MDF: Magnetic Particle Imaging Data Format

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Abstract

Magnetic particle imaging (MPI) is a tomographic method to determine the spatial distribution of magnetic nanoparticles. In this document a file format for the standardized storage of MPI data is introduced. The aim of the Magnetic Particle Imaging Data Format (MDF) is to provide a coherent way of exchanging MPI data acquired with different MPI scanners worldwide. The focus of the file format is on sequence parameters, raw measurement data, calibration data, and reconstruction data. The format is based on the hierarchical document format (HDF) in version 5 (HDF5).

Introduction

The purpose of this document is to introduce a file format for exchanging in version 5 (HDF5) [1]. HDF5 allows to store multiple datasets within Magnetic Particle Imaging (MPI) data. The Magnetic Particle Imaging a single file and is thus very flexible to use. To allow the exchange of Data Format (MDF) is based on the hierarchical document format (HDF) MPI data, one has to specify a naming scheme within HDF5 files which is the purpose of this document. In order to create and access HDF5 data, an Open Source C library is available. For most programming languages bindings to this library exist. Matlab supports HDF5 by the functions h5read and h5write. For Python the h5py package exists. The Julia programming language provides access to HDF5 files via the HDF5 package. For languages based on the .NET framework the HDF5DotNet library is available.

In this initial version of the file format the focus is on sequence parameters, raw measurement data, calibration data, and reconstruction data. The format can store three different dataset types

- 1. Measurement data
- 2. System calibration data
- 3. Reconstruction data

It is possible to combine measurement data and reconstruction data into a single file. However, calibration data has to be stored in an independent HDF5 file.

1.1 Datatypes

For most parameters a fixed datatype is used, i.e. the drive-field amplitudes are stored as H5T_NATIVE_DOUBLE values. For our convinience we refer to the HDF5 datatypes H5T_STRING, H5T_NATIVE_DOUBLE and H5T_NATIVE_INT64 as String, Float64 and Int64. The datatype of the measurement data and the calibration data is not restricted such that maximum flexibility is given. In case of no restrictions Any HDF5 data type can be choosen.

MPI parameters are stored as regular *HDF5 datasets*. *HDF5 attributes* are not used in the current specification of the MDF.

Since storing complex data in HDF5 is not standardized, we extend the dimensionality of an existing array and store the real and imaginary part in the last dimension with size 2 (index 0 = real part, index 1 = imaginary part). In this way the real and imaginary part of a complex datum is stored

sequentially on disk. When loading the data it is possible to cast it to a complex array in most programming languages.

1.2 Units

Physical quantities are given in SI units with one exception. The field strength is reported in $T\mu_0^{-1}=4~\pi~{\rm Am}^{-1}\mu_0^{-1}$. This convention has been proposed in the first MPI publication and since that time consistently used in most MPI related publications. The aim of this convention is to report the numbers on a Tesla scale, which most readers with a background in MRI are familiar with, but, on the other hand still use the correct unit for the magnetic field strength.

1.3 Sanity Check

In order to check if a generated MDF file is valid, we provide a sanity check script that can be found in the gitub repository:

https://github.com/MagneticParticleImaging/MDF

The code is written in the Julia programming language [2, 3, 4], which has to be downloaded from:

http://julialang.org.

More detailed instructions can be found in the README of the repository.

1.4 Contact

If you find mistakes in this document or the specified file format or if you want to discuss extensions to this specification, please open an issue on GitHub:

https://github.com/MagneticParticleImaging/MDF

As the file format is versionized it will be possible to extend it for future needs of MPI. The current version discussed in this document is version 2.0.0-pre.

1.5 arXiv

As of version 1.0.1 the most recent release of these specifications can also be also found on the arXiv:

http://arxiv.org/abs/1602.06072

If you use MDF please cite us using the arXiv reference, which is also available for download as MDF.bib from GitHub.

Changelog

1.6.1 v2.0

• Infrastructure for storing background data directly with MDF data has been added for both regular measurements and calibration measurements.

- In v1.x the MDF allowed certain fields to have varying dimensions depending on the context. This has been removed such that starting from v2.0 all dimensions have to be specified. This change makes implementations of the MDF less complex.
- Support for multiple excitation frequencies on a drive-field channel has been added. Additionally we added support for fully arbitrary excitation waveforms.

Data (group: /)

Remarks: Within the root group metadata about the file itself is stored. in dedicated groups on measurement data, calibration data, and/or recon-Within several subgroups, metadata about the experimental setting, the struction data. MPI tracer, and the MPI scanner are stored. The actual data is stored

Parameter	Type	Dim	Unit/Format	Optional	Description
version	String	1	0.1	no	Version of the file format
uuid	String	1	f81d4fae-7dec-11d0-a765-00a0c91e6bf6	no	Universally Unique Identifier (RFC 4122)
date	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC creation time of MDF data set

Study Description (group: /study/)

Remarks: The study description group describes the experimental setting under which the MPI data was recorded. The study field may be used as a name tag for several experiments, which are related. The dataset at hand may then be described by a number and a short description. Addi- the scanner was recorded.

tionally, the name of the imaged subject can be provided and the starting time of the MPI measurement can be provided.

The reference field may be used to indicate, if the background signal of

Parameter	Type	\mathbf{Dim}	$\mathbf{Unit}/\mathbf{Format}$	Optional	Description
name	String	1		yes	Name of the study
experiment	String	1		yes	Experiment number within study
description	String	1		yes	Short description of the experiment
subject	String	1		yes	Name of the subject that was imaged
reference	Int64	1		yes	Flag indicating if field of view was empty during the measurement
simulation	Int64	1		yes	Flag indicating if the data in this file is simulated rather than measured

2.2 Tracer Parameters (group: /tracer/)

Remarks: The tracer parameter group contains information about the MPI tracer used during the experiment such as the tracer name, its vendor, the tracer concentration, and the total volume applied.

Note that the injection clock recording the injection time should be synchronized with the clock, which provides the starting time of the measurement.

Parameter	Type	Dim	${ m Unit/Format}$	Optional	Description
name	String	1		yes	Name of tracer used in experiment
batch	String	1		yes	Batch of tracer
vendor	String	1		yes	Name of tracer supplier
volume	Float64	1	L	yes	Total volume of applied tracer
concentration	Float64	1	mol(solute)/L	yes	Molar concentration of solute per litre
solute	String	1		yes	Solute, e.g. Fe
time	String	1	yyyy-mm-ddThh:mm:ss.ms	yes	UTC time at which tracer injection started

2.3 Scanner Parameters (group: /scanner/)

Remarks: The scanner parameter group contains information about the MPI scanner used such as the manufacturer, the model, and the facility where the scanner is installed.

Parameter	\mathbf{Type}	Dim	${f Unit/Format}$	Optional	Description
facility	String	1		no	Facility where the MPI scanner is installed
operator	String	1		no	User who operates the MPI scanner
manufacturer	String	1		no	Scanner manufacturer
model	String	1		no	Scanner model
topology	String	1		no	Scanner topology (e.g. FFP or FFL)

2.4 Acquisition Parameters (group: /acquisition/)

Remarks: The acquisition parameter group can describe different imaging protocols and trajectory settings. The corresponding data is organized into general information, a subgroup containing data on the particle excitation and a subgroup containing data on the receive channels.

In general each MPI dataset consists of the measurement data of L frames. A frame groups all data together that will be used to reconstruct an

image/volume. On certain MPI scanners the drive-field field-of-view (FOV) can be shifted either by magnetic fields or by mechanical movement. Therefore, a frame may consist of J sub-measurements. For instance a Cartesian 2D trajectory with 100 lines would be realized by setting $\mathtt{numPatches} = 100$.

Parameter	\mathbf{Type}	Dim	Unit/Format	Optional	Description
numFrames	Int64	1	1	no	Number of available frames, denoted by L
framePeriod	Float64	1	S	no	Complete time to acquire a full frame
numPatches	Int64	1	1	no	Number of patches within a frame denoted by J
gradient	Float64	$J \times 3$	$\mathrm{Tm}^{-1}\mu_0^{-1}$	no	Gradient strength of the selection field in x, y , and z directions
time	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC start time of MPI measurement

2.4.1 Drive Field (group: /acquisition/drivefield/)

Remarks: The drive field subgroup describes the details on the imaging protocol and trajectory settings. On the lowest level each MPI scanner contains D channels for particle excitation. Since most drive-field parameters may change from patch to patch they have a leading J dimension.

These excitation signals are usually sinusoidal and can be described by D amplitudes (drive field strengths), D phases, a base frequency, and D dividers. In a more general setting the drive-field in channel d is described by

$$H_d(t) = \sum_{l=1}^{F} A_l \Lambda_l (2\pi f_l t + \varphi_l)$$

where F is the number of frequencies on the channel, A_l is the drive-field strength, ϕ_l is the phase, f_l is the frequency (described by the base frequency and the divider), and Λ_l is the waveform. The waveform is specified by a dedicated parameter waveform. If waveform is set to "CUSTOM", one can specify a custom waveform using the parameter customWaveform.

The center of the drive-field is specified in the parameter fieldOfViewCenter. The shift of the FOV is induced by a certain offset field that can be reported in the parameter offsetField

Parameter	\mathbf{Type}	Dim	Unit/Format	Optional	Description
numChannels	Int64	1	1	no	Number of drive field channels, denoted by D
strength	Float64	$J \times D$	$T\mu_0^{-1}$	no	Applied drive field strength
phase	Float64	$J\times D\times F$	$T\mu_0^{-1}$	no	Applied drive field phase φ in radians in the range $[-\pi,\pi)$
baseFrequency	Float64	1	$_{ m Hz}$	no	Base frequency to derive drive field frequencies
divider	Int64	$D \times F$	1	no	Divider for drive fields frequencies (baseFrequency / divider)
waveform	String	$D \times F$	1	no	Waveform type: "SINE", "TRIANGLE" or "CUSTOM"
customWaveform	Float64	$D \times F \times U$	1	yes	Custom waveform table
period	Float64	1	s	no	Drive field trajectory period
numAverages	Int64	1		no	Number of internal averages (applied in hardware/software)
repetitionTime	Float64	1	s	no	Time to complete averaged DF trajectory (averages * period)
fieldOfView	Float64	$J \times 3$	m	no	Approximate size of the area/volume captured by the trajectory
fieldOfViewCenter	Float64	$J \times 3$	m	no	Center of the drive field trajectory (relative to origin/center)
offsetField	Float64	$J \times 3$	$T\mu_0^{-1}$	yes	Applied offset field that yielded the fieldOfViewCenter

2.4.2 Receiver (group: /acquisition/receiver/)

Remarks: The receiver subgroup describes details on the MPI receiver. For a multi-patch sequence it is assumed, that signal acquisition only takes place during particle excitation. During each drive-field cycle, C receive channels record the superposition of the change of the particle magneti-

zation at Z equidistant time points. If the receive characteristics are the same for all receive channels then a single value is sufficient to describe all channels at once, else the C channels can be characterized individually.

Parameter	Type	Dim	$\mathbf{Unit}/\mathbf{Format}$	Optional	Description
numChannels	Int64	1		no	Number of receive channels C
bandwidth	Float64	C	Hz	no	Bandwidth of the receiver unit
numSamplingPoints	Int64	C		no	Number of sampling point within one drive-field period denoted by Z
frequencies	Float64	$C \times K$	Hz	yes	Vector containing recorded frequencies
transferFunction	Float64	$C \times K \times 2$		yes	Transfer function of the receive channel

2.5 Measurements (group: /measurement/)

Remarks: Measured data can be stored in Fourier domain (FD) representation as well as time domain (TD) representation. Usually only one of the representation is stored and one has to calculate the missing representation if it is needed but not available.

One measurement consists of the voltages recorded in all receive channels for all patches. The number of measurements in time domain is thus

given by JCZ. In frequency domain one measurement has KCZ data points. On disc the temporal/frequency index is the fastest, while the index over the patches is the slowest. If several measurements are acquired (indicated by numFrames), the measurements are concatenated. The number of measurements is denoted by L.

Parameter	\mathbf{Type}	Dim	$\mathbf{Unit}/\mathbf{Format}$	Optional	Description
dataFD	Any	$L\times J\times C\times K\times 2$		yes	Measurement data stored in Fourier domain representation. The last dimension is used for storing the complex data.
dataTD	Any	$L\times J\times C\times Z$		yes	Measurement data stored in time domain representation

2.6 Calibration (group: /calibration/)

Remarks: Calibration data is usually acquired by a combination of N calibration and M background measurements. Each calibration measurement is taken with a delta sample at a fixed position inside the FOV of the scanner. Each background measurement is taken with the delta sample outside of the FOV of the scanner. To accurately capture any possible drift in the background signal, background measurements are usually performed frequently throughout the whole calibration procedure. Each measurement of the complete procedure can be assigned an integer number $o=1,2,\ldots,N+M$ ordering the measurements with respect to the time points at which they were taken, with 1 beeing assigned to the first measurement and N+M beeing assigned to the last measurement.

The resulting N calibration measurements can be stored in time or frequency domain. Often, the calibration measurements are reorded with respect to the corresponding spatial position of the delta sample. Hence, the time ordering numbers o corresponding to each measurement are stored

separately. For practical reasons the calibration data is stored such that the index over the positions is the fastest while the index over all data points of a particular measurement is the slowest. Depending on the programming language used (column-major or row-major order) the system matrix may appear in a transposed representation when loaded into main memory. The M background measurements can also be stored in time or frequency domain. These measurements are stored without any changes to the storage order. Similar to the calibration measurements the time ordering number o is stored for each background measurement.

If a regular grid is used for sampling, by default the fastest index is in x direction, the second fastest index is in y direction, while the slowest index is in z direction. If a different ordering is used this can be documented using the optional parameter order. For non-regular sampling points there is the possibility to explicitly store all N positions.

Parameter	Type	Dim	Unit/Format	Optional	Description
dataTimeOrder	Int64	N		yes	Time ordering number for calibration measurements in system matrix
dataFD	Any	$J \times C \times K \times N \times 2$		yes	System matrix stored in its Fourier space representation with the last dimension storing complex data
dataTD	Any	$J\times C\times Z\times N$		yes	System matrix stored in its time domain representation
backgroundDataTimeOrder	Int64	M		yes	Time ordering number for background measurements
backgroundDataFD	Any	$M\times J\times C\times K\times 2$		yes	${\cal M}$ background measurements stored in Fourier space representation with the last dimension storing complex data
backgroundDataTD	Any	$M\times J\times C\times Z$		yes	background measurements stored in time domain representation
snrFD	Float64	$C \times K$		yes	Signal-to-noise estimate for recorded frequency components
fieldOfView	Float64	3	m	yes	Field of view of system matrix
fieldOfViewCenter	Float64	3	m	yes	Center of the system matrix (relative to origin/center)
size	Int64	3		yes	Number of voxels in each dimension
order	String	1		yes	Ordering of the dimensions, default is xyz
positions	Float64	$N \times 3$	m	yes	Position of each of the grid points, stored as (x, y, z) triples
offsetField	Float64	$N \times 3$	$T\mu_0^{-1}$	yes	Applied offset field strength to emulate a spatial position, stored as (x, y, z) triples
deltaSampleSize	Float64	3	m	yes	Size of delta sample used for calibration scan
method	String	1		yes	Method used to obtain calibration data. Can for instance be robot, hybrid, or simulation

Reconstruction Results (group: /reconstruction/)

Reconstruction results are stored in the parameter data. Dependent system matrix grid, the grid parameter are mirrored in the reconstruction on the number of individual channels S obtained by the reconstruction the results can be stored in a $L \times N$ array for S = 1 or in a $L \times N \times S$ array for S > 1. Since the grid of the reconstruction data can be different than the to store complex data if the reconstruction output is complex.

parameter group.

Usually the data is stored in a real data format but it is also possible

Parameter	Type	Dim	Unit/Format	Optional	Description
data	Any	$L\times N\times S$		yes	Reconstructed data
fieldOfView	Float64	3	m	yes	Field of view of reconstructed data
fieldOfViewCenter	Float64	3	m	yes	Center of the reconstructed data (relative to origin/center)
size	Int64	3		yes	Number of voxels in each dimension
order	String	1		yes	Ordering of the dimensions, default is xyz
positions	Float64	$N \times 3$	m	yes	Position of each of the grid points, stored as (x, y, z) tripels

References

- [1] The HDF Group. Hierarchical Data Format, version 5, 1997-2016. http://www.hdfgroup.org/HDF5/.
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