes

File Name

.txt

Text

Save Selected Data to Mango

Save N

FIBEr DAQ Manager

Upload Wizzard

Select Experiment

Select an existing experiment or create a new one. Experiments shown/created are based on the device used.

Experiment: Demo ManGo User Day 2024 | 2024-10-04 14:16

New Experiment

Title: * Demo ManGo User Day 2024

Description:

☒ Remember experiment?

+ Create

Next Cancel

10

FIBEr - KU Leuven Core Facility for Biomechanical Experimentation

KU LEUVEN

Test Data Acquisition

- Metadata file (json) added to dataset for upload
- Dataset with metadata moved to drop location for upload to ManGO



1105210056-2410041417

```
{
  "acquisition_datetime": "2024-10-04T14:17:47",
  "device": {
    "model": "Biaxial Testing Machine, Messphysik - Zwick/Roell",
    "name": "BIAX-01"
  },
  "experiment": {
    "id": "5f7c7fdda75a8711261e4ea7",
    "name": "Demo ManGO User Day 2024"
  },
  "operator": {
    "name": " ",
    "surname": " ",
    "uid": " "
  },
  "project": {
    "id": "b85cf558-f560-4d15-a72d-36e1fbce1ed5",
    "name": "FIBEr_oefenstaal"
  },
  "sample": {
    "id": "1105210056",
    "name": "Human brain 8/23 Exp3.1"
  }
}
```

Data Ingestion into ManGO



ManGO Ingestor



- Linux-based device designed to facilitate the **ingestion of instrument data and metadata from multiple devices** into the ManGO active data platform.
- Purpose
 - Streamline the process of ingesting and managing scientific data **across different platforms and environments with central control**.
 - Avoid installation of software on instrument computers by **pulling data directly from SMB/CIFS (or NFS) share(s) defined on the instrument computers**.
 - **Extendable** with custom handlers for metadata extraction

ManGO Ingestor



- Foundation
 - **Built upon the iRODS Capability Automated Ingest (iCAI)** to provide a library of common ingestion handlers with enhanced configuration features.
 - Includes base **handler classes** for different types of data ingestion, such as RunFolderIngestHandler, BCLIngestHandler, and FASTQIngestHandler.
 - Inspired by bihealth/rodeos-ingest: Code for ingesting omics data into omics storage based on iRODS capabilities (github.com)
- Cloud-based deployment of software components
 - K3s lightweight Kubernetes distro great for edge deployments in labs
 - ManGO Ingest Docker image
 - ManGO Ingest Helm chart to facilitate configuration, deployment and updating of all software components



Data Ingestion into ManGO (ingress collections)

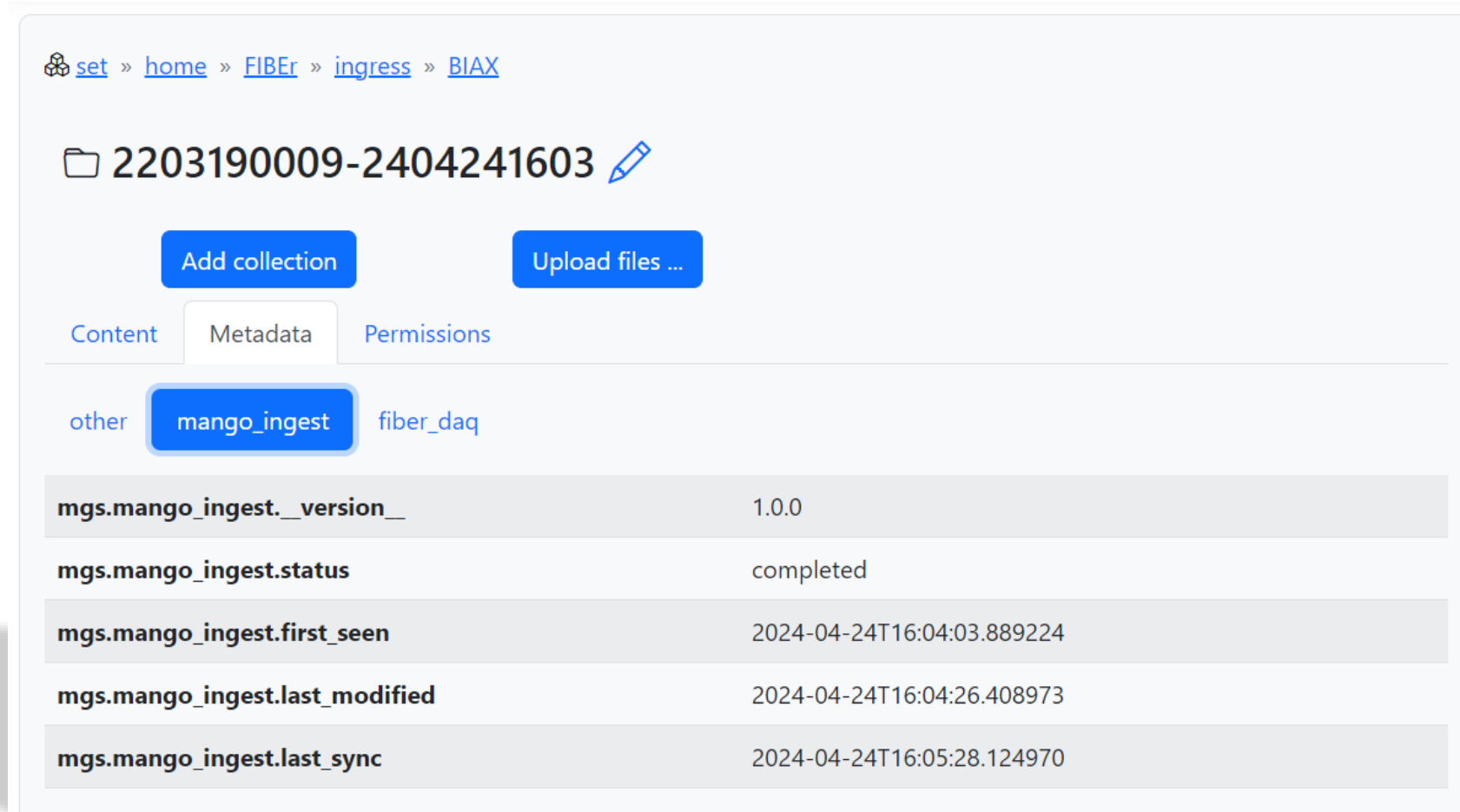
- The ManGO Ingestor syncs datasets from the DAQ device drop locations to an **ingress collection per source device**

The screenshot displays the ManGO web interface for an ingress collection. The breadcrumb navigation at the top reads: [set](#) » [home](#) » [FIBEr](#) » [ingress](#) » [BIAX](#). Below this, the collection ID **2203190009-2404241603** is shown with a pencil icon for editing. Two blue buttons are present: **Add collection** and **Upload files ...**. A tabbed interface shows **Content**, **Metadata**, and **Permissions**, with **Content** selected. Action icons for **Delete**, **Move**, **Copy**, and **Download** are available. A warning message states: "Copying/Download is only available for data objects." Below this is a table listing the collection's contents.

<input type="checkbox"/>	Name	Owner	Created	Modified	Size	
<input type="checkbox"/>	test20211109	FIBEr_ingress	2024-04-24 16:04:04	2024-04-24 16:04:05		
<input type="checkbox"/>	change500hz.PNG	FIBEr_ingress	2024-04-24 16:04:04	2024-04-24 16:04:04	45.0 kB	↓
<input type="checkbox"/>	fiber_daq.json	FIBEr_ingress	2024-04-24 16:04:04	2024-04-24 16:04:04	558 Bytes	↓
<input type="checkbox"/>	input_PB_protocol_DSM.txt	FIBEr_ingress	2024-04-24 16:04:05	2024-04-24 16:04:05	683 Bytes	↓
<input type="checkbox"/>	input_PB_protocol_SampleRateTest.txt	FIBEr_ingress	2024-04-24 16:04:05	2024-04-24 16:04:05	327 Bytes	↓

Data Ingestion into ManGO (ingest metadata)

- ManGO Ingestor adds metadata to datasets about the sync status
- Ingestor uses customizable hook method to detect completion of a test/measurement sequence



The screenshot displays the ManGO web interface for a dataset. The breadcrumb navigation shows the path: [set](#) » [home](#) » [FIBEr](#) » [ingress](#) » [BLAX](#). The dataset identifier is 2203190009-2404241603, with an edit icon. Two buttons are visible: "Add collection" and "Upload files ...". Below these are tabs for "Content", "Metadata", and "Permissions", with "Metadata" currently selected. Under the "Metadata" tab, there are three buttons: "other", "mango_ingest" (which is highlighted), and "fiber_daq". A table below lists the metadata for the "mango_ingest" collection:

mgs.mango_ingest.__version__	1.0.0
mgs.mango_ingest.status	completed
mgs.mango_ingest.first_seen	2024-04-24T16:04:03.889224
mgs.mango_ingest.last_modified	2024-04-24T16:04:26.408973
mgs.mango_ingest.last_sync	2024-04-24T16:05:28.124970

Data Ingestion into ManGO (other metadata)

- Acquisition metadata is added to the dataset collection
- ManGO Ingestor can be extended with custom handlers to extract and add metadata for specific instruments

set » home » FIBEr » ingress » BIAx

2203190009-2404241603

Add collection

Upload files ...

Content

Metadata

Permissions

other

mango_ingest

fiber_daq

mgs.fiber_daq.__version__	1.0.0	
mgs.fiber_daq.sample.id	2203190009	1
mgs.fiber_daq.sample.name	cerebellum	1
mgs.fiber_daq.project.id	a4943114-de7f-4690-b946-e4aba55bdb67	1
mgs.fiber_daq.project.name	Oefenstaal STB	1
mgs.fiber_daq.acquisition_datetime	2024-04-24T16:03:27	
mgs.fiber_daq.experiment.id	5dea7e7c37f5b86413b15267	1
mgs.fiber_daq.experiment.name	Pia Mater	1
mgs.fiber_daq.device.model	Biaxial Tester	1
mgs.fiber_daq.device.name	Biax	1
mgs.fiber_daq.operator.name		1
mgs.fiber_daq.operator.uid		1

Move Datasets to Project Collections

Work in Progress

- **ManGO Flow** moves completed data ingests from ingress collection to raw collection of the associated project

set » home » FIBEr

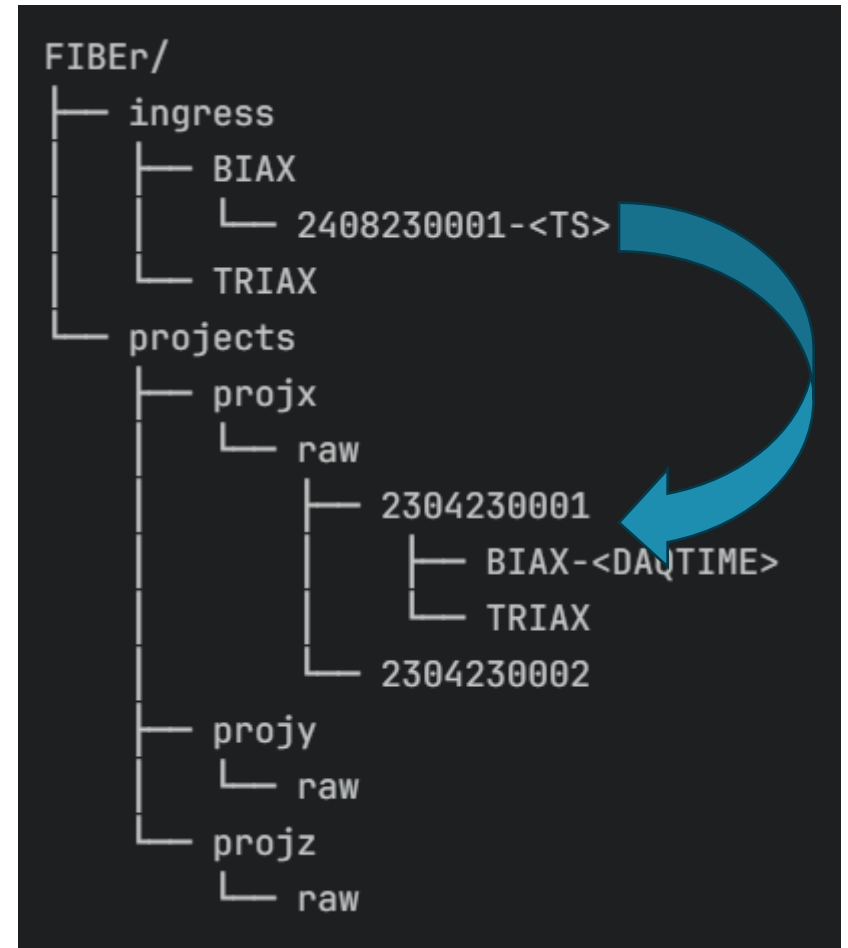
projects

Add collection Upload files ...

Content Metadata Permissions

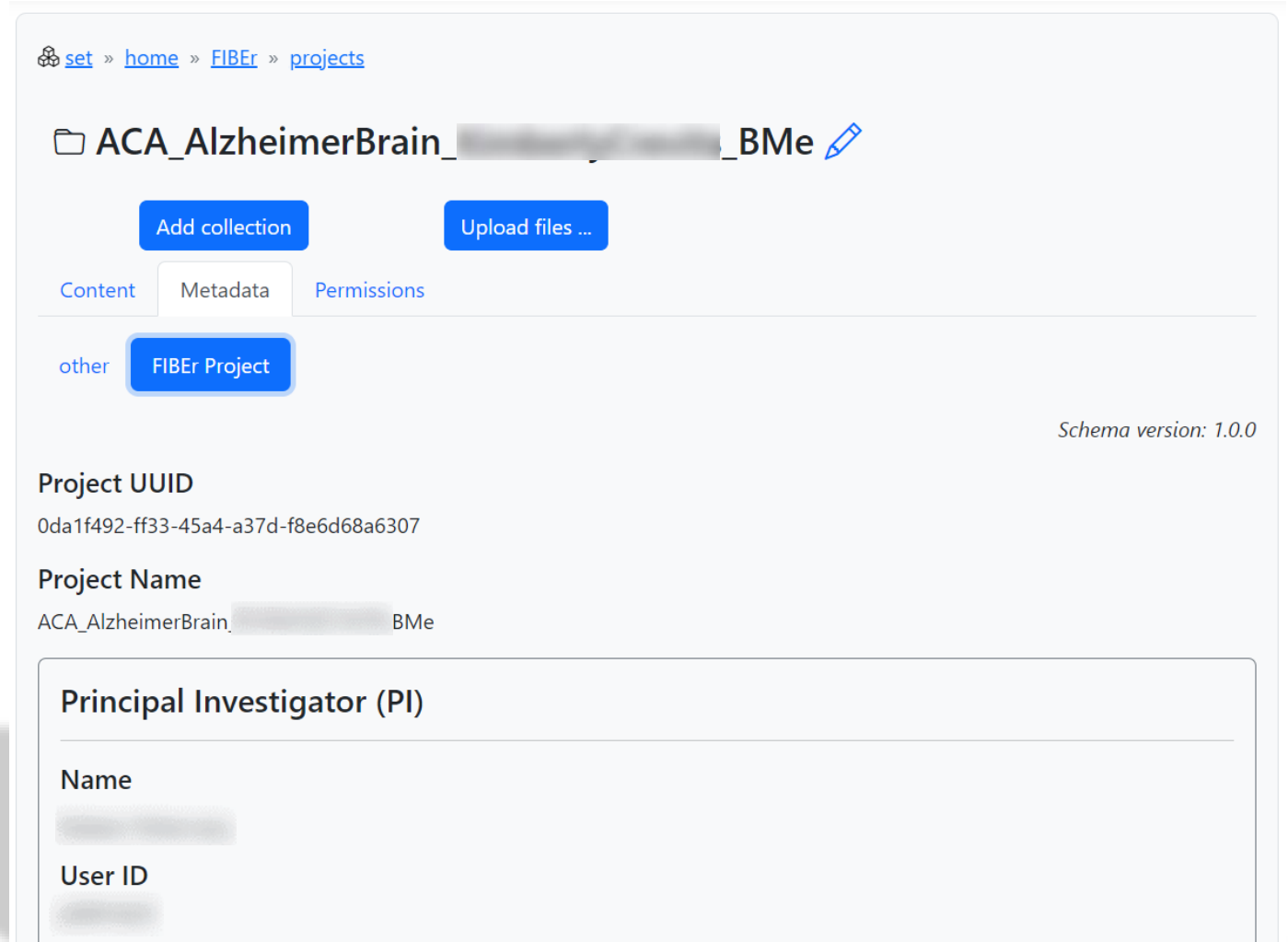
Delete Move Copy Download ⚠ Copying/Download is only available for data objects.

<input type="checkbox"/>	Name	Owner	Created	Modified	Size
<input type="checkbox"/>	ACA AlzheimerBrain BMe		2024-09-12 11:19:52	2024-09-12 11:19:52	
<input type="checkbox"/>	ACA CompressionOfSferoidsInMicroCT ACA		2024-09-12 12:05:08	2024-09-12 12:05:08	



Move Datasets to Project Collections (project metadata)

- Target project collection is determined by project metadata set on project collections and the acquisition metadata set on the ingested dataset



The screenshot shows the FIBEr project metadata interface. At the top, there is a breadcrumb navigation: [set](#) » [home](#) » [FIBEr](#) » [projects](#). Below this, the project name is displayed as "ACA_AlzheimerBrain_ [redacted] _BMe" with an edit icon. Two blue buttons are present: "Add collection" and "Upload files ...". Below these are three tabs: "Content", "Metadata" (which is active), and "Permissions". Under the "Metadata" tab, there is a section labeled "other" with a button "FIBEr Project". To the right of this section, it says "Schema version: 1.0.0". The "Project UUID" is shown as "0da1f492-ff33-45a4-a37d-f8e6d68a6307". The "Project Name" is "ACA_AlzheimerBrain_ [redacted] BMe". Below this is a section for the "Principal Investigator (PI)" with fields for "Name" and "User ID", both of which are redacted.

Data Processing



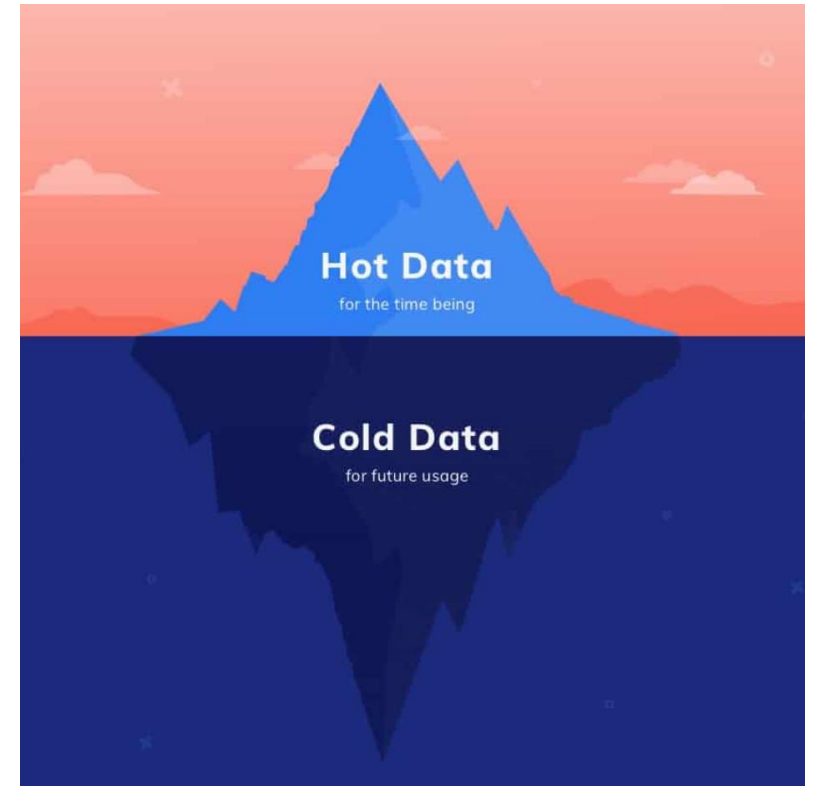
- Workflow depends on project and data types
- Generic workflow using Globus for data transfers
 - Transfer raw data to workstation or HPC for processing
 - Upload of results
 - Still early-stage ideas to be worked out



Archival of completed projects (in the future)



- Move data of completed projects to **cold storage**
 - Long-term storage
 - *Qualified* and well described *immutable datasets*
 - May be re-used or re-examined in the future
 - Enough *metadata* provided, to allow the datasets to be re-used
 - *Searchable* in the long-term





Any Questions?

References

- <https://fiber.biomech.be>
- <https://gitlab.kuleuven.be/setit/rdm/mango-ingest>
- <https://gitlab.kuleuven.be/setit/rdm/mango-ingest-helm-chart>
- https://github.com/irods/irods_capability_automated_ingest
- <https://github.com/kuleuven/mango-mdschema>
- <https://rdm-docs.icts.kuleuven.be/mango/>
- <https://rdm-docs.icts.kuleuven.be/globus/>