FAIR Data Management Workflow for MRI Data

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Abstract. We present a workflow to improve the management of Magnetic Resonance Imaging data and to increase its compliance with the FAIR principles. This involves using the JSON Metadata Mapping Tool we have developed to map metadata from a domain-specific file format to a JSON schema based format, and storing the data and the mapped metadata in repositories. Some steps in the workflow are automated, while others require human intervention, facilitated by Graphical User Interfaces for each service. We assessed the compliance of our curated data to the FAIR principles, both manually and using the F-UJI tool. We obtain a FAIR assessment score of 79% for both datasets, which is the highest compared to similar ones in the same field. According to these results, we conclude that the workflow we have implemented can provide a significant improvement towards FAIR data management.

Keywords: FAIR Data Management, Metadata Schema, Metadata Mapping, Magnetic Resonance Imaging.

1 Introduction

Magnetic Resonance Imaging (MRI) is a non-destructive, (mostly) non-invasive technique which exploits the phenomenon of Nuclear Magnetic Resonance (NMR) in which nuclear spin is manipulated to reveal a picture of the spin density. Certainly popular in medicine, MRI additionally finds utility in engineering and materials sciences, including applications to get insights on processes and transport in biological and technical systems, biofouling, and electrochemical device characterization. The variety of applications presents a challenge in the context of MRI data management standardization. Despite the Digital Imaging and Communications in Medicine (DICOM) format [1] being broadly used to store MRI data, there is still a large variety of data curation and management methods in the materials science community, making it difficult to fully exploit the valuable potential of this research data.

MRI is one of the techniques available in the catalogue of the Nanoscience Foundries and Fine Analysis-Europe Pilot (NEP) [2]. The aim of the project is not only to provide user access to facilities, but also to develop methods, services and infrastructure for the management of the produced data.

Thus, within the frame of the NEP project, in this work we want to introduce a data management workflow, consisting of a sequence of clear steps, in order to curate MRI datasets

and make them comply with the FAIR (Findable, Accessible, Interoperable, Reusable) principles [3] as much as possible. The steps comprise: (i) extraction of selected metadata attributes from the DICOM format, (ii) mapping of the attributes to an open standard file format, i.e. JSON, according to the metadata schema we have developed, (iii) upload of the MRI dataset to a data repository, (iv) registration of the metadata document in a metadata repository that validates it against the schema. For all software components, we also developed Graphical User Interfaces (GUIs), which ease the scientists in executing the steps which are not automated and require manual interaction. With the help of this workflow, the data generated in the laboratory can be easily enriched with complete and structured metadata, which are essential for interoperability and reusability. Data and metadata can then be stored in appropriate repositories to be findable and accessible by future generations of researchers in the field.

2 Data Description

2.1 Glossary

To develop and contextualize the metadata schema describing the MRI data, we first defined the semantic model, i.e., we described the meaning of the terms in this specific domain [4]. Whenever possible, we adopted or adapted existing definitions which already reached a consensus in the MRI community or at least under the umbrella of the materials science related projects we are involved in: NEP [2], the Joint Lab "Integrated Model and Data-driven Materials Characterization" (JL-MDMC) [5], and the Nationale Forschungs-dateninfrastruktur für Materialwissenschaft und Werkstofftechnik (NFDI-MatWerk) [6]. Our main references were: the DICOM definitions available in the DICOM Standard Browser by Innolitics [7], the NEP Glossary [8], and the Joint Lab "Integrated Model and Data-driven Materials Characterization" (MDMC) Glossary [9]. The terms are used in the metadata schema and throughout the text (indicated with initial capital letters from now on) according to the definitions reported in [4].

2.2 MRI Data

The MRI Measurements were performed on a 15.2 T Bruker BioSpec AVANCE NEO imaging Instrument [10] controlled by ParaVision 360 V3.3, using a 35 mm proton RF probe and a Sample phantom consisting of seven 5 mm NMR tubes filled with copper sulfate solution (CuSO₄, concentration = 0, 5, 10, 25, 50, 75, 100 mM) or a Glucose solution. A variety of imaging Protocols were used in order to generate experimental DICOM Files populating Protocol-specific attributes. These Protocols included: FLASH, RARE (with RARE factor 1 and 4), MSME (with 1 and 4 echo Images), B1map, CSI, and FieldMap. Image resolutions were always 100 μ m isotropic, except for B1map (200 μ m isotropic), CSI (500 μ m isotropic), and FieldMap (200 μ m isotropic). The special feature of the CSI Protocol is that for every pixel of the produced Image, a NMR Spectrum is measured and stored in a separate DICOM File. In this case, all the DICOM Files containing the Spectra are still part of the single imaging Experiment, i.e. part of the same Series.

The DICOM standard comprises a large set of Metadata attributes that can be included in the file header. For a given imaging application, MRI in our case, the acquisition software collects a predefined subset of attributes, but allows the User to select additional ones from the whole standard. For the sake of generality, we limited the attributes to the default settings in the software.

In total, we yielded two MRI Studies: the Study on the Glucose solution with 10 Series, and the Study on the $CuSO_4$ solution with 19 Series. After the Measurements, the DICOM Files of each Study were collected in a folder, which was compressed in a ZIP file. The two final output ZIP files from the Experiments were uploaded to the Zenodo [11] data repository. More details are provided in subsection 3.3.

3 Results

3.1 MRI Metadata Schema

A Metadata schema defines the structure, the semantics, and the constraints of the attributes used to describe a resource. Metadata schemas are recommended by the FAIR principles, as their adoption facilitates the reuse and exchange of data. In the field of MRI, some standards describing imaging Experiments exist which are compatible with the DI-COM standard [12,13]. However, all of them are mainly applied in the medical domain. To the best of our knowledge, no standard exists to describe MRI Experiments in materials science applications. Thus, we defined a Metadata schema which extends the DICOM standard with a set of attributes suitable for the materials science domain [14].

Metadata contained in the header of binary files such as DICOM are limited in their accessibility. To improve this aspect and to address interoperability, we developed the schema in JSON. Being an open standard text file format, it does not require any specialized software, which makes the Metadata broadly accessible and machine actionable. The Metadata attributes selected for our schema are intended to enable the reproducibility of a MRI Study and to facilitate the analysis and the search of the results. To address interoperability and reuse in the materials science domain, we harmonized the naming convention, as explained in subsection 2.1, and we aligned the structure of the MRI schema to the existing results and the ongoing efforts (e.g. [15]) in NEP [2], JL-MDMC [5] and NFDI-MatWerk [6]. The schema resembles the structure of a DICOM MRI Study, reported in Figure 1. A Study, the entry object of the schema, contains one or more Series. All the Series of a Study are described by the same common Study-related attribute values. Each Series, in

study are described by the same common Study-related attribute values. Each Series, in turn, contains one or more Images or Spectra. Also in this case, all the Images (or Spectra) of a Series are described by the same common Series-related attribute values. In addition, a specific "perImage" set of attributes is present for each Image (or Spectrum). It is worth noticing that every DICOM header stores the minimum and maximum pixel value of the Images (or Spectra) in the file. It was mentioned in subsection 2.2 that, depending on the imaging Protocol, a Series might be enclosed in a single DICOM File or distributed across multiple ones. Thus, to keep consistency between these two possible data configurations, we assigned as common Series-related Metadata attributes the minimum and maximum pixel value in a Series, independently of the values reported in the header of individual DICOM Files.

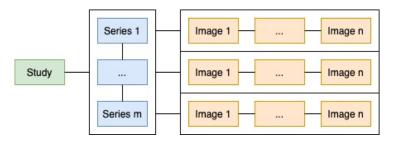


Fig. 1: The structure of a MRI Study. Each Study consists of one or multiple Series. Each Series contains one or multiple Images or Spectra.

3.2 The JSON Metadata Mapping Tool

Metadata mapping is the process of associating equivalent Metadata attributes of an origin and a target schema. In this way, the attribute values can be transferred between Metadata documents, even in different file formats, when they are following different structures. In our specific case, we intend to map the attributes from the DICOM standard to the MRI schema presented in subsection 3.1. Overall, some tools exist that either support the users in the mapping process [16,17,18], or transfer Metadata from DICOM to JSON [13,19]. They are either very discipline specific, too general for our purpose, or do not allow to include custom Metadata schemas.

Therefore, out of the work in the Helmholtz Metadata Collaboration (HMC) [20], we developed our own tool as part of the NEP data services: the JSON Metadata Mapping Tool (JaMMaTo) [21]. This tool can be implemented using the corresponding Python package via PIP [22], or using the plugin-based KIT Data Manager (KITDM) Mapping Service [23], which offers the additional benefit of a GUI. The tool takes as input a ZIP file containing all the DICOM Files belonging to a Study, the JSON map and the MRI schema. It then returns as output the mapped metadata as JSON document containing the attributes from the DICOM headers structured as the MRI schema. As a final result for our specific case, two Metadata document were generated, one for each of the two MRI Studies [24,25], and ingested to MetaRepo [26], the NEP Metadata repository, further described in subsection 3.3.

The essential steps of our tool, shown in Figure 2, are: extracting the attribute values from origin schema O (DICOM standard), associating them with the corresponding ones in target schema T (as key:value pairs in a JSON map), and inserting the attribute values at the corresponding position according to JSON schema T (in our case, the MRI Schema). In special cases, multiple attributes in schema O are processed before being mapped to one attribute in schema T (many-to-one relation). For example, as already mentioned in subsection 3.1, in case of multiple DICOM Files belonging to the same Series, the minimum and maximum pixel values were collected from the headers of each file, and only the minimum and maximum (respectively) ones among them were assigned to the common Series-related Metadata attributes.

The software is written in Python3 and uses the Pydicom [27] module as an auxiliary component. It sequentially processes all the input DICOM Files, regardless of whether they contain a Series of Images or individual Spectra, reads the Metadata attributes from

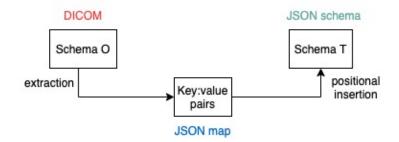


Fig. 2: The basic principle of mapping Metadata attributes between an origin schema O and a target schema T applied to JaMMaTo. The schemas and map files used in our specific case are coloured.

the header of each file, and groups together all Series and Images (or Spectra) attributes that are related to a Study, as shown in Figure 1.

The code consists of several classes for the different mapping steps, which can also be used independently. The most relevant classes are the schema_reader class, the dicom_reader class, the attribute_mapper class, and the attribute_inserter class (Figure 3).

Metadata Extraction The schema_reader class takes the MRI schema as input and creates a skeleton of its structure as a Python dictionary. The dicom_reader class takes a DICOM File as input and implements the Pydicom module. The output is further processed and all attributes of the DICOM File are stored in the Series object.

Metadata Mapping All the relevant attributes in the DICOM header and the corresponding attributes in the MRI schema, together with the Uniform Resource Identifier (URI) of the schema location in the Metadata repository ([26], see also subsection 3.3) can be found in the JSON map as key:value pairs [4]. The MRI schema is retrieved by JaMMaTo at run-time.

The attribute_mapper class takes as input the JSON map and the Series objects containing the Metadata attributes from the DICOM header, and creates a class instance object in a modular way for each Image (or Spectrum), each Series, and the Study itself, containing the corresponding attributes from the MRI schema and the values from the DICOM Files, which are then hierarchically appended according to the MRI Study structure shown in (Figure 1).

The attribute_inserter class takes the MRI schema skeleton and the Study object as input. Going through the MRI schema structure, the attribute values are fetched from the Study, the Series and the Image objects, and placed at the proper position. The class returns the mapped Metadata Python dictionary, which is eventually written into a JSON document.

Plugin for the Mapping Service The application and the usage of JaMMaTo was facilitated by the employment of the KITDM Mapping Service [23], which provides a GUI.

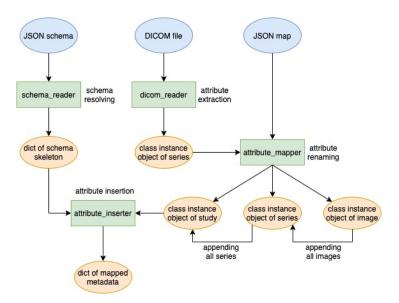


Fig. 3: The workflow of JaMMaTo. Blue ovals represent files used as input to the software. The green rectangles represent the classes performing tasks on the input files. The orange ovals represent the software-internal variables output from the classes, which can be further processed.

Thus, we also implemented JaMMaTo as a plugin for the Mapping Service. Figure 4 shows how the components act on the input files uploaded to the GUI by the User, and return the mapped Metadata document as output.

3.3 Data and Metadata Repositories

Storing data or Metadata in a database or in local devices makes them hard to be found, accessed, or shared. The use of repositories highly contribute to improve and facilitate these management aspects.

Repositories are information systems used to store, manage and provide access to digital resources, following a policy or a set of rules that define storage and access norms [9]. Many data repositories automatically assign globally unique Persistent Identifiers (PIDs) to deposited resources. This makes them particularly suitable for research data which are not likely to be altered again. Metadata repositories also exist, which are specialized in the storage and management of Metadata schemas and documents linked to the research data via PIDs.

We stored each of our two MRI Studies described in subsection 2.2 as ZIP files in Zenodo [11], a domain-agnostic data repository which provides a basic set of administrative Metadata and automatically assigns Digital Object Identifiers (DOIs) to resources. Each of our MRI Studies has been made accessible [28,29] and can be downloaded.

The MRI Metadata schema described in subsection 3.1 and the two Metadata documents generated as output of JaMMaTo (subsection 3.2) were stored in MetaRepo [26], the NEP

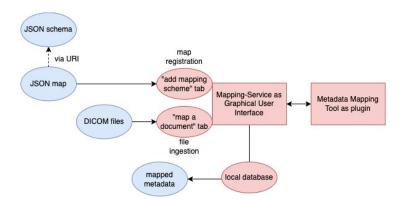


Fig. 4: JaMMaTo (right red rectangle) as a plugin for the Mapping Service (left red rectangle). Blue ovals represent input and output files. Red ovals represent the components of the Mapping Service initiated on the GUI by the User to act on the input files or which are involved to return the resulting output file.

instance of the KITDM MetaStore2 [30]. This is a Metadata repository and schema registry providing a set of basic administrative Metadata and performing validation of Metadata documents against the corresponding schema at ingest time. Schemas and Metadata documents can be accessed via URIs and visualized or edited, according to the granted access rights. Each of the two Metadata documents we ingested [24,25] includes in the administrative Metadata both the URI of the MRI schema [14] it is based on, as well as the DOI of the corresponding Study it describes [28,29].

4 Discussion of Results

4.1 Workflow for MRI Data

The workflow we suggest for managing the MRI data consists of four main steps: DICOM attributes extraction, Metadata mapping to the MRI schema, data upload to Zenodo, and Metadata document registration in MetaRepo. In addition, some preliminary steps are required: the design of a MRI schema (later registered in MetaRepo) and the attribute assignment (i.e., the creation of the JSON map associating the DICOM attributes to the MRI schema as key:value pairs). Both these steps benefit from an important contribution by domain experts, who know the semantics of the Metadata attributes and can decide which ones are required to describe the Experiments. In general, the preliminary steps need to be performed only once. In fact, a new attribute assignment is only necessary in case the MRI schema or the DICOM attributes change.

In some phases of the workflow, the contribution of the User is required. For example, the steps of JaMMaTo are automatically performed, but they must be manually triggered. Two options are possible, each one offering advantages and limitations: the plugin for the Mapping Service eases the data ingestion but currently supports the mapping of only one Study at a time. On the other hand, the Python package allows to automatically perform mappings of multiple Studies even with different JSON maps, but needs to be executed

from the command line.

The upload of the DICOM Files to Zenodo, as well as the registration of the MRI schema and of the Metadata documents to MetaRepo have to be performed manually, too. These actions are greatly facilitated by the user-friendly GUIs available for both the services. In this work, we only covered the mapping from DICOM to JSON format. Nevertheless, the components of JaMMaTo are modular and largely independent of one another. Therefore, the tool can be easily generalized and extended to other measurement techniques, providing additional reader classes in order to extract the Metadata from other origin file formats.

4.2 FAIR Assessment Evaluation

Many tools exist to assess the FAIRness of data resources, i.e., to quantify how much they comply with the FAIR principles, according to a specific implementation of the FAIR metrics. Some of the available tools enable manual assessment [31,32,33,34], while others are automated frameworks [35,36,37,38]. Among the latter, F-UJI [38] assesses 13 over 15 FAIR principles, which correspond to 17 core FAIR metrics defined by FAIRsFAIR [39], following domain-agnostic web standards (e.g., [40,41,42,43,44]). Being specifically suited for research datasets, this tool was used to evaluate a set of pilot repositories [45] and of Helmholtz data repositories [46] to globally identify gaps among them. Supported by its broad adoption and the available literature, we decided to use F-UJI [38] to evaluate the FAIRness of our curated datasets.

Both our MRI datasets reach a FAIRness score of 79%, based on the following breakdown: Findability (F)=7/7, Accessibility (A)=3/3, Interoperability (I)=3/4, Reusability (R)=6/10. To evaluate the quality of this score, we compared our datasets with similar ones in the same field. In order to avoid any bias due to possible differences in data management among repositories [46], we selected from Zenodo a sample of 71 MRI-related datasets [47] and performed the same FAIR assessment on them. The breakdown of the results is shown in Figure 5. The average score of the sample is 52%, the minimum being 18% and the maximum 79%. Thus, our MRI datasets display the highest score in the evaluated sample, which is achieved by only 7 other datasets out of 71.

All the datasets with the highest score, including ours, display the same breakdown. The detailed report provided by F-UJI highlights a lack of requirements, especially I2 (usage of vocabularies that follow the FAIR principles), R1 (plurality of accurate and relevant attributes), and R1.2 (detailed provenance). We deduce that some of the requirements cannot be fulfilled because F-UJI cannot retrieve the information from Zenodo.

It must be noticed that F-UJI tests only the administrative Metadata, based on domainagnostic standards, of deposited datasets: any additional domain-specific Metadata is not taken into account. Thus, we manually evaluated the FAIRness of our datasets, following the definitions provided by GO-FAIR [48]. We report in the following the criteria which could not be assessed by F-UJI:

- I2 (usage of vocabularies that follow the FAIR principles): partially fulfilled. The terms used in the MRI schema to describe the datasets are defined in the publicly available glossary [4], and have been agreed in the community. The individual terms are not yet included in a vocabulary to be resolvable using globally unique and persistent identifiers. This work is ongoing.

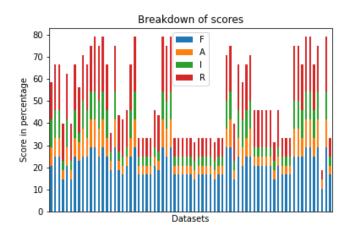


Fig. 5: The distribution of the score assessments for each FAIR principle of 71 MRI-related datasets on Zenodo. The scores were assessed using F-UJI.

- R1 (plurality of accurate and relevant attributes): completely fulfilled. The MRI schema [14], designed in collaboration with experts in the field, contain rich Metadata, including the scope of the Study, the date and time of the Experiment, the User who performed the Measurements, the Sample, the Measurement conditions, the Instrument, the Protocol parameters, and the features of each Series and of each Image. A definition is provided for each term, if the name is not self-explanatory.
- R1.2 (detailed provenance): completely fulfilled. The MRI schema includes all the details needed to perform the imaging Experiment and reproduce the output.

5 Conclusions

In this work, we presented a data management workflow to improve the FAIRness of MRI data. As a preliminary step, we collaborated with experienced research Users on the design of a Metadata schema [14] to describe the MRI Studies for materials science applications. The terms and the hierarchical structure we used in the MRI schema are consistent with both the DICOM standard [7] and other materials science projects (NEP [2], JL-MDMC [5] and NFDI-MatWerk [6]): this aspect favours the data reusability (principle R1.3) and enables new opportunities for interdisciplinary research.

The MRI schema includes a large number of relevant metadata (principles F2 and R1) needed to reproduce the results of an imaging Experiment: to ease the Users in the tedious and error-prone task of manually filling all the corresponding values, we developed JaMMaTo. For each Study, the tool extracts the required attributes from the files in the DICOM format and maps them according to the MRI schema structure. The mapped Metadata document, written in JSON, offers the big advantage to collect the descriptive attributes in an open, standard, machine-readable file format, favouring interoperability (principle I1).

The Metadata documents, the MRI schema they are based on, and the datasets they describe, were stored in MetaRepo and Zenodo, respectively. The combined use of reliable data and Metadata repositories allows to manage granular access and usage rights (principles A1.2 and R1.1), enriches the contextual knowledge about the Raw Data thanks to cross-references (principle I3), ensures the resource findability (principles F3 and F4) and guarantees the persistence of the Metadata, even in case the data might be restricted or no longer available (principle A2).

Finally, based on both the F-UJI score and our manual assessment (subsection 4.2), we can conclude that the FAIRness of the produced MRI datasets was sensitively improved thanks to the use of our data management workflow. Therefore, we propose it as a valuable example of the FAIRification process [49]. The components and the tools shown in this work can be used by the MRI community or extended to serve other scientific laboratories in the materials science domain and beyond.

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