## MDF: Magnetic Particle Imaging Data Format

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June 1, 2017

Version 2.0.0-pre

#### 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 and MPS data is introduced. The aim of the Magnetic Particle Imaging Data Format (MDF) is to provide a coherent way of exchanging MPI and MPS data acquired with different 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).

## 1 Introduction

The purpose of this document is to introduce a file format for exchanging Magnetic Particle Imaging (MPI) and Magnetic Particle Spectroscopy on the hierarchical document format (HDF) in version 5 (HDF5) [1]. HDF5

allows to store multiple datasets within a single file and is thus very flexible to use. To allow the exchange of 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.

The current version is mainly focused on storing raw measurement data, system matrices, or reconstruction data together with corresponding sequence parameters and meta data. Though it is possible to combine measurement data and reconstruction data into a single file it is recommended to use a single file for each of the following dataset types:

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

#### 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 offers more freedom and is denoted by Number, which can be any of the following HDF5 data types: H5T\_NATIVE\_FLOAT, H5T\_NATIVE\_DOUBLE, H5T\_NATIVE\_INT8, H5T\_NATIVE\_INT16, H5T\_NATIVE\_INT32, and H5T\_NATIVE\_INT64. Whenever Boolean data has to be stored we use H5T\_NATIVE\_INT8 for storage.

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 Parameter Extension

Often you will find that you want to store parameters or meta data which are specific to your side. For example the temperature of the room in which your MPI device is operated. In this case you are free to add a new parameters to any of the existing groups. Moreover if necessary you are also free to introduce new groups. To be able to distinguish these datasets

and groups from the specified ones we recommend to use the prefix E for needs of MPI. The current version discussed in this document is version all parameters and groups. In our example I could add a new group Eroom 2.0.0-pre. and within the dataset Etemperature.

#### 1.5Contact

If you find mistakes in this document or the specified file format or if you As of version 1.0.1 the most recent release of these specifications can also 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

#### 1.6 arXiv

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.

## Data (group: /)

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

reconstruction data.

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)
time	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC creation time of MDF data set

#### 2.1 Study Description (group: /study/)

**Remarks:** A study is supposed to group a series of experiments to support, refute, or validate a hypothesis. The study group may contain name, number, and description of the study.

Parameter	Type	Dim	${ m Unit/Format}$	Optional	Description
name	String	1		yes	Name of the study
number	Int64	1		yes	Experiment number within study
description	String	1		yes	Short description of the experiment

#### 2.2 Experiment Description (group: /experiment/)

**Remarks:** For each experiment within a study name, number, and ject and a flag indicating if data has been obtained via simulations can be description may be provided. Additionally, the name of the imaged substored.

Parameter	$\mathbf{Type}$	$\mathbf{Dim}$	${ m Unit/Format}$	Optional	Description
name	String	1		yes	Experiment name
number	Int64	1		yes	Experiment number
description	String	1		yes	Short description of the experiment
subject	String	1		yes	Name of the subject that was imaged
isSimulation	Int8	1		yes	Flag indicating if the data in this file is simulated rather than measured

## 2.3 Tracer Parameters (group: /tracer/)

Remarks: The tracer parameter group contains information about the MPI tracers used during the experiment. For each tracer its name, batch, vendor, its volume, its molar concentration of solute per litre and the time point of injection can be provided.

This version of the MDF can handle two basic scenarios. In the first one static tracer phantoms are used. In this case the phantom contains A distinct tracers. These might be particles of different core sizes, mobile

or immobilized particles for example. In this case injectionTime is not used. In the second case A boli (e.g. pulsed boli) are administrated during the measurement, in which case the approximate administration volume, tracer type and time point of injection can be provided. 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	A		yes	Name of tracer used in experiment
batch	String	A		yes	Batch of tracer
vendor	String	A		yes	Name of tracer supplier
volume	Float64	A	L	yes	Total volume of applied tracer
concentration	Float64	A	mol(solute)/L	yes	Molar concentration of solute per litre
solute	String	A		yes	Solute, e.g. Fe
injectionTime	String	A	yyyy-mm-ddThh:mm:ss.ms	yes	UTC time at which tracer injection started

# 2.4 Scanner Parameters (group: /scanner/)

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

Parameter	$\mathbf{Type}$	$\mathbf{Dim}$	${f Unit/Format}$	Optional	Description
facility	String	1		yes	Facility where the MPI scanner is installed
operator	String	1		yes	User who operates the MPI scanner
manufacturer	String	1		yes	Scanner manufacturer
model	String	1		yes	Scanner model
topology	String	1		no	Scanner topology (e.g. FFP, FFL, MPS)
boreSize	Float64	1		yes	Scanner model

## 2.5 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 within this group, a subgroup containing information on the D excitation channels and a subgroup containing information on the C receive channels.

In general each MPI dataset consists of measurement data of N+Mframes, where N is the number of subject measurements and M is the number of background measurements. A frame groups together all data that will can used to reconstruct a single MPI image/tomogram. In the simplest scenario a frame consist of the data acquired during a single drive field cy-

cle. If averaging is applied at the receiver the time it takes to capture a single frame increases by receiver/numAverages, but the amount of data captured remains the same. In a multi patch setting J offsetFields or mechanical movements shift the gradient field by offsetFieldShift to different spatial positions. Here J is the number patches of a multi patch measurement. In such a scenario a frame may consist of J sub-measurements, each of which is acquired and averaged over receiver/numAverages drive field cycles. For instance a Cartesian 2D trajectory with 100 lines would be realized by setting numPatches = 100.

Parameter	$\mathbf{Type}$	Dim	Unit/Format	Optional	Description
startTime	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC start time of MPI measurement
numFrames	Int64	1	1	no	Number of available measurement frames, denoted by $N$
${\tt numBackgroundFrames}$	Int64	1	1	no	Number of available background measurement frames, denoted by ${\cal M}$
framePeriod	Float64	1	S	no	Complete time to acquire data of a full frame (product of drive field period, numPatches, and numAverages)
numPatches	Int64	1	1	no	Number of patches within a frame denoted by $J$
gradient	Float64	$J \times 3$	${\rm Tm}^{-1}\mu_0^{-1}$	yes	Gradient strength of the selection field in $x$ , $y$ , and $z$ directions
offsetField	Float64	$J \times 3$	$\mathrm{T}\mu_0^{-1}$	yes	Offset field applied for each patch in the measurement sequence
offsetFieldShift	Float64	$J \times 3$	m	yes	Position of the field free point (relative to origin/center)

### 2.5.1 Drive Field (group: /acquisition/drivefield/)

**Remarks:** The drive field subgroup describes the excitation details of the nels for particle excitation. Since most drive-field parameters may change imaging protocol. On the lowest level each MPI scanner contains D chanfrom patch to patch they have a leading dimension J.

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 generated drive-fields of channel d can be 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,  $\phi_l$  is the phase,  $f_l$  is the frequency (described by the base fre-

quency and the divider), and  $\Lambda_l$  is the waveform. The waveform is specified by a dedicated parameter waveform. it can be set to *sine*, *triangle* or *custom*. If set to *custom*, one can specify a custom waveform using the parameter customWaveform. The number of sampling points of the customWaveform is denoted by U. The triangle is defined to be a  $2\pi$  periodization of the triangle function:

$$\Lambda_{\rm tri}(t) = \left| t + \frac{\pi}{2} \right| - \frac{\pi}{2} \quad \text{for} \quad -\frac{3}{2}\pi \le t \le \frac{\pi}{2}$$

Type	Dim	${ m Unit/Format}$	Optional	Description
Int64	1	1	no	Number of drive field channels, denoted by $D$
Float64	$J\times D\times F$	$T\mu_0^{-1}$	no	Applied drive field strength
Float64	$J \times D \times F$	rad	no	Applied drive field phase $\varphi$ in radians in the range $[-\pi,\pi)$
Float64	1	Hz	no	Base frequency to derive drive field frequencies
Float64	$D \times F \times U$	1	yes	Custom waveform table
Int64	$D \times F$	1	no	Divider for drive fields frequencies (baseFrequency / divider)
String	$D \times F$	1	no	Waveform type: sine, triangle or custom
Float64	1	s	no	Drive field trajectory period
	Int64 Float64 Float64 Float64 Int64 String	Int64 1 Float64 $J \times D \times F$ Float64 $J \times D \times F$ Float64 1 Float64 $D \times F \times U$ Int64 $D \times F$ String $D \times F$	Int64 1 1  Float64 $J \times D \times F$ $T\mu_0^{-1}$ Float64 $J \times D \times F$ rad  Float64 1 Hz  Float64 $D \times F \times U$ 1  Int64 $D \times F$ 1  String $D \times F$ 1	Int64 1 1 no  Float64 $J \times D \times F$ $T\mu_0^{-1}$ no  Float64 $J \times D \times F$ rad no  Float64 1 Hz no  Float64 $D \times F \times U$ 1 yes  Int64 $D \times F$ 1 no  String $D \times F$ 1 no

#### 2.5.2 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 some quantity related to the magnetization dynamic. In most cases these will be a voltage signals induced into the C receive coils, which are proportional to the change of the particle magnetization.

The MPI signal is obtained at Z equidistant time points. Note that in most cases the voltages are not measured directly at the receive coils but amplified and filtered first. To be able to compensate these changes the transfer function can optionally be stored in the parameter transferFunction. It is stored in frequency space representation where  $K = \frac{Z}{2} + 1$  is the number of discrete frequency components.

Parameter	$\mathbf{Type}$	$\mathbf{Dim}$	Unit/Format	Optional	Description	
numChannels	Int64	1		no	Number of receive channels $C$	
numAverages	Int64	1		no	Internal block averaging over a number of drive field cycles	
bandwidth	Float64	1	$_{ m Hz}$	no	Bandwidth of the receiver unit	
numSamplingPoints	Int64	1		no	Number of sampling point within one drive-field period denoted by ${\cal Z}$	
transferFunction	Float64	$C\times K\times 2$		yes	Transfer function of the receive channel	

#### 2.6 Measurement (group: /measurement/)

Remarks: TODO Tobi: Update group with the changes from latest discussion. MPI data is usually acquired by a series of N measurements and M background measurements. Here we refer to background measurements as MPI data captured, when any signal generating material, e.g. a phantom or a delta sample is removed from the scanner bore. Both the N measurements and the M background measurements can be stored in an arbitrary order, e.g. with respect to the spatial position of a delta sample if the data corresponds to a calibration measurement. To be able to recover the time order in which the measurements were taken each of the N+M data sets can be assigned an integer number  $o=1,2,\ldots,N+M$  ordering the measurements and background measurements with respect to time. I.e. data set  $o_1$  is acquired prior to data set  $o_2$ , if and only if  $o_1 < o_2$ .

The resulting N measurements and M background measurements should be stored in time domain, where the data of a single frame consists

of the signal recorded for all patches in each receive channel, i.e.  $J \times C \times Z$  data points per set with the temporal index being the fastest to access. If several measurements are acquired (indicated by numFrames), the N measurements and M background measurements are concatenated along the slowest dimension respectively.

During measurements the analog signal measured is usually converted into  $(r_1,\ldots,r_{JZ})\in\mathbb{Z}^J\times\mathbb{Z}^Z$  integer values per channel  $c\in C$  and frame using analog to digital converters. Often this raw data is stored instead of the physical quantities they represent. To bring the raw values into a physical representation one can map  $r_i\mapsto (a_cr_i+b_c)U$ , where  $a_c$  and  $b_c$  are the characteristic dimensionless scaling factor and offset the receive channel  $c\in C$  and U is the corresponding unit of measurement, i.e. usually voltages.

Parameter	$\mathbf{Type}$	Dim	${ m Unit/Format}$	Optional	Description
unit	String	1		yes	SI unit of the measured quantity, usually V
dataConversionFactor	Number	$C \times 2$		yes	Dimension less scaling factor and offset $(a_c, b_c)$ to convert raw data into a physical quantity with corresponding unit of measurement unit
data	Number	$N+M\times J\times C\times Z$		yes	Measurement data stored in time domain representation
isBackgroundData	Int8	N + M		yes	Boolean mask indicating for each frame if it contains background data or not.

# 2.7 Processing (group: /processing/)

Parameter	$\mathbf{Type}$	Dim	${ m Unit/Format}$	Optional	Description
processedData	Number	$Q\times J\times C\times K\times 2$		yes	Processed data stored in frequency domain representation
processedDataTransposed	Number	$J \times C \times K \times Q \times 2$		yes	As processed data but transposed
isSpectralLeakageCorrected	Int8	1		yes	flag indicating if spectral leakage correction has been applied
isTransferFunctionCorrected	Int8	1		yes	flag indicating if the transfer function has been corrected
isAveraged	Int8	1		yes	flag indicating if the raw data has been averaged in a processing step
isFramesSelected	Int8	1		yes	flag indicating if the processed data contains only a selection of the raw data
isBackgroundCorrected	Int8	1		yes	flag indicating if a background has been corrected
permutation	Int64	Q		yes	Index vector indicating a permutation of the $Q$ frames

# 2.8 Calibration (group: /calibration/)

Remarks: TODO Tobi: Update group with the changes from latest discussion.

Parameter	Type	Dim	Unit/Format	Optional	Description
snr	Float64	$J\times C\times K$		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
orderDimensions	String	1		yes	Ordering of the dimensions, default is xyz
positions	Float64	$Q \times 3$	m	yes	Position of each of the grid points, stored as $(x, y, z)$ triples
offsetField	Float64	$Q \times 3$	$\mathrm{T}\mu_0^{-1}$	yes	Applied offset field strength to emulate a spatial position $(x, y, z)$
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 on the number of individual channels S obtained by the reconstruction the results can be stored in a  $L \times P$  array for S = 1 or in a  $L \times P \times S$  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.

system matrix grid, the grid parameter are mirrored in the reconstruction parameter group.

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

Parameter	Type	Dim	${f Unit/Format}$	Optional	Description
data	Number	$L\times P\times S$		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	$P \times 3$	m	yes	Position of each of the grid points, stored as $(x, y, z)$ tripels
overscanMask TODO martin :-)	Float64	$P \times 3$	m	yes	Position of each of the grid points, stored as $(x, y, z)$ tripels

### 3 Changelog

#### $3.1 \quad v2.0.0$

- Updated Affiliations in the MDF specification.
- Made extensive improvements to the descriptions of fields and groups.
- 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 should make implementations handling MDF files less complex.
- Specified supported data types for the storage of measurement data and reconstruction data.
- Rename /date to /time for consistency reasons.
- Remove /study/reference since this functionality is now covered by the integrated background measurements.
- Rename /study/simulation to /study/isSimulation for consistency reasons and changed type to Int8.
- Created new group /experiment with fields /experiment/name, /experiment/number and /experiment/description to be able to provide more fine grained information on study and experiment.
- Moved /study/subject and /study/isSimulation to /experiment/subject and /experiment/isSimulation.
- $\bullet$  Renamed /tracer/time to /tracer/injectionTime.
- Added the possibility store the tracer concentration also for non iron based tracer materials by adding the /tracer/solute field and redefining the field tracer/concentration.
- Renamed field /tracer/time to /tracer/injectionTime to be more specific.

- Added the dimension A to all fields of the tracer group to be able to describe settings where multiple tracers are used or tracers are administered multiple times.
- Added field /scanner/boreSize to describe the scanner.
- Set all fields but topology in the /scanner group to be optional.
- Rename /acquisition/time to /acquisition/startTime.
- /acquisition/gradient is now optional since it is now mandatory for MPS measurements.
- Added field /acquisition/numBackgroungFrames as counter for the number of measurements used for background subtraction.
- Added /acquisition/offsetField and /acquisition/offsetFieldShift to describe homogeneous offset fields.
- Support for triangle wave forms and fully arbitrary excitation waveforms has been added by adding the fields /drivefield/phase, /drivefield/customWaveform, /drivefield/waveform.
- ullet Support for multiple excitation frequencies on a drive-field channel has been added by intoducing a new dimension F to the fields /drivefield/strength, /drivefield/phase, /drivefield/customWaveform, /drivefield/waveform, and /drivefield/divider.
- Removed fieldOfView and fieldOfViewCenter from /drivefield group. /acquisition/offsetField and /acquisition/offsetFieldShift replace fieldOfViewCenter. The fieldOfView can be derived from the gradient strength and drive field strength.
- Moved /drivefield/averages to /receiver/numAverages

- Remove /acquisition/receiver/frequencies since it can be 3.4 v1.0.3 directly derived from /acquisition/receiver/bandwidth and /acquisition/receiver/numSamplingPoints.
- TODO Tobi: record changes to /measurement group here. Added possibility to store the transformation from raw data to a physical representation with units. Signal to noise ratios can now be stored for each patch indivisually. To do so the dimension J was added to this field.
- TODO Tobi: record changes to /calibration group here.
- Added new section changelog to the MDF documentation to record the development of the MDF.

#### $3.2 \quad v1.0.5$

- Added the possibility to store different channels of reconstructed data.
- Added support for receive channels with different characteristics (e.g. bandwidth).
- Made dataset /acquisition/receiver/frequencies optional.
- Extended the description on the data types, which are used to store data.
- Added references for Julia and HDF5 to the specifications.

#### 3.3 v1.0.4

• Clarify that HDF5 datasets are used to store MPI parameters.

- Updated Affiliations in the MDF specification.
- Included data download into the Python and Matlab example code.
- Changes in the Python and Matlab example code to be better comparable to the Julia example code.

#### 3.5 v1.0.2

• Added reference to arXiv paper and bibtex file for reference.

#### 3.6 v1.0.1

- A sanity check within the Julia code shipped alongside the specifications.
- An update to the specification documenting the availability of a sanity check.
- Updated MDF files on https://www.tuhh.de/ibi/research/mpi-dataformat.html.
- Updated documentation to the Julia, Matlab and Python reconstruction scripts.
- Improved Julia reconstruction script, automatically downloading the required MDF files.

### References

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

- [2] Jeff Bezanson, Stefan Karpinski, Viral B. Shah, and Alan Edelman. Julia: A fast dynamic language for technical computing. CoRR, abs/1209.5145, 2012.
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