Fairspace

Fairspace is a secure place for managing research data. Research teams have their own workspaces in which they can manage research data collections. Researchers can upload directories and files to data collections. Data access is organised on data collection level. Collections can be shared with other teams or individual researchers. Also, collections can be published for all researchers in the organisation.

Collections and files can be annotated with descriptive metadata. The metadata is stored using the Resource Description Framework (RDF) in an Apache Jena database. For the metadata, a data model can be configured that suits the data management needs of the organisation. The data model is specified using the Shapes Constraint Language (SHACL), see the section on Data model and view configuration. Descriptive metadata entities (e.g., subjects, projects, samples) should be added to the database by a careful process, ensuring that duplicates and inconsistencies are avoided and all entities have proper unique identifiers. The application provides overviews of the available metadata entities. In the collection browser, researchers can link their collections and file to these entities or add textual descriptions and key words.

Key features

- Fairspace is a data repository that enables researchers to securely **store** and **organise** their research data sets, and **share** the data with collaborators.
- Fairspace lets researchers annotate their data collections with relevant metadata properties and link the data to associated metadata entities (subjects, samples, projects, etc.). This helps researchers find their own data and make it **findable** for others, contributing to implementation of the FAIR principles.
- Fairspace ensures that all metadata entities have a unique identifier and validates metadata consistency and validity upon data entry.
- Fairspace allows organisations to use **customise** the configured data model, by specifying custom entity types and constraints. This enables the adoption of community standards for metadata relevant for the research domain, which contributes to the **reusability** of the data.
- Fairspace uses the Resource Description Framework (RDF) and WebDAV standards for data exchange, and stimulates the uses of standard vocabularies, contributing to **interoperability** of data.

Table of contents

Usage . . . 3
- User interface . . . 3
  - Login . . . 3
  - Workspaces . . . 3
  - Collections . . . 4
  - Metadata . . . 8
- Interfaces for accessing and querying data (API) . . . 8
  - Authentication . . . 9
  - WebDAV . . . 13
  - SPARQL . . . 22
  - RDF metadata . . . 23
  - Metadata views . . . 29
  - Workspace management . . . 31
  - Users and permissions . . . 33
  - Configuration endpoints . . . 34

Structure and terminology . . . 36
- Workflow and access modes . . . 37
- Roles and permissions . . . 38

Data model and view configuration . . . 40
- Metadata . . . 40
  - Types of metadata . . . 40
  - Purpose . . . 40
- Data model . . . 41
  - Data domains . . . 41
- Data model configuration . . . 42
  - Limitations . . . 47
  - Controlled vocabularies . . . 47
- View configuration . . . 48

Installation and configuration . . . 49
- Local development . . . 49
- Kubernetes and helm . . . 49
  - Instructions for deploying to Google Cloud . . . 49

Design . . . 52
- Storage . . . 52

License . . . 53

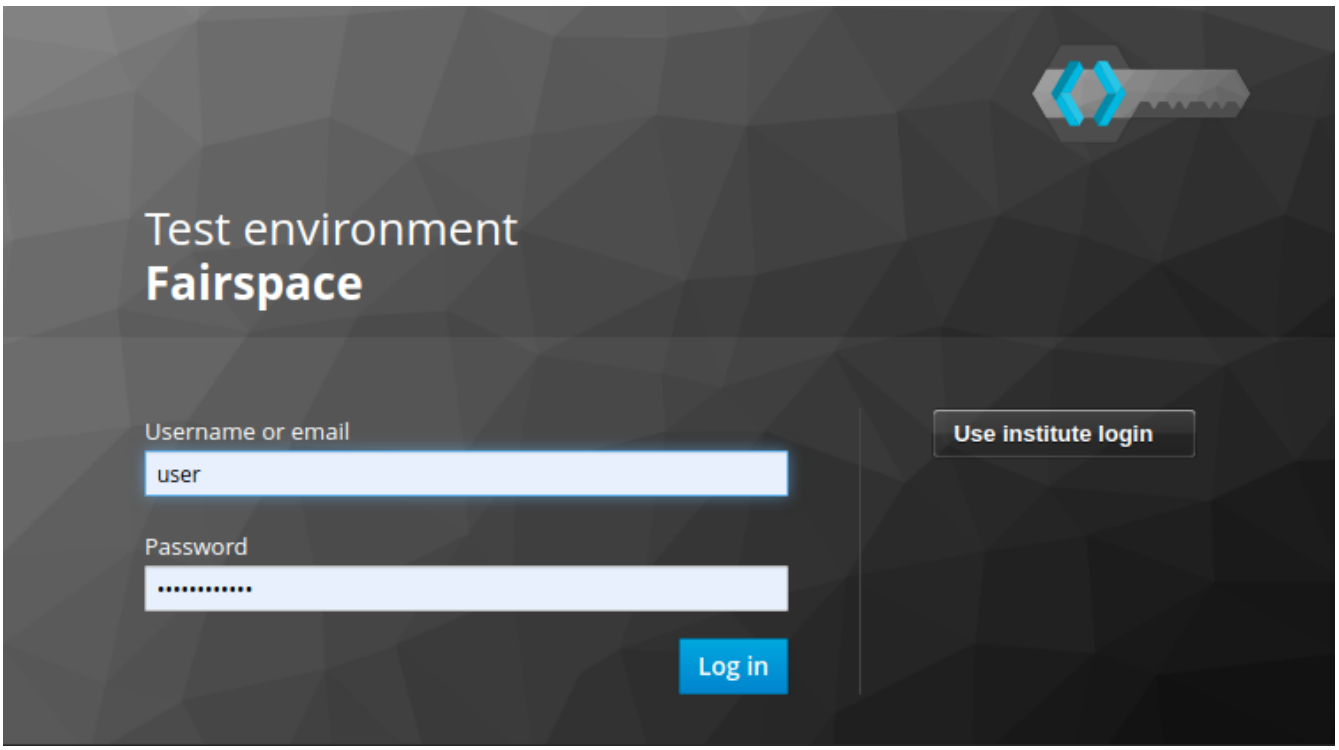
Usage

User interface

Login

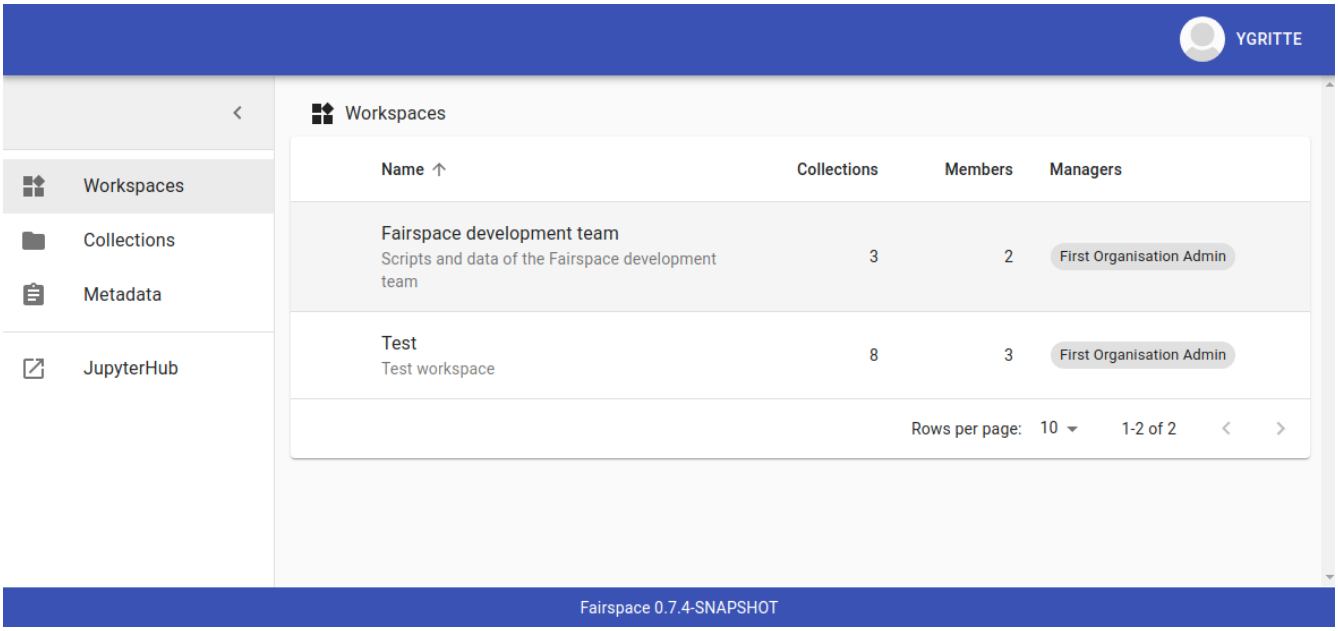
Users are authenticated using Keycloak, an open-source identity provider that provides secure authentication methods and can be configured to integrate with institutional identity providers using user federation or identity brokering, see the Keycloak server administration pages.

The user either logs in directly using Keycloak or is forwarded to a configured external login:

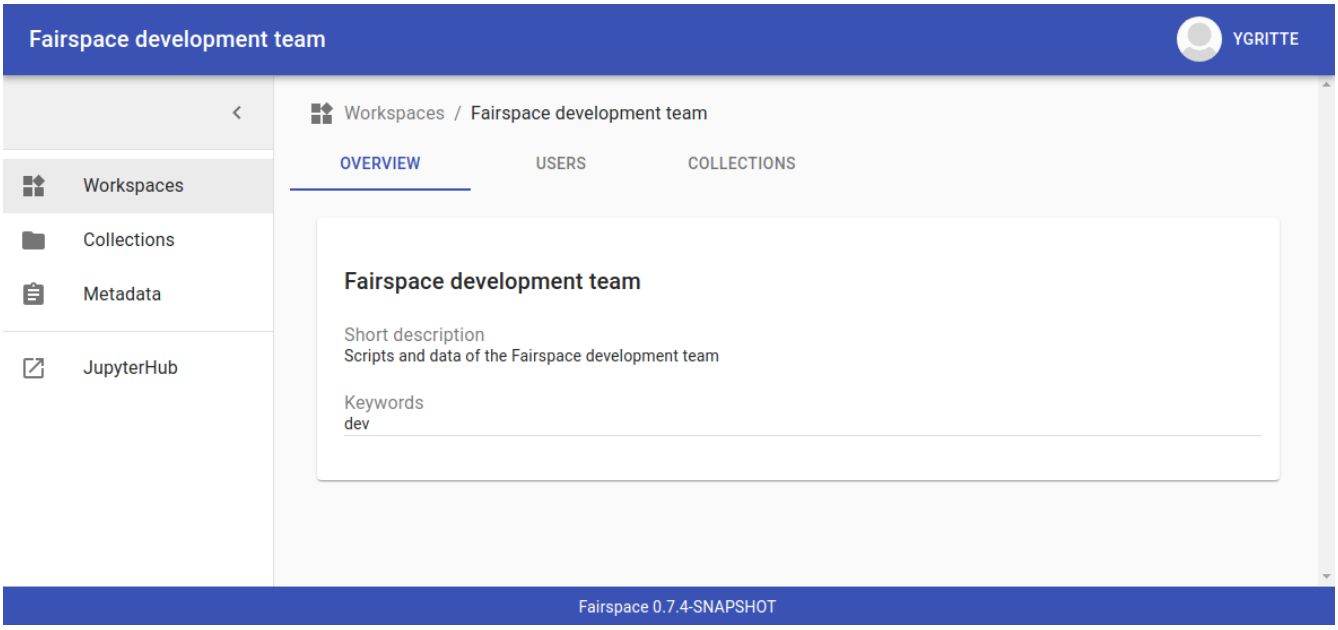


Workspaces

Users enter Fairspace on the workspaces page that lists all workspaces. A workspace represents a team in the organisation that collaborates on research data collections.



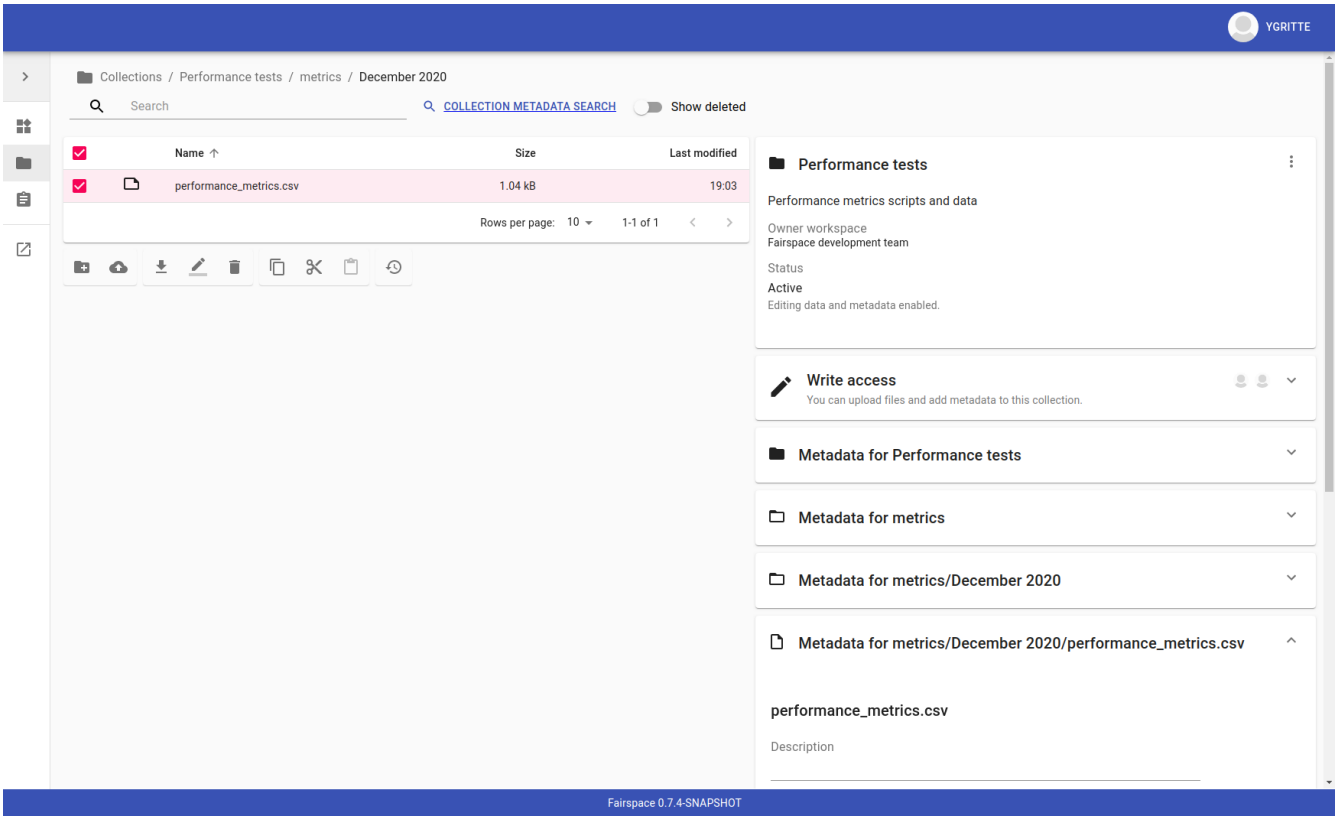
Workspace administrators can edit the workspace overview page and manage workspace membership. All workspace members can add collections to the workspace.



Collections

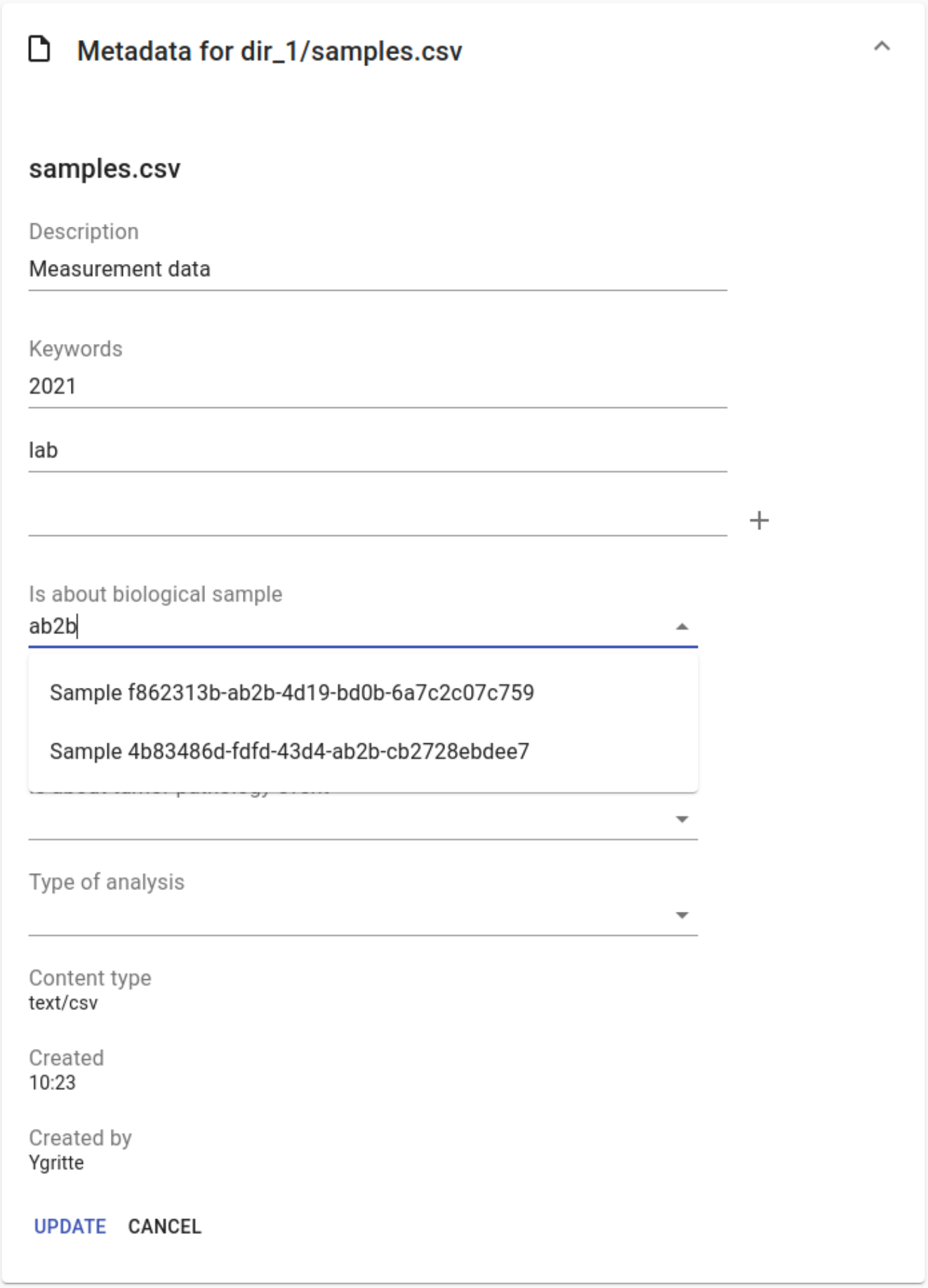
The contents of collections can be navigated in the collections browser. It behaves like a regular file browser. Click to select a directory or file and see its metadata, double click to navigate into directories or open a file.

Access is managed on collection level. Users with at least write access to a collection can upload files or directories, rename or delete files, restore old file versions, and edit the associated metadata.



Metadata forms

Users with write access to the collection can annotate collections, directories and files using *metadata forms*. Free text fields, like description and key words, can be entered freely, links to shared entities, like subjects, samples and projects, or values from a controlled vocabulary, like taxonomy or analysis type, can be selected from a list:



The shared metadata entities and controlled vocabularies cannot be added via the user interface. The RDF metadata API should be used for that instead.

Metadata upload

Another way to annotate directories and files is by uploading a comma-separated values (CSV) file with metadata. This section describes the CSV-based format used for bulk metadata uploads.

The file should be a valid CSV-file:

- Records are separated with a `,`-character.
- Values may be enclosed in double quotes: `"value"`.
- In values that contain a double, the double quotes need to be escaped by replacing them with double double quotes: `Example "quoted" text` becomes `"Example ""quoted"" text"`.

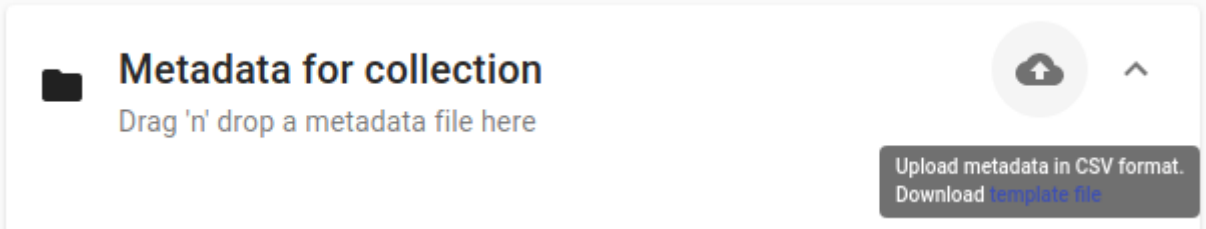
In the metadata upload, lines starting with `#` are ignored. These lines are considered to be comments.

The file should have a header row containing the names of the columns. The mandatory `Path` column is used for the file path. For the property columns, the name should match exactly the name of the property in the database.

The format of the values is as follows:

- *Path*: the relative path to a file or a directory (relative to the collection or directory where the file is uploaded). Use `./` for the current directory or collection.
- *Entity types* can be referenced by ID or unique label.
- Multiple values must be separated by the pipe symbol `|`, e.g., use `test|lab` to enter the values `test` and `lab`.

The file can be uploaded to the current directory by dropping the file in the metadata panel of the directory, or by selecting the metadata upload button.
By hovering over the metadata upload button, a link to a *metadata template file* becomes available:



The file describes the format in commented lines and contains the available properties in the header row.

Example 1. Example metadata file

An example comma-separated values file with metadata about the current directory `./`, which is annotated with a description and two key words (`sample` and `lab`), and the file `test.txt` which is linked to Subject 1 by the unique subject label and to the RNA-seq analysis type by the analysis type identifier (`O6-12`).

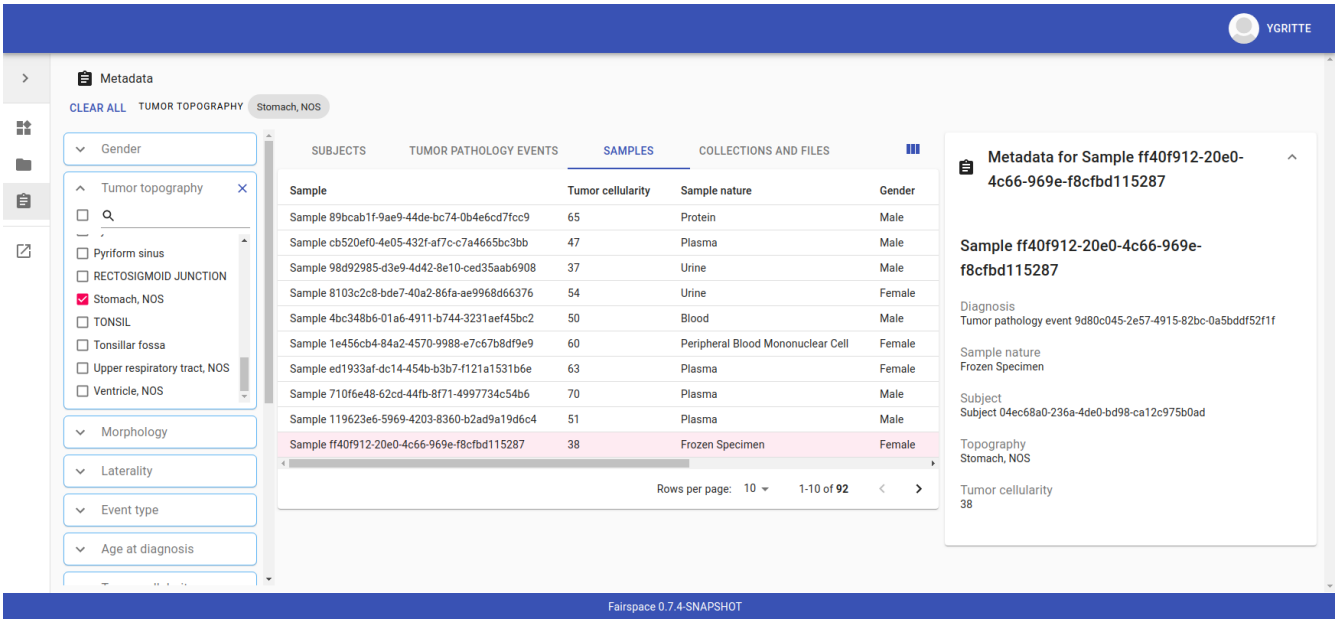
```
Path,Is about subject,Type of analysis,Description,Keywords
./,,,Directory with samples,sample|lab,
test.txt,Subject 1,https://institut-curie.org/analysis#O6-12,,
```

This specified the table:

Path	Is about subject	Type of analysis	Description	Keywords
./			Directory with samples	sample|lab
	test.txt	Subject 1	https://institut-curie.org/analysis#O6-12	

Metadata

Explore metadata and find associated collections and files.



Interfaces for accessing and querying data (API)

The data in Fairspace can be accessed via Application Programming Interfaces (APIs). The user interfaces application uses those APIs, but also other programs can use them, e.g., for automated data uploading or for exporting data for further processing or for synchronisation with other systems.

Authentication

All API endpoints require authentication via an authorisation header. To enable WebDAV clients to connect to Fairspace, also so-called *Basic authentication* is supported.

For secure authentication, it is strongly advised to use the *OpenID Connect (OICD) / OAuth2* workflow. The user interface application also uses this workflow.

When using the APIs in automated scripts, ensure that an account is used with only the required privileges (conform the *principle of least privilege*). I.e., when an admin account is not needed, use a non-admin account. For adding shared metadata, an account with *Add shared metadata* role is required, see Uploading metadata.

When an action is done on behalf of a specific user, do not use a service account or system account for the action directly, but obtain a token for that user first, e.g., by using the impersonation feature of Keycloak. That way the audit logging still captures which user did what.

OpenID Connect (OICD) / OAuth2 workflow

Fairspace supports OpenID Connect authentication via Keycloak. The workflow for API access is roughly as follows.

- The client authenticates with the token endpoint of the identity provider (Keycloak) and obtains a signed access token
- The client uses the access token in the request header when connecting to the Fairspace API
- Fairspace receives the request with the access token and validates if the token is valid, using the public key of the identity provider.

The token endpoint of Keycloak supports refreshing the token if it is close to expiry. However, checking the token expiration and refreshing make the authentication logic quite complex.

You can either obtain a fresh token before every API request or use an existing library that implements the authentication workflow. For finding available client-side libraries, check the Securing applications and services guide of Keycloak.

For use in scripts, it is advised to obtain a token for offline access, using the Offline access feature of OpenID Connect.

Code to obtain the OpenID Connect authorisation header (Python)

```python
import logging
import os
import requests

log = logging.getLogger()

def fetch_access_token(keycloak_url: str,
                       realm: str,
                       client_id: str,
                       client_secret: str,
                       username: str,
                       password: str) -> str:
    """
    Obtain access token from Keycloak
    :return: the access token as string.
    """
    params = {
        'client_id': client_id,
        'client_secret': client_secret,
        'username': username,
        'password': password,
        'grant_type': 'password'
    }
    headers = {
        'Content-type': 'application/x-www-form-urlencoded',
        'Accept': 'application/json'
    }
    response = requests.post(f'{keycloak_url}/auth/realms/{realm}/protocol/openid-connect/token',
                             data=params,
                             headers=headers)
    if not response.ok:
        log.error('Error fetching token!', response.json())
        raise Exception('Error fetching token.')
    data = response.json()
    token = data['access_token']
    log.info(f"Token obtained successfully. It will expire in {data['expires_in']} seconds")
    return token

def auth():
    keycloak_url = os.environ.get('KEYCLOAK_URL')
    realm = os.environ.get('KEYCLOAK_REALM')
    client_id = os.environ.get('KEYCLOAK_CLIENT_ID')
    client_secret = os.environ.get('KEYCLOAK_CLIENT_SECRET')
    username = os.environ.get('USERNAME')
    password = os.environ.get('PASSWORD')
    token = fetch_access_token(keycloak_url, realm, client_id, client_secret, username, password)
    return f'Bearer: {token}'
```

Code to obtain the OpenID Connect authorisation header (bash, curl)

Requires the jq JSON parser.

```
fetch_access_token() {
  curl -s \
    -d "client_id=${KEYCLOAK_CLIENT_ID}" \
    -d "client_secret=${KEYCLOAK_CLIENT_SECRET}" \
    -d "username=${USERNAME}" \
    -d "password=${PASSWORD}" \
    -d 'grant_type=password' \
    "${KEYCLOAK_SERVER_URL}/auth/realms/${KEYCLOAK_REALM}/protocol/openid-
connect/token" | jq -r '.access_token'
}
ACCESS_TOKEN=$(fetch_access_token)
```

Basic authentication

For WebDAV client access and for a simpler authentication method during testing, Fairspace also supports *Basic authentication*, which means that the `base64` encoded `username:password` string is sent in the `Authorization` header together with a prefix `Basic` .

This authentication method is considered to be less secure than token based authentication, because it requires scripts to have a plain text password stored somewhere. Also, users may have to retype their passwords when logging in, tempting them to choose less secure, easier to remember, passwords.

Code to generate the Basic authorisation header (Python)

```
import base64
import os

def auth():
    username = os.environ.get('USERNAME')
    password = os.environ.get('PASSWORD')
    return f"Basic {base64.b64encode(f'{username}:{password}'.encode()).decode()}"
```

Code to generate the Basic authorisation header (bash)

```
AUTH_HEADER="Basic $(echo -n "${USERNAME}:${PASSWORD}" | base64)"
```

Examples

In the examples in this documentation, we assume one of both methods to be available.

This means for the Python examples that a function `auth()` should be implemented that returns the authorisation header value, see the examples above.

```
import os
from requests import Response, Session

def auth():
    """ Returns authorisation header
    Replace this with an implementation from one of the sections above.
    """
    pass

server_url = os.environ.get('FAIRSPACE_URL')
headers = {
    'Authorization': auth()
}
response = Session().get(f'{server_url}/api/users/current', headers)
if not response.ok:
    raise Exception(f"Error fetching current user: {response.status_code} {response
.reason}")
print(response.json())
```

For examples using curl, an authorisation header needs to be passed using the `-H` option.

For basic authentation:

```
AUTH_HEADER="Basic $(echo -n "${USERNAME}:${PASSWORD}" | base64)"
curl -i -H "Authorization: ${AUTH_HEADER}" "${FAIRSPACE_URL}/api/users/current"
```

For OpenID Connect:

```
# ACCESS_TOKEN=...
AUTH_HEADER="Bearer ${ACCESS_TOKEN}"
curl -i -H "Authorization: ${AUTH_HEADER}" "${FAIRSPACE_URL}/api/users/current"
```

Automatic authentication in Jupyter Hub

In Jupyter Hub, users are automatically authenticated and can directly connect to the local API address without adding authentication headers.

WebDAV

A file storage API is exposed via the WebDAV protocol for accessing the file system via the web. It runs on `/api/webdav/`.

This endpoint can be used by many file explorers, including Windows Explorer, and by tools like FileZilla and Cyberduck. Use `https://fairspace.example.com/api/webdav/` or

`davs://fairspace.example.com/api/webdav/` as location, with `fairspace.example.com` replaced by the server name.

All visible collections in the system are exposed as top-level directories. Creating a top-level directory via WebDAV will result in an error message, see Create collection or directory.

The Web-based Distributed Authoring and Versioning (WebDAV) protocol allows users to operate on collections and files. Fairspace exposes a WebDAV API for accessing the file systems, while restricting access to only the files accessible by the user.

The WebDAV API allows to upload and download files and to perform standard file operations such as copying or moving, as well as custom operations, such as collection lifecycle management and advanced data loss prevention features such as versioning and undeletion.

Directory listing and path properties

`PROPFIND /api/webdav/{path}/`	
Request headers:	
`Depth`	When `0` only the information about the path is returned, when `1` the contents of the directory is returned, if the path is a directory.
`Show-Deleted`	Include deleted paths when the value is `on`. (*Optional*)
`Version`	Specify a version number to request properties of a specific file version. The first version has number `1`. If not specific, the current version is returned.
Request body:	
To include also custom Fairspace attributes in the response, like the collection description, send the following request body: `<propfind><allprop /></propfind>`	

Code examples

Check if path exists (Python)

```
import logging
import os
from requests import Request, Response, Session

log = logging.getLogger()

server_url = os.environ.get('FAIRSPACE_URL')

def exists(path):
    """ Check if a path exists
    """
    headers = {
        'Depth': '0',
        'Authorization': auth()
    }
    session = Session()
    req = Request('PROPFIND', f'{server_url}/api/webdav/{path}/', headers,
cookies=session.cookies)
    response: Response = session.send(req.prepare())
    return response.ok
```

Fetch directory listing (Python)

```
import logging
import os
from requests import Request, Response, Session
from xml.etree.ElementTree import fromstring

log = logging.getLogger()

server_url = os.environ.get('FAIRSPACE_URL')

def ls(path: str):
    """ List contents of path
    """
    headers = {
        'Depth': '1',
        'Authorization': auth()
    }
    session = Session()
    req = Request('PROPFIND', f'{server_url}/api/webdav/{path}', headers, cookies
=session.cookies)
    response: Response = session.send(req.prepare())
    if not response.ok:
        raise Exception(f"Error fetching directory '{path}': {response.
status_code} {response.reason}")
    tree = fromstring(response.content.decode())
    for item in tree.findall('{DAV:}response'):
        print(item.find('{DAV:}href').text)
```

Fetch directory listing (curl)

Requires the xmlstarlet tool.

```
curl -s -H "Authorization: ${AUTH_HEADER}" -X PROPFIND -H "Depth: 1" "
${FAIRSPACE_URL}/api/webdav/${path}" -d '<propfind><allprop /></propfind>' \
| xmlstarlet sel -T -t -m d:multistatus/d:response -v
d:propstat/d:prop/d:displayname -n
```

Example response

Example `PROPFIND` response

Example response using `PROPFIND` on the root location `https://fairspace.ci.fairway.app/api/webdav` with `Depth: 1` and request body `<propfind><allprop /></propfind>`. Adding the `<allprop />` in the request results in custom Fairspace properties, like the description (`ns1:comment`), to be included in the WebDAV response.

```
<?xml version="1.0" encoding="utf-8" ?>
<d:multistatus xmlns:ns1="https://fairspace.nl/ontology#" xmlns:d="DAV:">
    <d:response>
        <d:href>/api/webdav/</d:href>
        <d:propstat>
            <d:prop>
                <d:getcontenttype></d:getcontenttype>
                <d:getetag>
"https://fairspace.ci.fairway.app/api/webdav"</d:getetag>
                <d:iscollection>TRUE</d:iscollection>
                <d:displayname></d:displayname>
                <d:isreadonly>TRUE</d:isreadonly>
                <d:name></d:name>
                <d:supported-report-set></d:supported-report-set>
                <d:resourcetype>
                    <d:collection/>
                </d:resourcetype>
            </d:prop>
            <d:status>HTTP/1.1 200 OK</d:status>
        </d:propstat>
    </d:response>
    <d:response>
        <d:href>/api/webdav/Demonstration/</d:href>
        <d:propstat>
            <d:prop>
                <ns1:access>Write</ns1:access>
                <ns1:canRead>TRUE</ns1:canRead>
                <ns1:userPermissions>http://fairspace.ci.fairway.app/iri/user-iri
Manage
                </ns1:userPermissions>
                <ns1:accessMode>Restricted</ns1:accessMode>
                <ns1:availableStatuses>Active</ns1:availableStatuses>
                <ns1:canDelete>FALSE</ns1:canDelete>
                <ns1:iri>
https://fairspace.ci.fairway.app/api/webdav/Demonstration</ns1:iri>
                <ns1:canWrite>TRUE</ns1:canWrite>
                <ns1:ownedByName>Demo</ns1:ownedByName>
                <ns1:canManage>FALSE</ns1:canManage>
                <ns1:canUndelete>FALSE</ns1:canUndelete>

<ns1:workspacePermissions>http://fairspace.ci.fairway.app/iri/workspace-iri
                    Write
                </ns1:workspacePermissions>
```

```
                <ns1:createdBy>http://fairspace.ci.fairway.app/iri/user-
iri</ns1:createdBy>
                <ns1:comment>Demonstration collection</ns1:comment>
                <ns1:availableAccessModes>Restricted</ns1:availableAccessModes>
                <ns1:ownedBy>http://fairspace.ci.fairway.app/iri/workspace-
iri</ns1:ownedBy>
                <ns1:status>Active</ns1:status>
                <d:getcreated>2021-02-02T12:12:33Z</d:getcreated>
                <d:creationdate>2021-02-02T12:12:33Z</d:creationdate>
                <d:getcontenttype>text/html</d:getcontenttype>

<d:getetag>"https://fairspace.ci.fairway.app/api/webdav/Demonstration"</d:getetag>
                <d:iscollection>TRUE</d:iscollection>
                <d:displayname>Demonstration collection</d:displayname>
                <d:isreadonly>FALSE</d:isreadonly>
                <d:name>Demonstration collection</d:name>
                <d:supported-report-set></d:supported-report-set>
                <d:resourcetype>
                    <d:collection/>
                </d:resourcetype>
            </d:prop>
            <d:status>HTTP/1.1 200 OK</d:status>
        </d:propstat>
    </d:response>
</d:multistatus>
```

Create collection or directory

`MKCOL /api/webdav/{path}/`	
Create collection or directory	
Request headers:	
`Owner`	Specify the identifier of the owner workspace when creating a collection.

Example create collection or directory (Python)

```
import logging
import os
from requests import Request, Response, Session

log = logging.getLogger()

server_url = os.environ.get('FAIRSPACE_URL')

def mkdir(path: str, workspace_iri: str=None):
    # Create directory
    headers = {
        'Authorization': auth()
    }
    if workspace is not None:
        headers['Owner'] = workspace_iri
    req = Request('MKCOL', f'{server_url}/api/webdav/{path}/', headers, cookies
=self.session().cookies)
    response: Response = Session().send(req.prepare())
    if not response.ok:
        raise Exception(f"Error creating directory '{path}': {response.
status_code} {response.reason}")
```

Example create collection or directory (curl)

```
# Create a new collection, owned by workspace WORKSPACE_IRI
NEW_COLLECTION=New collection
WORKSPACE_IRI=http://fairspace.ci.fairway.app/iri/workspace-iri
curl -i -H "Authorization: ${AUTH_HEADER}" -X MKCOL -H "Owner: ${WORKSPACE_IRI}"
"${FAIRSPACE_URL}/api/webdav/${NEW_COLLECTION}"
# Create a new directory in the newly created collection
curl -i -H "Authorization: ${AUTH_HEADER}" -X MKCOL "${FAIRSPACE_URL}
/api/webdav/${NEW_COLLECTION}/Test directory"
```

Upload files

`POST /api/webdav/{path}/` `action=upload_files`	
Request data:	
`action`	`upload_files`
`files`	Send files with the target file names as keys, see the examples below.

Example uploading files (Python)

```
import logging
import os
from requests import Response, Session

log = logging.getLogger()

server_url = os.environ.get('FAIRSPACE_URL')

def upload_files(path: str, files: Dict[str, any]):
    # Upload files
    response: Response = Session().post(f'{server_url}/api/webdav/{path}/',
            headers={'Authorization': auth()},
            data={'action': 'upload_files'},
            files=files)
    if not response.ok:
        raise Exception(f"Error uploading files into '{path}': {response
.status_code} {response.reason}")
```

Example uploading files (curl)

```
# Upload files 'coffee.jpg' and 'coffee 2.jpg' to a collection
path="new collection"
curl -i -H "Authorization: ${AUTH_HEADER}" -X POST -F 'action=upload_files' -F
'coffee.jpg=@coffee.jpg' -F 'coffee 2.jpg=@coffee 2.jpg'"${FAIRSPACE_URL
}/api/webdav/${path}"
```

Copy and move a directory or file

`COPY /api/webdav/{path}/`	
Copy a directory or file.	
Request headers:	
`Destination`	The destination path relative to the server, URL encoded, e.g., `/api/webdav/collection%20abc/test.txt`.

Example copy path (curl)

```
# Copy 'Examples/Test dir/test 1.txt' to 'Examples/Test dir/test 2.txt'
path="Examples/Test dir/test 1.txt"
target="/api/webdav/Examples/Test%20dir/test%202.txt"
curl -i -H "Authorization: ${AUTH_HEADER}" -X COPY -H "Destination: ${target}" "
${FAIRSPACE_URL}/api/webdav/${path}"
```

`MOVE /api/webdav/{path}/`	
Move or rename a directory or file	
Request headers:	
`Destination`	The destination path relative to the server, URL encoded, e.g., `/api/webdav/collection%20abc/test.txt`.

Example copy path (curl)

```
# Move 'Examples/Test dir/test 1.txt' to 'Examples/Test dir/test 2.txt'
path="Examples/Test dir/test 1.txt"
target="/api/webdav/Examples/Test%20dir/test%202.txt"
curl -i -H "Authorization: ${AUTH_HEADER}" -X MOVE -H "Destination: ${target}" "
${FAIRSPACE_URL}/api/webdav/${path}"
```

Undelete a directory or file

`POST /api/webdav/{path}/` `action=undelete`	
Undelete a directory or file	
Request headers:	
`Show-deleted`	`on`
Request data:	
`action`	`undelete`

Example undelete path (curl)

```
curl -i -H "Authorization: ${AUTH_HEADER}" -X POST -F "action=undelete" "
${FAIRSPACE_URL}/api/webdav/${path}"
```

Revert to a file version

`POST /api/webdav/{path}/` `action=revert`	
Restore a previous file version	
Request data:	
`action`	`revert`
`version`	The version number to restore.

Example revert file version (curl)

```
curl -i -H "Authorization: ${AUTH_HEADER}" -X POST -F "action=revert" -F
"version=${version}" "${FAIRSPACE_URL}/api/webdav/${path}"
```

Other collection actions

On collections, a number of actions is available. These are not documented here in detail, but can be used from the user interface instead.

Action	Description
`set_access_mode`	Change the access mode of a collection.
`set_status`	Change the status of a collection.
`set_permission`	Change the permission of the specified user or workspace on a collection.
`set_owned_by`	Transfer ownership of a collection to another workspace.
`unpublish`	Unpublish a published collection.

SPARQL

The SPARQL API is a standard API for querying RDF databases. This endpoint is read-only and can be used for advanced search, analytics, data extraction, etc.

`POST /api/rdf/query`		
SPARQL query		
Parameters:		
`query`	SPARQL	Query.
`aggregate`	boolean	Include aggregates.

Example SPARQL query using curl

```
curl -X POST -H 'Content-Type: application/sparql-query' -H 'Accept:
application/json' \
-d '{
  "query": "
    PREFIX example: <https://example.com/ontology#>
    PREFIX fs:    <https://fairspace.nl/ontology#>

    SELECT DISTINCT ?sample
    WHERE {
      ?sample a example:BiologicalSample .
      FILTER NOT EXISTS { ?sample fs:dateDeleted ?anyDateDeleted }
    }
    # ORDER BY ?sample
    LIMIT 500",
  "aggregate": True
}' \
"http://localhost:8080/api/rdf/query"
```

RDF metadata

For reading and writing metadata to the database, the `/api/metadata` endpoint supports a number of operations:

- `GET`: Retrieve metadata for a specified subject, predicate or object.
- `PUT`: Add metadata
- `PATCH`: Update metadata
- `DELETE`: Delete specified triples or all metadata linked to a subject.

The metadata is stored as subject-predicate-object triples. The API supports several serialisation formats for sending :

- Turtle (`text/turtle`)
- JSON-LD (`application/ld+json`, JSON schema)
- N-Triples (`application/n-triples`)

After any update, the metadata must be consistent with the data model, see Data model and view configuration. If an update would violate the data model constraints, the request is rejected with a status `400` response, with a message indicating the violation.

Uploading metadata

Shared metadata entities will in most cases come from other systems and will be added to Fairspace exclusively by an ETL process which will extract data from the laboratory and clinical systems, perform pseudonymization of identifiers, convert the metadata to some RDF-native format

conforming the data model and send them to Fairspace.

Fairspace will validate the uploaded metadata against the constraints defined in the data model and returns a detailed error message in case of violations. The validations include all the necessary type checks, referential consistency (validity of identifiers) checks, validation of mandatory fields, etc. If any entity violates the constraints, the entire bulk upload will be rejected.

The ETL process will use a special technical account with the *Add shared metadata* role. Regular users will not be able to add or modify shared metadata entities. Regular users can link files to shared metadata entities, see Metadata forms and Metadata upload.

In addition to the main ETL workflow, data managers needs a possibility to add or modify certain properties of top-level metadata entities. This can be done using the RDF-based metadata API.

A number of guidelines for uploading shared metadata:

- Entities must have a type, a globally unique identifier, and a unique label for the type.
  It is advised to use a unique identifier from an existing reference system for this purpose.
- Because of the nature of linked data, it is advised to add shared metatdata entities in an append-only fashion: only adding entities and avoid updating or deleting entities.
- By nature of RDF, metadata is typically added on the level of triples. E.g., when adding a property `dcat:keyword` to a file, this will add a key word to the (possibly) already existing list of key words.
  If you want to completely replace (or remove) a property from an entity, use the `PATCH` method instead of `PUT`.

Example metadata file in turtle format: `testdata.ttl`:

```
@prefix example: <https://example.com/ontology#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix subject: <http://example.com/subjects#> .
@prefix file: <http://example.com/api/webdav/> .
@prefix gender: <http://hl7.org/fhir/administrative-gender#> .
@prefix ncbitaxon: <https://bioportal.bioontology.org/ontologies/NCBITAXON/> .
@prefix dcat: <http://www.w3.org/ns/dcat#> .

subject:s1 a example:Subject ;
    rdfs:label "Subject 1" ;
    example:isOfSpecies ncbitaxon:9606 .

file:coll1\/coffee.jpg
    dcat:keyword "fairspace", "java" ;
    example:aboutSubject example:s1 .
```

Example uploading metadata file using Python.

```
import logging
import os
from requests import Response, Session

log = logging.getLogger()

server_url = os.environ.get('FAIRSPACE_URL')

with open('testdata.ttl') as testdata:
    response: Response = Session().put(f"{server_url}/api/metadata/",
        data=testdata.read(),
        headers={
            'Authorization': auth(),
            'Content-type': 'text/turtle'
        })
    if not response.ok:
        raise Exception(f"Error uploading metadata: {response.status_code}
{response.reason}")
```

Example uploading metadata file using curl.

```
curl -v -X PUT -H "Authorization: Basic $(echo -n "${USERNAME}:${PASSWORD}" |
base64)" \
  -H "Content-type: text/turtle" --data @testdata.ttl "${FAIRSPACE_URL
}/api/metadata/"
```

API specification

`GET /api/metadata/`		
Retrieve metadata		
Parameters:		
`subject`	string	The subject to filter on.
`predicate`	string	The predicate to filter on, not required.
`object`	string	The object to filter on, not required.

`GET /api/metadata/`		
`includeObjectProperties`	boolean	If set, the response will include several properties for the included objects. The properties to be included are marked with `fs:importantProperty` in the vocabulary.
Response:		
Returns serialised triples matching the query parameters.		

Example of retrieving metadata using curl

Request metadata for the triple with subject 'a', predicate 'b' and object 'c'.

```
curl -G -H "Accept: application/ld+json" \
--data-urlencode "subject=a" \
--data-urlencode "predicate=b" \
--data-urlencode "object=c" \
--data-urlencode "withValueProperties=true" \
"http://localhost:8080/api/metadata/"
```

`PUT /api/metadata/`
Add metadata. Existing metadata is left untouched. The data must be consistent with the data model after the update (see Data model and view configuration), otherwise `400` is returned. Only available for users with *Add shared metadata* role.
Request body:
Serialised RDF triples.
Response:
Response contains the workspace name and newly assigned IRI.

Example of adding metadata using curl

```
curl -X PUT -H "Content-type: application/ld+json" -d \
'{
  "@graph" : [ {
    "@id" : "ws:7f0ed5bb-7a96-4715-8727-6b4b7f1facfd",
    "hasData" : "ws:4bcd1780-c9cd-4bdd-0000-1ce966ff9ac3"
   } ],
  "@context" : {
    "hasData" : {
      "@id" : "http://fairspace.ci.fairway.app/vocabulary/hasData",
      "@type" : "@id"
    },
    "ws" : "http://fairspace.ci.fairway.app/iri/"
  }
}' \
"http://localhost:8080/api/metadata/"
```

`PATCH /api/metadata/`
Update metadata. Any existing metadata for a given subject/predicate combination will be overwritten with the provided values. The data must be consistent with the data model after the update (see Data model and view configuration), otherwise `400` is returned. Only available for users with *Add shared metadata* role.
Request body:
Serialised RDF triples.
Response:
Response contains the workspace name and newly assigned IRI.

Example of updating metadata using curl

```
curl -X PATCH -H "Content-type: application/ld+json" -d \
'{
  "@graph" : [ {
    "@id" : "ws:7f0ed5bb-7a96-4715-8727-6b4b7f1facfd",
    "hasData" : "ws:4bcd1780-c9cd-4bdd-0000-1ce966ff9ac3"
   } ],
  "@context" : {
    "hasData" : {
      "@id" : "http://fairspace.ci.fairway.app/vocabulary/hasData",
      "@type" : "@id"
    },
    "ws" : "http://fairspace.ci.fairway.app/iri/"
  }
}' \
"http://localhost:8080/api/metadata/"
```

`DELETE /api/metadata/`		
Delete metadata. If a request body is provided, the triples specified in the body will be deleted. Otherwise, the subject specified in the subject parameter will be marked as deleted. Please note that the subject will still exist in the database. Only available for users with *Add shared metadata* role.		
Parameters:		
`subject`	string	The subject to filter on. (*Optional*)
Request body:		
Serialised RDF triples. (*Optional*)		

Example of deleting metadata using curl

```
curl -X DELETE -H "Content-Type: application/ld+json" -d \
'{
  "@graph" : [ {
    "@id" : "ws:7f0ed5bb-7a96-4715-8727-6b4b7f1facfd",
    "hasData" : "ws:4bcd1780-c9cd-4bdd-0000-1ce966ff9ac3"
   } ],
  "@context" : {
    "hasData" : {
      "@id" : "http://fairspace.ci.fairway.app/vocabulary/hasData",
      "@type" : "@id"
    },
    "ws" : "http://fairspace.ci.fairway.app/iri/"
  }
}' \
"http://localhost:8080/api/metadata/"
```

Metadata views

Metadata views endpoint used for metadata-based search.

`GET /api/views/`
List all views with available columns per each view.

Example using curl

```
curl -H "Accept: application/json" "http://localhost:8080/api/views/"
```

`POST /api/views/`		
Fetch page of rows of a view matching the request filters.		
Parameters:		
`view`	string	Name of the view.
`filters`	List of filters, based on available facets and their values. Each filter has to contain a "field" property, matching the name of a facet, and list of values to filter on.	
`page`	integer	Requested page
`size`	integer	Page size

Example fetching page of view rows using curl

```
curl -X POST -H 'Content-type: application/json' -H 'Accept: application/json' -d
\
'{
  "view":"Resource",
  "filters":[
    {
      "field":"Resource_type",
      "values":["https://fairspace.nl/ontology#Collection"]
    }
  ],
  "page":1,
  "size":100
}' \
"http://localhost:8080/api/views/"
```

`POST /api/views/count`		
Count rows of a view matching request filters.		
Parameters:		
`view`	string	Name of the view.
`filters`	List of filters, based on available facets and their values. Each filter has to contain a "field" property, matching the name of a facet, and list of values to filter on.	

Example counting view rows using curl

```
curl -X POST -H 'Content-type: application/json' -H 'Accept: application/json' -d
\
'{
  "view":"Resource",
  "filters":[
    {
      "field":"Resource_type",
      "values":["https://fairspace.nl/ontology#Collection"]
    }
  ]
}' \
'http://localhost:8080/api/views/count'
```

`GET /api/views/facets`
List all facets with available values per each facet.

Example retrieving facets with values using curl

```
curl -H "Accept: application/json" "http://localhost:8080/api/views/facets"
```

Workspace management

Operations on workspace entities.

`GET /api/workspaces/`	
List all available workspaces.	
Response contains the following data:	
`iri`	Unique workspace IRI.
`name`	Unique workspace name.
`comment`	Workspace description in markdown format.
`managers`	List of workspace managers.
`summary`	Short summary on the workspace - how many collections and how many users it has.
`canCollaborate`	If a current user is added to the workspace as a collaborator.
`canManage`	If a current user is a workspace manager.

Example of listing available workspaces using curl

```
curl -H "Accept: application/json" "http://localhost:8080/api/workspaces/"
```

`PUT /api/workspaces/`		
Add a workspace. Available only to administrators.		
Parameters:		
`name`	string	Unique workspace name.
Response:		
Response contains the workspace name and newly assigned IRI.		

Example of adding a workspace using curl

```
curl -X PUT -H "Accept: application/json" -d '{"name": "test workspace"}'
"http://localhost:8080/api/workspaces/"
```

`PATCH /api/workspaces/`		
Update a workspace.		
Parameters:		
`iri`	string	Unique workspace IRI *(required)*.
`name`	string	Unique workspace name.
`comment`	Markdown	Workspace description in markdown format.

Example of updating a workspace using curl

```
curl -X PATCH -H "Accept: application/json" -d \
'{
  "iri": "http://fairspace.com/iri/123,
  "name": "new test name",
  "comment": "New description"
}"' \
"http://localhost:8080/api/workspaces/"
```

`DELETE /api/workspaces/`		
Delete a workspace. Available only to administrators.		
Parameters:		
`workspace`	string	Workspace IRI (URL-encoded).

Example of deleting a workspace using curl

```
curl -X DELETE --data-urlencode "workspace=http://fairspace.com/iri/123"
"http://localhost:8080/api/workspaces/"
```

Workspace users

`GET /api/workspaces/users`		
List all workspace users with workspace roles.		
Parameters:		
`workspace`	string	Workspace IRI (URL-encoded).
Response:		
Response contains list of workspace users with their workspace roles.		

Example of listing workspace users using curl

```
curl -H 'Accept: application/json'
'http://localhost:8080/api/workspaces/users?workspace=http://fairspace.com/iri/123
'
```

`PATCH /api/workspaces/users`		
Update workspace users and their workspace roles.		
Parameters:		
`workspace`	string	Workspace IRI (URL-encoded).
Response:		
Response contains list of workspace users with their updated workspace roles.		

Example of updating workspace users using curl

```
curl -H 'Accept: application/json' --data-urlencode
"workspace=http://fairspace.com/iri/123"
"http://localhost:8080/api/workspaces/users"
```

Users and permissions

`GET /api/users/`
List all organisation users.
Response:
Returns list of users with user's unique ID, name, email, username and user's organisation-level permissions: if a user is an administrator, super-administrator or can view public metadata, view public data or add shared metadata.

Example listing users using curl

```
curl -H 'Accept: application/json' 'http://localhost:8080/api/users/'
```

`PATCH /api/users/`		
Update user roles.		
Parameters:		
`id`	string	Id of the user for which roles will be updated.

PATCH /api/users/		
"role name"	boolean	Role name is any of `isAdmin`, `canViewPublicData`, `canViewPublicMetadata` or `canAddSharedMetadata`. The value determines whether the user has the role or not.

Example updating user roles using curl

```
curl -X PATCH -H "Accept: application/json" -d \
'{
  "id": "xyz-0000",
  "canViewPublicData": false,
  "canViewPublicMetadata": true
}' \
"http://localhost:8080/api/users/"
```

GET /api/users/current
Get current user.
Response:
Returns current user's unique ID, name, email, username and user's organisation-level permissions: if the user is an administrator, super-administrator or can view public metadata, view public data or add shared metadata.

Example getting current user using curl

```
curl -H "Accept: application/json" "http://localhost:8080/api/users/current"
```

POST /api/users/current/logout
logout the current user.

Example logging out using curl

```
curl -X POST "http://localhost:8080/api/users/current/logout"
```

Configuration endpoints

Vocabulary

The vocabulary contains a description of the structure of the metadata. It contains the types of

entities that can be created, along with the data types for the fields. It is stored in SHACL format.

`GET /api/vocabulary/`
Retrieve a representation of the vocabulary.

Example fetching the vocabulary in turtle format using curl

```
curl -H 'Accept: text/turtle' 'http://localhost:8080/api/vocabulary/'
```

Example fetching the vocabulary in json-ld format using curl

```
curl -H 'Accept: application/json+ld' 'http://localhost:8080/api/vocabulary/'
```

Features

`GET /api/features/`
List available application features.

Response contains list of additional features that are currently available in the application, e.g., metadata editing in the user interface.

Example listing features using curl

```
curl -H 'Accept: application/json' 'http://localhost:8080/api/features/'
```

Services

`GET /api/services/`
List linked services.

Response contains list of external services linked to Fairspace, e.g. JupyterHub, cBioPortal, etc.

Example listing services using curl

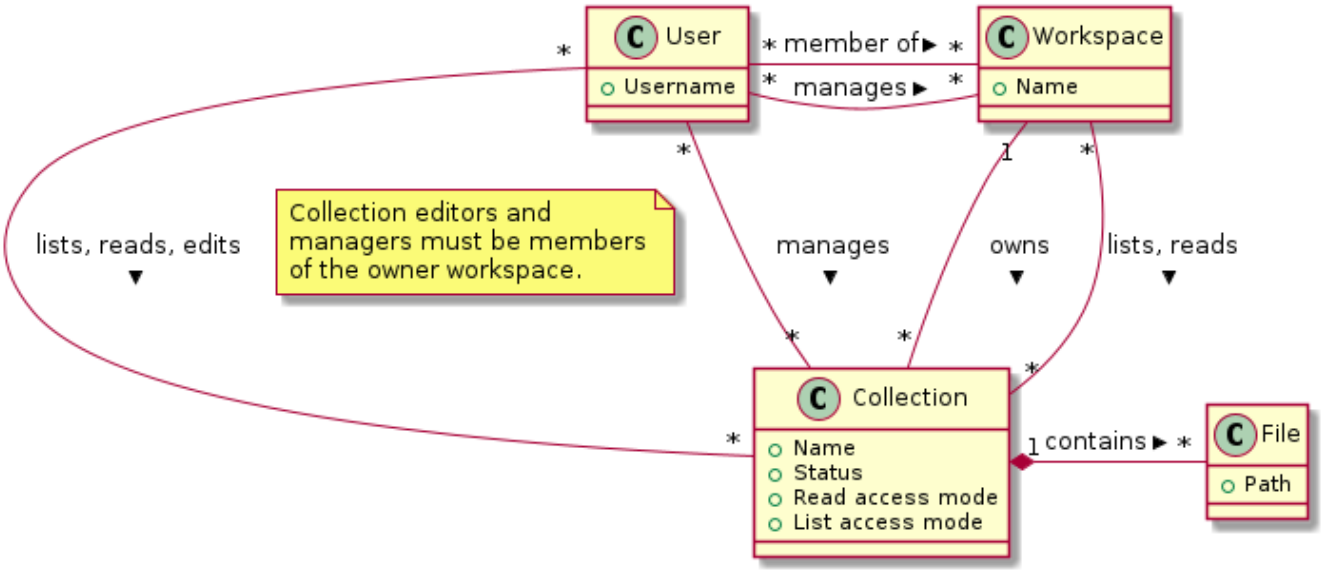
```
curl -H 'Accept: application/json' 'http://localhost:8080/api/services/'
```

Structure and terminology

In this section we describe in detail the main concepts and components of the Fairspace data repository and how they relate to each other.

The core entities of the data repository are:

- *Users*: individual users in the organisation, looking for data, contributing to data collections or managing data.
- *Workspaces* (for projects, teams): entities in the system linked, representing a group of users, to organise data collections and data access.
- *Collections*: entities in the system to group data files. These are the minimal units of data for data access and data modification rules.
- *Files*: The smallest units of data that the system processes. Files always belong to a single collection. Files can be added, changed and deleted, but not in all collection states. Changing a file creates a new version. Access to a file is based on access to the collection the file belongs to. Files can be organised in *Directories*, which we will leave out of most descriptions for brevity.



The diagram above sketches the relevant entities and actors. The basic structure consists of users, workspaces, collections and files as represented in the system. Collections are the basic units of data access management. A collection is owned by a workspace. The responsibility for a collection is organised via the owner workspace: members of the owner workspace can be assigned as editors or managers of the collection. This reflects the situation where in an organisation, a data collection belongs to a project or a research team. This way the workspace represents the organisational unit that is responsible for a number of data collections (e.g., a research team or project). Data can be shared with other workspaces or individual users (for reading) and ownership may be transferred to another workspace (e.g., in the case the workspace is temporary, or when the organisation changes).

Fairspace provides a *data catalogue*, containing all the metadata, which is visible for all users with catalogue access (*View public metadata*). Users with metadata write access (*Add shared metadata*) can add metadata to the catalogue. Preferably this is done by an automated process that ensures

the consistency of the metadata and uniqueness of metadata entities. Metadata on collection and file level is protected by the access policy of the collections.

User administration is organised in an external component ([Keycloak]), but user permissions are stored in Fairspace. A back end application is responsible for storing the data and metadata, and for providing APIs for securely retrieving and adding data and metadata using standard data formats and protocols. A user interface application provides an interactive file manager and (meta)data browser and data entry forms based on the back end APIs. Besides the data storage and data management, Fairspace offers *analysis environments* using Jupyter Hub. In Jupyter Hub, the data repository is accessible. Every user has a private working directory. We do no assumptions on the structure of the data or on the permissions of the external file systems that are connected to the data repository and referenced in the data catalogue. The organisation structure may be replicated in the different systems in incompatible ways, and the permissions may not be aligned.

Workflow and access modes

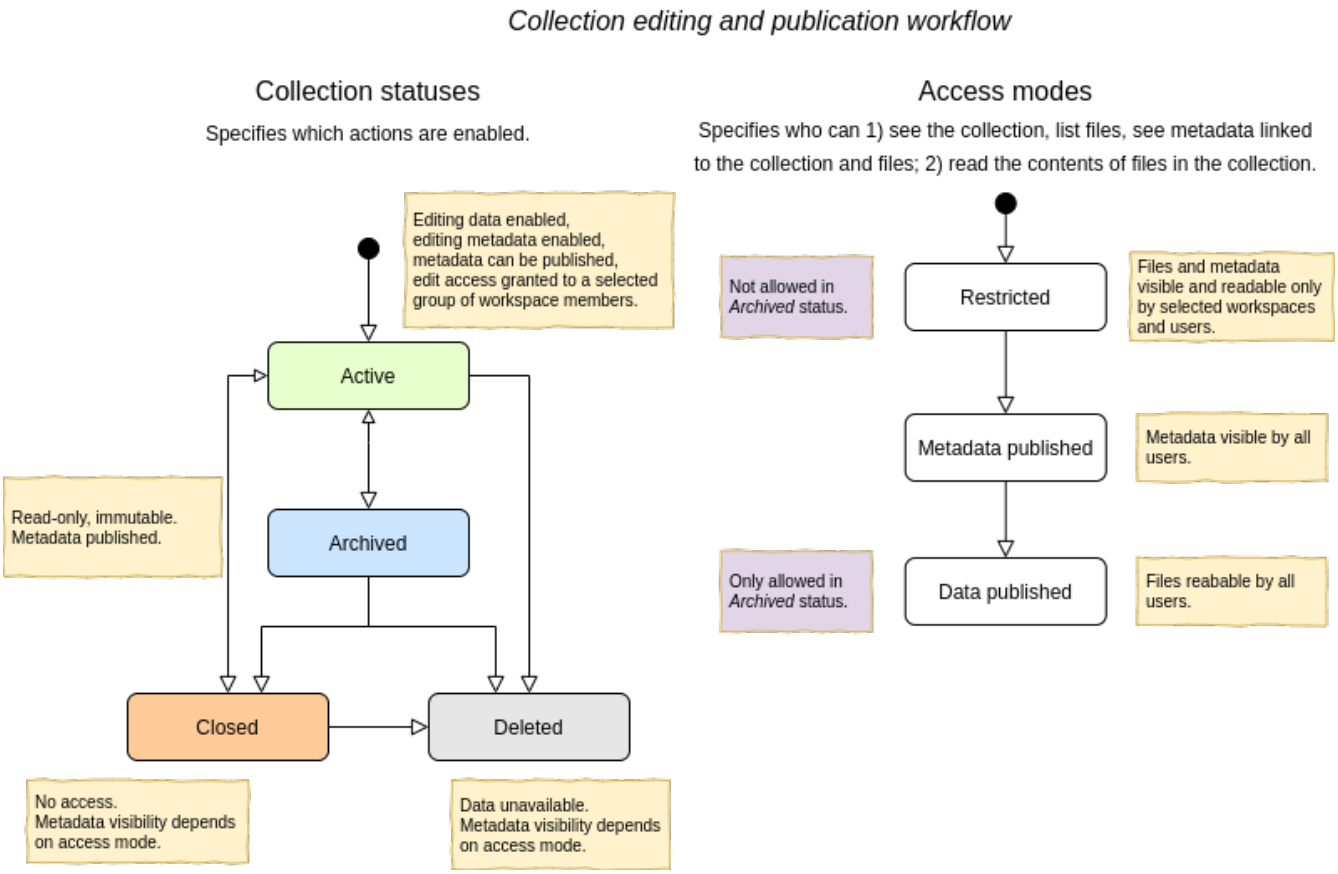
During the lifetime of a collection, different rules may be applicable for data modification and data access. In Fairspace, collections follow a workflow with the following statuses:

- *Active*: for the phase of data collection, data production and data processing;
- *Archived*: for when the data set is complete and is available for reuse;
- *Closed*: for when the data set should not be available for reading, but still needs to be preserved;
- *Deleted*: for when the data set needs to be permanently made unavailable. This status is irreversible. There is one exception to this rule – for the sake of data loss prevention, in special cases, administrators can still undelete a collection that was already deleted.

In these different statuses, different actions on the data are enabled or disabled. Also, visibility of the data and linked metadata depends partly on the collection status. We also distinguish three access modes for reading and listing files in a collection (where listing also includes seeing the metadata):

- *Restricted*: only access to explicitly selected workspaces and users;
- *Metadata published*: the collection and its files are visible, metadata linked to them is visible for all users;
- *Data published*: the files in the collection are readable for all users. This mode is irreversible. There is one exception to this rule – there might be a special situation, resulting from, e.g., a legal reason, when a collection has to be unpublished. This action is available to administrators, but it is highly discouraged, since the collection (meta)data may already be referenced in other systems.

The statuses and access modes, and the transitions between them are shown in the following diagram.



Roles and permissions

We distinguish the following roles in the solution:

- *User*: regular users can only view their own workspaces and collections.
- *View public metadata*: the user can view public metadata, workspaces, collections and files;
- *View public data*: the user can read public files;
- *Admin*: can create workspaces, assign roles and permissions;
- *Add shared metadata*: can add, modify and delete shared metadata entities.

Most users should have the *View public data* role. Only when the shared metadata may contain sensitive information that should not be visible for some users, the public data and public metadata roles should be discarded for those users.

Workspaces are used to organise collections in a hierarchy. On workspace level there are two access levels:

- *Manager*: can edit workspace details, manage workspace access and manage access to all collections that belong to the workspace;
- *Member*: can create a collection in the workspace.

Access to collections and files is managed on collection level. We distinguish the following access levels on collections:

- *List*: see collection, directory and file names and metadata properties/relations (only applicable

for collections shared via the *Metadata published* access mode);

- *Read*: read file contents;
- *Write*: add files, add new file versions, mark files as deleted;
- *Manage*: grant, revoke access to the collection, change collection status and modes.

Access levels are hierarchical: the *Read* level includes the *List* level; the *Edit* level includes *Read* level; the *Manage* level includes *Edit* and *Read* level access. The user that creates the collection gets *Manage* access.

Data model and view configuration

Metadata

Metadata is data about data. Metadata is used to describe data assets, e.g., for making it easier to find or use certain data. Because metadata is data itself, it can be difficult to make a proper distinction between data and metadata in a system.

Types of metadata

In a digital archive, *technical metadata* is linked to data assets, like file type, location, size, creation or modification dates, checksums for checking data integrity, ownership. Such metadata is essential for a system to store and retrieve data files. Technical metadata can also include data format specific properties, like encoding, data layout, resolution, etc., required to correctly read the data.
With most publications, *bibliographic metadata* is associated, such as author, title, abstract, publication details, keywords and subject categories. Such metadata makes it possible to find relevant publications. This is the kind of metadata used by libraries and archives and numerous standards exist for such data, such as Dublin Core and METS.

More detailed *descriptive metadata* provides information about the contents of the data, e.g., description of rows and columns, summary statistics, project information, geographical information, results, study design, methods, materials or equipment. In the extreme case, the entire content of the file is captured in descriptive metadata.

We can distinguish different kinds of descriptive metadata, such as:

- Description of the *contents* (rows, columns, values, summary statistics)
- Description of the *subject*, what the data is about (subject, topic, project, study design, object of study, time, location)
- Description of *data sources* (for derived or processed data)
- Description of the *methods* or technology used to produce or capture the data, such as scripts and versions.

In the context of health research data, it is essential to link data to research subjects, i.e., patients and samples.

The values of the metadata can be of any type, numerical, free text, date, conform to a controlled vocabulary (e.g., ICD or SNOMED codes, units, file types) or a reference to a typed entity within the database, or external entities.

Likewise, the data the metadata is about can be of any type, a file system, a tabular file, image, genomic data, a relational database, etc.

Purpose

Metadata is used for several purposes:

- Descriptors to enable use of the data (file type, file format, encoding, how it was created/generated). The metadata may be used by users or scripts to read or interpret a particular file or data set.
- Finding relevant data for analysis:
  - Metadata may be used to organise data within a data set that a researcher is working on, by using (study specific) categories linked to individual files.
  - Metadata may be used in search queries or navigation to find out if data is available that meets certain selection criteria (e.g., data types, categories, cohort characteristics), for inclusion in a new analysis.
  - Metadata may be used to identify data that is linked to a specific entity, such as a patient or a sample, to determine if such data has already been analysed, in order to avoid duplicate analysis.

It is important to identify for which purpose metadata is collected and used, as it may affect which types of metadata are collected, how they are navigated and if access control on metadata is desired or required.

Data model

To enable validation of (meta)data, and to enable intuitive navigation and search within the metadata, it is essential to have a good data model.
The data model consists of the entity types (classes), their properties (with types) and relationships between entities that can be represented in the system.

The data model needs to be broad (expressive) enough to allow users to express all relevant facts about data sets conveniently and accurately, but it needs to be specific enough to allow validation and the generation of useful overviews and information pages. International data standards should be used as much as possible to enable interoperability between systems.

E.g., it is probably better to use a specific field ‘disease’ where the value must be a valid ICD-10 code, than using a generic ‘description’ field where a disease is described in a free text field.

Data domains

We distinguish different data domains in order to clearly separate the data that is system specific and the metadata that is more flexible.

Workspaces and collection-level data

Users, workspaces, collections, directories and files are system-level entities, representing the file system of the system. Access to these entities is restricted by the workspace-level and collection-level access control. These entities cannot be changed on demand, but are inherent to the system. However, custom properties and relations may be added, e.g., to link files to patients.

Metadata

The data model for the other (non system-level) entities, the shared metadata, can be configured, in

order to make the metadata suitable for the environment where it is used. These metadata are used to link entities in the file system to entities in the research domain, such as samples, patients, diseases, diagnoses, or to entities in the organisation domain, such as projects. These entities may be displayed and navigated in the application and can be explored through the API (for technical users).

Controlled vocabularies

The data model may contain controlled vocabularies (e.g., disease codes, file types, project phases) that can be used as values in the metadata. Every value in a controlled vocabulary has a unique identifier and a label. Using such vocabularies enables standardisation and validation of metadata values.

Reference data

The data model may support domain specific entity types (patients, samples, genes, treatments, studies, etc.) or generic entity types (project, organisation, person, etc), defining the metadata objects that collection-level data assets can refer to. The reference data can also be linked.

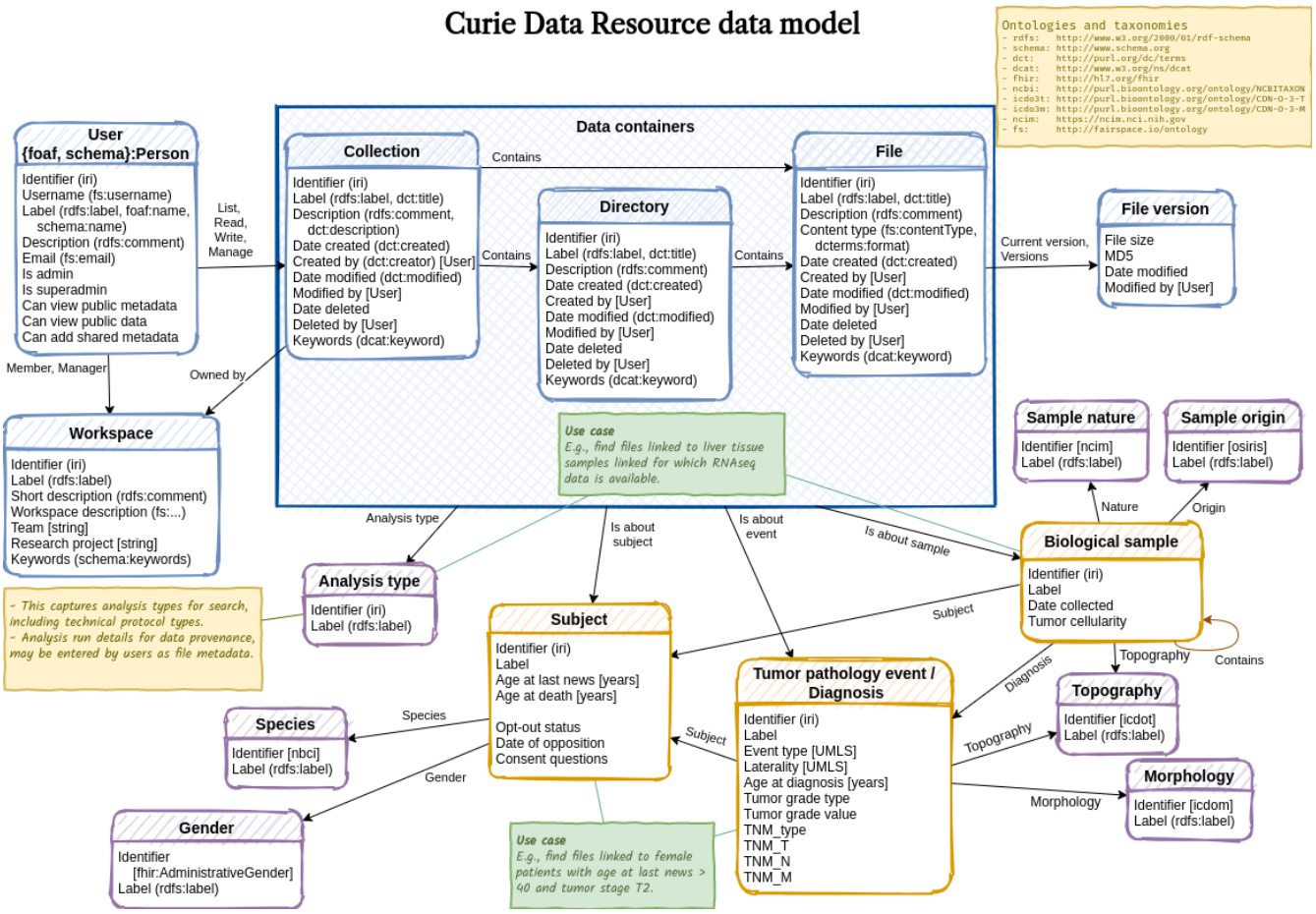
Every entity has a unique identifier, a type, a label, and the properties and relations as specified by the type. These entities do not belong to a particular space that is owned by a specific group or user.

Data model configuration

Fairspace uses an Apache Jena database to store system metadata and the custom domain specific metadata. The data models for these metadata are defined using the Shapes Constraint Language (SHACL).

- The system metadata includes workspaces, collections, directories, files, file versions, users and access rights. The system data model is defined in system-vocabulary.ttl
- The customisable data model includes the custom (shared) metadata entities, custom controlled vocabulary types, and custom properties of the system entities. The default custom data model is defined in vocabulary.ttl. This data model can be overriden by a data more suitable for your organisation.

A schematic overview of the default data model in vocabulary.ttl:



The data model defines an entity-relationship model, specifying the entity types that are relevant to describe your data assets, the properties of the entities, and the relationships between entities.

Example 2. Example data model

In this example data model, the following custom entity types are defined:

- `example:Gender` with property *Label*;
- `example:Species` with property *Label*;
- `example:Subject` with properties *Gender*, *Species*, *Age at last news* and *Files*.

The system class `fs:File` is extended with the *Is about subject* property.

```
@prefix owl: <http://www.w3.org/2002/07/owl#> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix sh: <http://www.w3.org/ns/shacl#> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix dash: <http://datashapes.org/dash#> .
@prefix fs: <https://fairspace.nl/ontology#> .
@prefix example: <https://example.com/ontology#> .

example:Gender a rdfs:Class, sh:NodeShape ;
    sh:closed false ;
    sh:description "The gender of the subject." ;
    sh:name "Gender" ;
    sh:ignoredProperties ( rdf:type owl:sameAs ) ;
    sh:property
    [
        sh:name "Label" ;
        sh:description "Unique gender label." ;
        sh:datatype xsd:string ;
        sh:maxCount 1 ;
        dash:singleLine true ;
        fs:importantProperty true ;
        sh:path rdfs:label
    ] .

example:Species a rdfs:Class, sh:NodeShape ;
    sh:closed false ;
    sh:description "The species of the subject." ;
    sh:name "Species" ;
    sh:ignoredProperties ( rdf:type owl:sameAs ) ;
    sh:property
    [
        sh:name "Label" ;
        sh:description "Unique species label." ;
        sh:datatype xsd:string ;
        sh:maxCount 1 ;
        dash:singleLine true ;
        fs:importantProperty true ;
        sh:path rdfs:label
    ] .
```

```
example:isOfGender a rdf:Property .
example:isOfSpecies a rdf:Property .
example:ageAtLastNews a rdf:Property .

example:Subject a rdfs:Class, sh:NodeShape ;
    sh:closed false ;
    sh:description "A subject of research." ;
    sh:name "Subject" ;
    sh:ignoredProperties ( rdf:type owl:sameAs ) ;
    sh:property
    [
        sh:name "Label" ;
        sh:description "Unique subject label." ;
        sh:datatype xsd:string ;
        sh:maxCount 1 ;
        dash:singleLine true ;
        fs:importantProperty true ;
        sh:path rdfs:label;
        sh:order 0
    ],
    [
        sh:name "Gender" ;
        sh:description "The gender of the subject." ;
        sh:maxCount 1 ;
        sh:class example:Gender ;
        sh:path example:isOfGender
    ],
    [
        sh:name "Species" ;
        sh:description "The species of the subject." ;
        sh:maxCount 1 ;
        sh:class example:Species ;
        sh:path example:isOfSpecies
    ],
    [
        sh:name "Age at last news" ;
        sh:description "The age at last news." ;
        sh:datatype xsd:integer ;
        sh:maxCount 1 ;
        sh:path example:ageAtLastNews
    ],
    [
        sh:name "Files" ;
        sh:description "Linked files" ;
        sh:path [sh:inversePath example:aboutSubject];
    ] .

example:aboutSubject a rdf:Property .

# Augmented system class shapes
```

```
fs:File sh:property
    [
        sh:name "Is about subject" ;
        sh:description "Subjects that are featured in this collection." ;
        sh:class example:Subject ;
        sh:path example:aboutSubject
    ] .
```

All entity types have a unique label, specified using the `rdfs:label` predicate. The *Gender* and *Species* properties link the subject to an entity from the respective controlled vocabularies. The *Age at last news* property is a numerical (integer) value property.
The *Files* property of the *Subject* entity type is an example of an inverse relation. The link is defined on the file, but the link will be visible on the subject as well, because of this inverse relation.

The following guidelines should be followed when creating a custom data model.

- Define a namespace for your custom entities and properties, like `@prefix example: https://example.com/ontology# .` in the example.
- Each custom entity type must have types `rdfs:Class` and `sh:NodeShape`, the properties `sh:closed false` and `sh:ignoredProperties ( rdf:type owl:sameAs )`, and a valid value for `sh:name`. The `sh:description` property is optional.
- Controlled vocabulary or terminology types are modelled as entity types as well, having only the *Label* (`rdfs:label`) property, see `example:Gender` and `example:Species`.
- Properties are specified using the `sh:property` property.
  - Every entity type must have a property *Label* (`sh:path rdfs:label`) of data type `xsd:string`. The label of an entity must be unique for that type. The label property should be singleton and marked `fs:importantProperty true`. If there are multiple properties, the label should have `sh:order: 0`.
  - Properties must have a valid value for `sh:name`. The `sh:description` property is optional.
  - A property must either have a `sh:datatype` property, specifying one of `xsd:string`, `xsd:integer` or `xsd:date`, or a property `sh:class` specifying an entity type as the target of a relationship.
  - The predicate used for the property (the middle part of the RDF triple) is specified with the `sh:path` property, e.g., `example:aboutSubject` for the *Is about subject* relation.
  - If a relationship is bidirectional, the path of the inverse relation is specified using `sh:inversePath`, see the *Files* property on the *Subject* entity type.
  - A property can be marked *mandatory* by specifying `sh:minCount 1`. A property can be marked *singleton* by specifying `sh:maxCount 1`.
  - A text property (with `sh:datatype xsd:string`) can be limited to a single line text field using `dash:singleLine true`.

Limitations

Although assigning multiple types to an entity is easy in RDF, Fairspace assumes entities to have a single type.

Inheritance is possible in SHACL, but not supported by Fairspace. Instead of specifying an entity type as a subtype of another, a single type can be specified with a *type* property, indicating the sub type of the entity.

E.g., instead of defining entity types *DNASeqAssay* and *RNASeqAssay* as sub types of *Assay*, a property type *assayType* can be defined on *Assay*, using a controlled vocabulary type *AssayType* with the assay types as values.

Controlled vocabularies

For controlled vocabulary types, e.g., *Gender* and *Species* in the example, you should insert the allowed values in the database by uploading a taxonomies file using the [Metadata upload API]. An example taxonomy is in taxonomies.ttl.

It is preferred to use existing standard taxonomies and labels. If that is not possible, please define your own namespaces for your custom taxonomies.

Example 3. Example taxonomy

In this example we use existing standard ontologies for the *Gender* and *Species* controlled vocabulary types.

- The HL7 FHIR AdministrativeGender code system for *Gender*.
- The NCBI Organismal Classification for *Species*.

```
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix example: <https://example.com/ontology#> .
@prefix gender: <http://hl7.org/fhir/administrative-gender#> .
@prefix ncbitaxon: <https://bioportal.bioontology.org/ontologies/NCBITAXON/> .

gender:male a example:Gender ;
  rdfs:label "Male" .
gender:female a example:Gender ;
  rdfs:label "Female" .

ncbitaxon:562 a example:Species ;
  rdfs:label "Escherichia coli" .
ncbitaxon:1423 a example:Species ;
  rdfs:label "Bacillus subtilis" .
ncbitaxon:4896 a example:Species ;
  rdfs:label "Schizosaccharomyces pombe" .
ncbitaxon:4932 a example:Species ;
  rdfs:label "Saccharomyces cerevisiae" .
ncbitaxon:6239 a example:Species ;
  rdfs:label "Caenorhabditis elegans" .
ncbitaxon:7227 a example:Species ;
  rdfs:label "Drosophila melanogaster" .
ncbitaxon:7955 a example:Species ;
  rdfs:label "Zebrafish" .
ncbitaxon:8355 a example:Species ;
  rdfs:label "Xenopus laevis" .
ncbitaxon:9606 a example:Species ;
  rdfs:label "Homo sapiens" .
ncbitaxon:10090 a example:Species ;
  rdfs:label "Mus musculus" .
```

View configuration

For the metadata pages in the user interface, a view configuration needs to be created that specifies the tables and columns. An example can be found in views.yaml

Installation and configuration

Local development

Requires:

- yarn
- docker
- Java 15

To run the development version, checkout this repository, navigate to `projects/mercury` and run

```
yarn dev
```

If on MacOS, configure docker logging.... TODO As env variable, or in `.env` file: `DOCKER_LOGGING_DRIVER=json-file`.

This will start a Keycloak instance for authentication at port `5100`, the backend application named Saturn at port `8080` and the user interface at port `3000`.

At first run, you need to configure the service account in Keycloak.

- Navigate to http://localhost:5100
- Login with credentials `keycloak`, `keycloak`
- Grant `realm-management` roles in the Fairspace realm: `view-realm`, `manage-realm`, `manage-authorization`, `manage-users`.

Now everything should be ready to start using Fairspace:

- Navigate to http://localhost:3000 to open the application.
- Login with one of the following credentials:

Username	Password
organisation-admin	fairspace123
user	fairspace123

Kubernetes and helm

You can deploy Fairspace on a Kubernetes cluster using Helm. Helm charts for Fairspace are published to the public helm repository at https://storage.googleapis.com/fairspace-helm.

Instructions for deploying to Google Cloud

Download and install helm and gcloud

- Download `helm 2.14.3` from from https://github.com/helm/helm/releases/tag/v2.14.3
- Extract the downloaded archive to `~/bin/helm` and check with:

```
~/bin/helm/helm version
```

- Install kubectl.
- Download and install the Google Cloud SDK (requires Python).
- Obtain credentials for Kubernetes:

```
  gcloud container clusters get-credentials <cluster id> --zone europe-west1-b
```

  Use `fairspacecicluster` as cluster id for the CI environment. Ensure that your Google account has access to the `fairspace-207108` GCP project and log in using

```
  gcloud auth login
```

- Check if all tools are correctly installed:

```
# List available clusters
gcloud container clusters list
# List Kubernetes namespaces
kubectl get ns
# List helm releases (deployments)
~/bin/helm/helm list
```

Initialise helm and add fairspace repository

```
# Initialise helm
~/bin/helm/helm init --client-only --stable-repo-url https://charts.helm.sh/stable
# Add the fairspace repo for reading
~/bin/helm/helm repo add fairspace https://storage.googleapis.com/fairspace-helm
# (Optional) Add the fairspace repo via the GCS plugin for writing
~/bin/helm/helm plugin install https://github.com/hayorov/helm-gcs.git --version 0.2.2
gcloud iam service-accounts keys create credentials.json --iam-account fairspace-
207108@appspot.gserviceaccount.com
export GOOGLE_APPLICATION_CREDENTIALS=/path/to/credentials.json
~/bin/helm/helm repo add fairspace-gcs gs://fairspace-helm
```

Fetch chart

```
# Update repo
~/bin/helm/helm repo update
# Fetch the fairspace chart
~/bin/helm/helm fetch fairspace/fairspace --version 0.7.5
```

Deploy Fairspace

Create a new Kubernetes namespace:

```
kubectl create namespace fairspace-new
```

Create a new deployment (called *release* in helm terminology) and install the Fairspace chart:

```
~/bin/helm/helm install fairspace/fairspace --version 0.7.5 --name fairspace-new
--namespace=fairspace-new \
-f /path/to/values.yaml --set-file saturn.vocabulary=/path/to/vocabulary.ttl --set
-file saturn.views=/path/to/views.yaml
```

You can pass values files with `-f` and provide a file for a specified value with `--set-file`.

Update an existing deployment

To update a deployment using a new chart:

```
~/bin/helm/helm upgrade fairspace-new fairspace-0.7.5.tgz
```

With `helm upgrade` you can also pass new values files with `-f` and pass files with `--set-file` as for `helm install`.

Clean up deployment

To clean up an environment or completely reinstall an environment, you can use `helm del`. :warning: Be careful, you may lose data!

```
~/bin/helm/helm del --purge fairspace-test
```

Design

Storage

RDF database using Apache Jena for:

- File metadata
- Permissions
- User metadata

File system data stored as blocks on the file system in append-only fashion.

License

...