



High Data Rate Processing and Analysis Initiative (HDRI)



Helmholtz PNI Centres DESY Hamburg
FZ Jülich
FZ Karlsruhe
GKSS Geesthacht
GSI Darmstadt
HZB Berlin

Workpackages - WP1: Data Management (DESY, HZB)

- Standardization and Data Formats
- Data Access Strategies
- Data Lifetime Management and Archiving

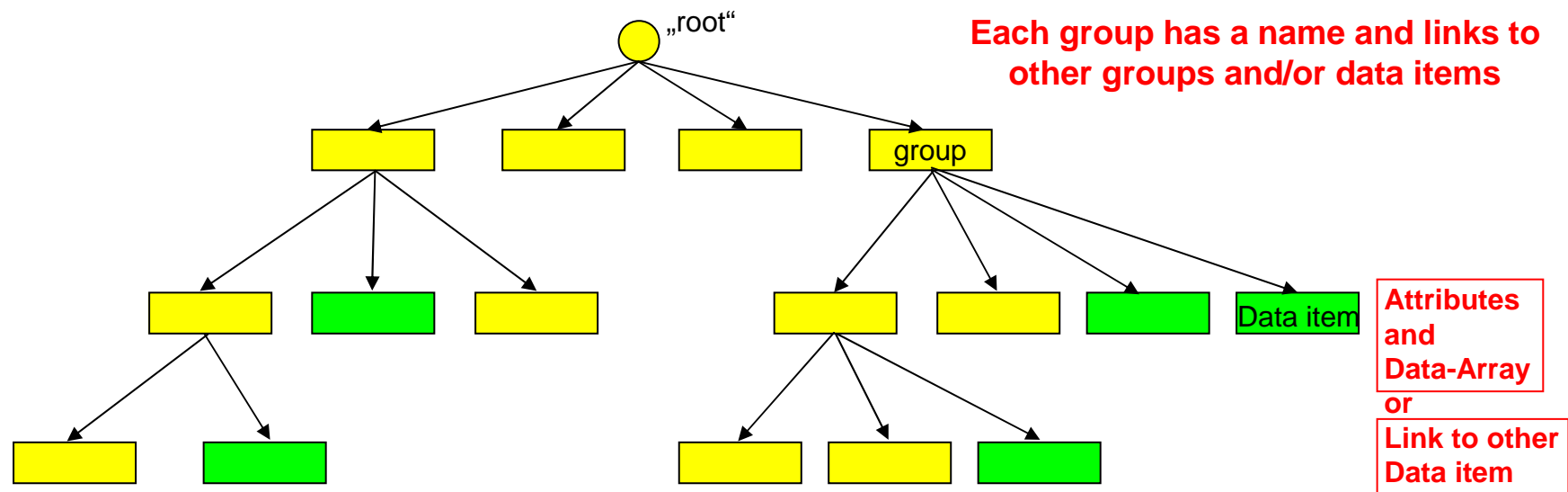
WP2: Real-time Data Processing (GSI, KIT)

- Data Processing with Dedicated Hardware
- Real-Time Data Assessment with Parallel Computing
- Analysis Methods and Applications

WP3: Data Analysis, Modelling, and Simulation (FZJ)

- Motivation:**
- Facilitate exchange of data
 - Provide a unified interface to data evaluation software
 - Enforce complete assembly of parameters, data, and meta-data to fully describe the experimental setup and the experiment

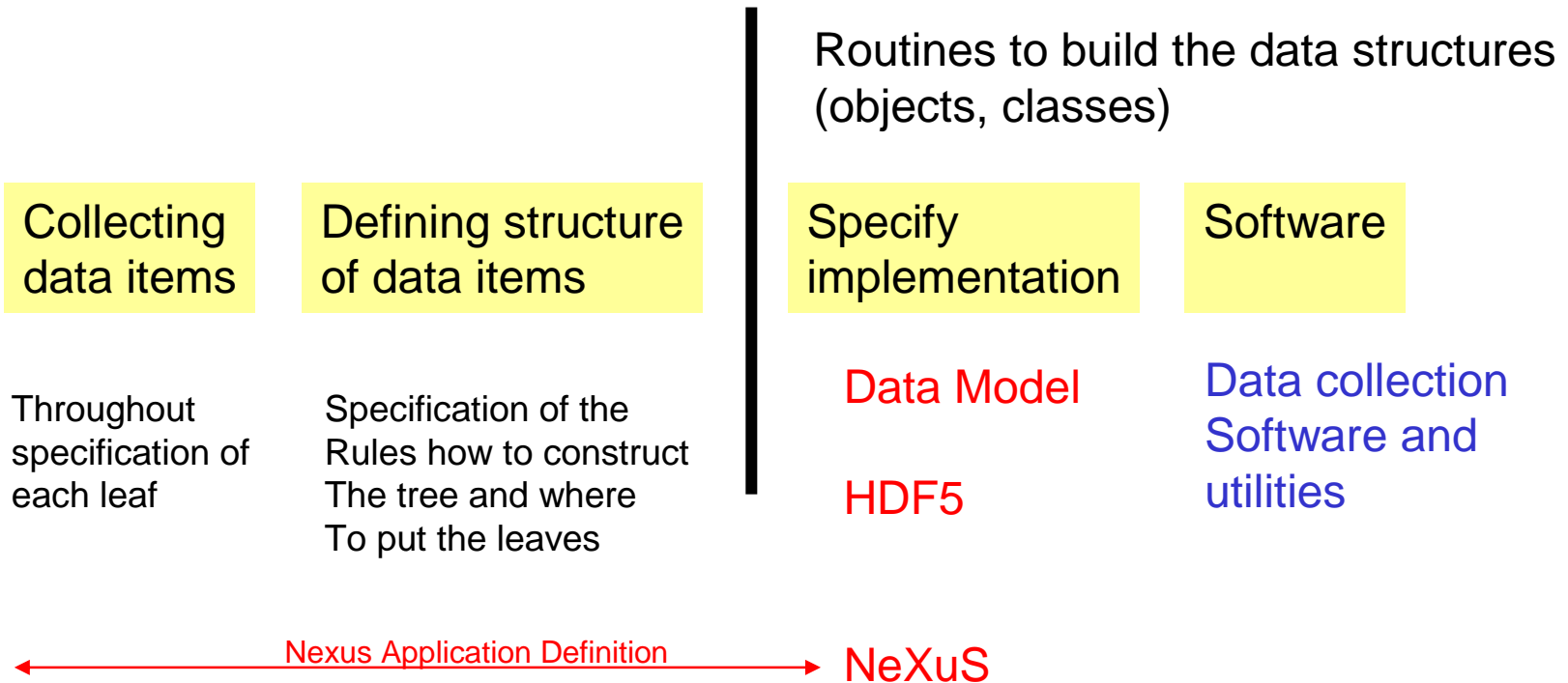
- Aims**
- Hierarchically structured and self-documenting
 - Flexible and extendible
 - **Efficient Access**
 - **High integrity**



A data item is identified by its path: „root“/xx/yy/..zz



Steps towards a data format





Catalogue of Names



Root group identifies class of experiment:

Protein crystallography, μ -Tomography, SAS/WAS, GISAS, μ -Fluorescence, ...

Task for each class:

Define as many group and data item identifiers as possible (names & placement in tree)

- Name
- Position in tree
- Definition of meaning
- Attributes [e.g. units] (for data items)
- Default attributes [e.g. wavelength in nm] (for data items)
- Format of representation [e.g. array of real numbers, flag] (for data items)

Data items are either

- In catalogue and mandatory for class
- In catalogue but optional (used only if required)
- Freely defined by user (unknown by catalogue)

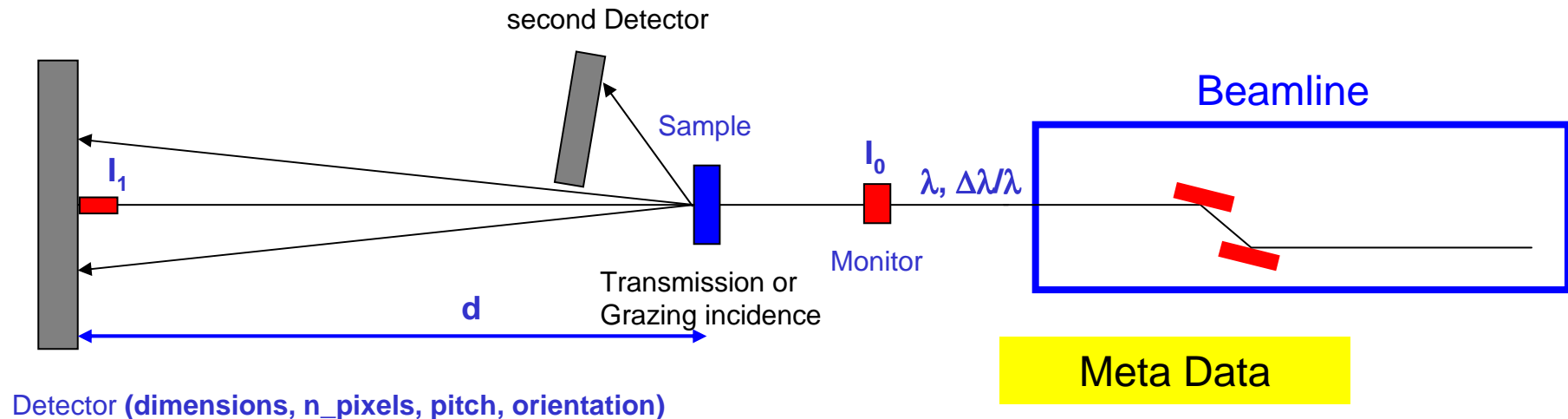


Workshop Agenda



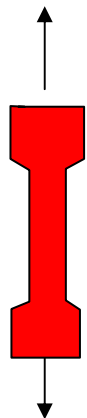
	Wednesday, Oct. 27	Thursday, Oct. 28	Friday, Oct. 29
09:00		Working Groups	Working Groups
15			
30			
45			
10:00	Welcome (E. Weckert)		
15	Workshop Motivation and SAXS (R. Gehrke)		
11:00	Coffee Break	Coffee Break	Coffee Break
30	Tomography (F. Beckmann)	Working Groups	Discussion of Working Group results
12:00	EXAFS and Fluorescence (G. Wellenreuther)		
30	PX (T. Schneider)		
13:00	Lunch	Lunch	Lunch
14:00	Common Data Model (A. Buteau)	Discussion of Working Group results	
45	Discussion		
15:00	NeXuS application definitions (M. Koennecke)	NeXuS (M. Koennecke)	
30	Discussion (Instrument definitions)		
45		Discussion	
16:00	Coffee Break	Coffee Break	
30	Discussion (Instrument definitions)	MetaData (N.N.)	
17:00	Wikis and Mindmaps (R. Gehrke)		
15		Discussion (Meta Data)	
30	Definition of Working Groups		
		Dinner 19:00 Bistro	

Working Groups in Rooms **456, 235, 116** (Bldg. 61), **L110** (Petra)



In-Situ measurements

- Example 1: Heating $\rightarrow T, t$
- Example 2: Sputter deposition
- Example 3: Stretching



Stress, strain
TV-image

Scanning measurements

- Example 1: μ -focus 2D raster scanning $\rightarrow x, y$
- Example 2: orientation scanning $\rightarrow \alpha$

Simultaneous measurements

- Example 1: Ellipsometry
- Example 2: DSC
- Example 3: Microscopy (optical, AFM)

Virtually any combination of this is possible
 \rightarrow **New (unpredictable) experiment strategies**

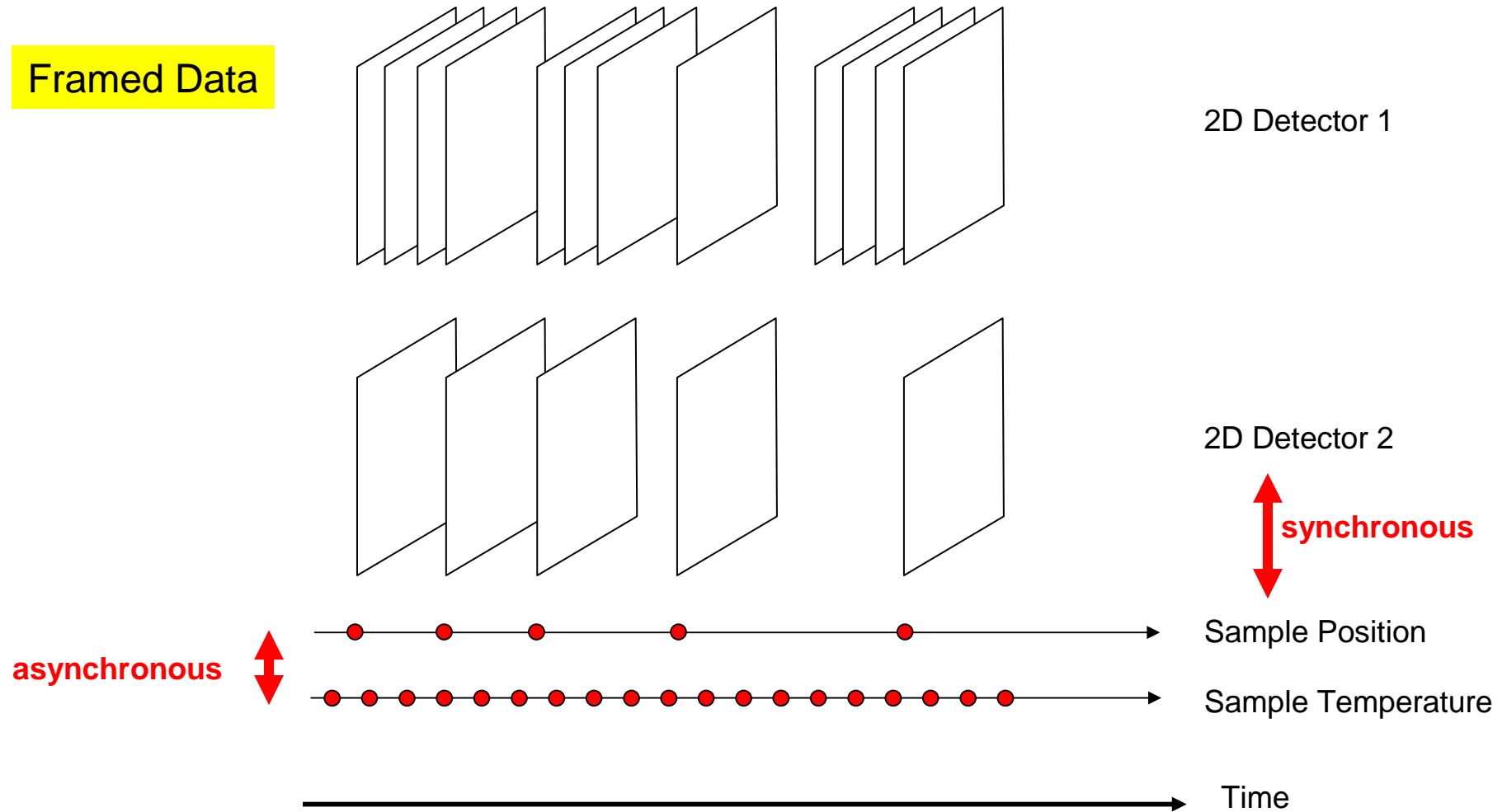


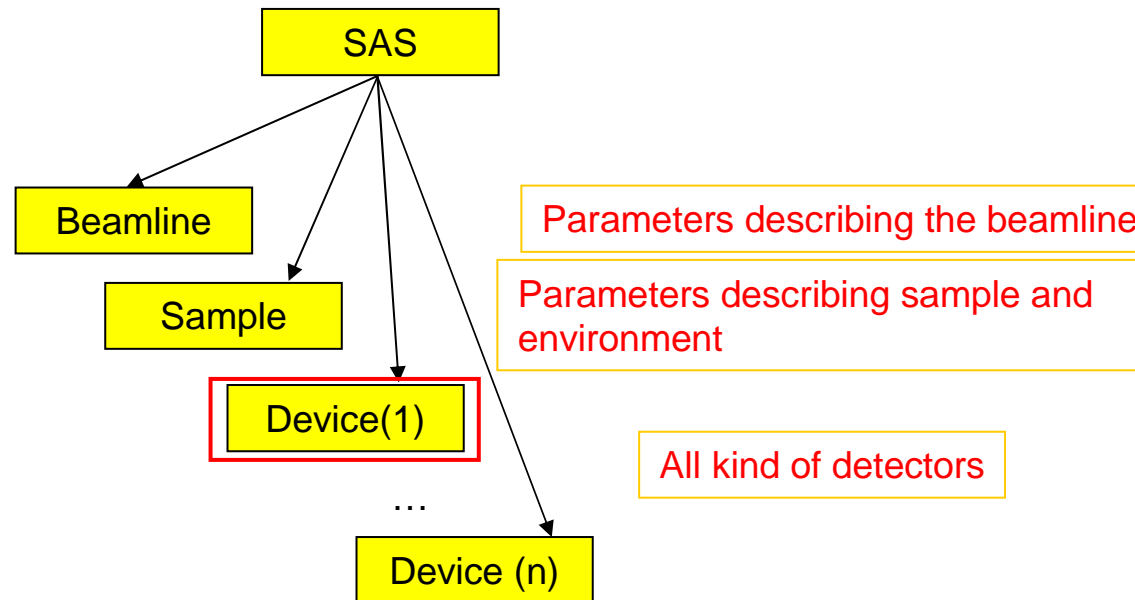
Static, synchronously and asynchronously framed data



Static Data

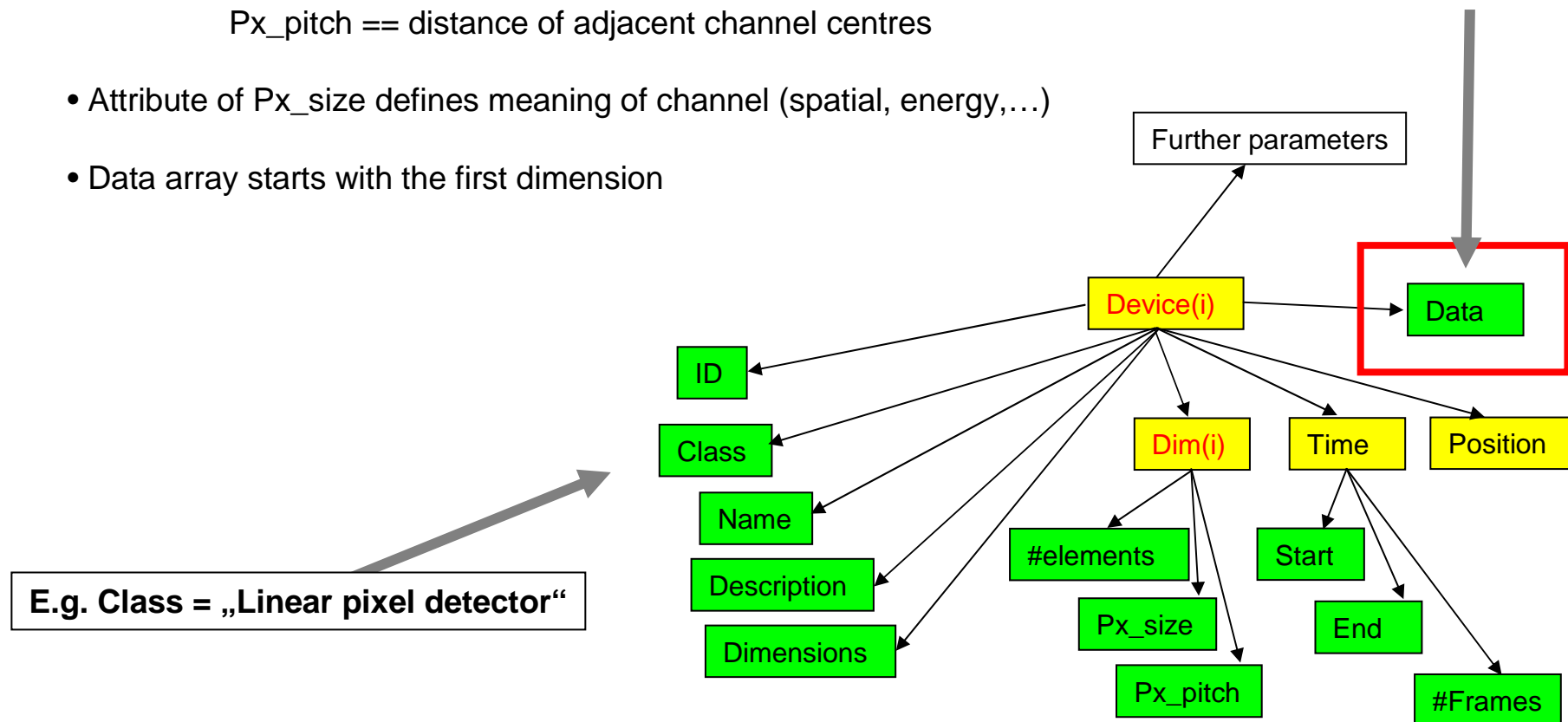
Framed Data





- „Linear“ means **equidistant** in all dimensions
- „Element“ represents a „**recording channel**“ !!!
 #elements == number of independent channels in that „dimension“
 Px_size == width of this channels
 Px_pitch == distance of adjacent channel centres
- Attribute of Px_size defines meaning of channel (spatial, energy,...)
- Data array starts with the first dimension

Array with
one index for
each dimension
(+Frame index)



Note: One group „Dim“ for each dimension !!!

Note: Group „time“ appears if data are framed !!!



Frame based Experiments



Series of subsequent measurements (frames) with index i

Example 1: Time Resolved Measurement

Data items are either static (n dimensions) or framed ($n+1$ dimensions)
with time as additional dimension

`../device(k)/data(x,y,i)`

`../device(k)/time/start(i)`

`../device(k)/time/stop(i)`

Example 1: 2D-Raster Scanning

Data items are either static (n dimensions) or framed ($n+1$ dimensions)
with sample position as additional dimension

`../device(k)/data(x,y,i)`

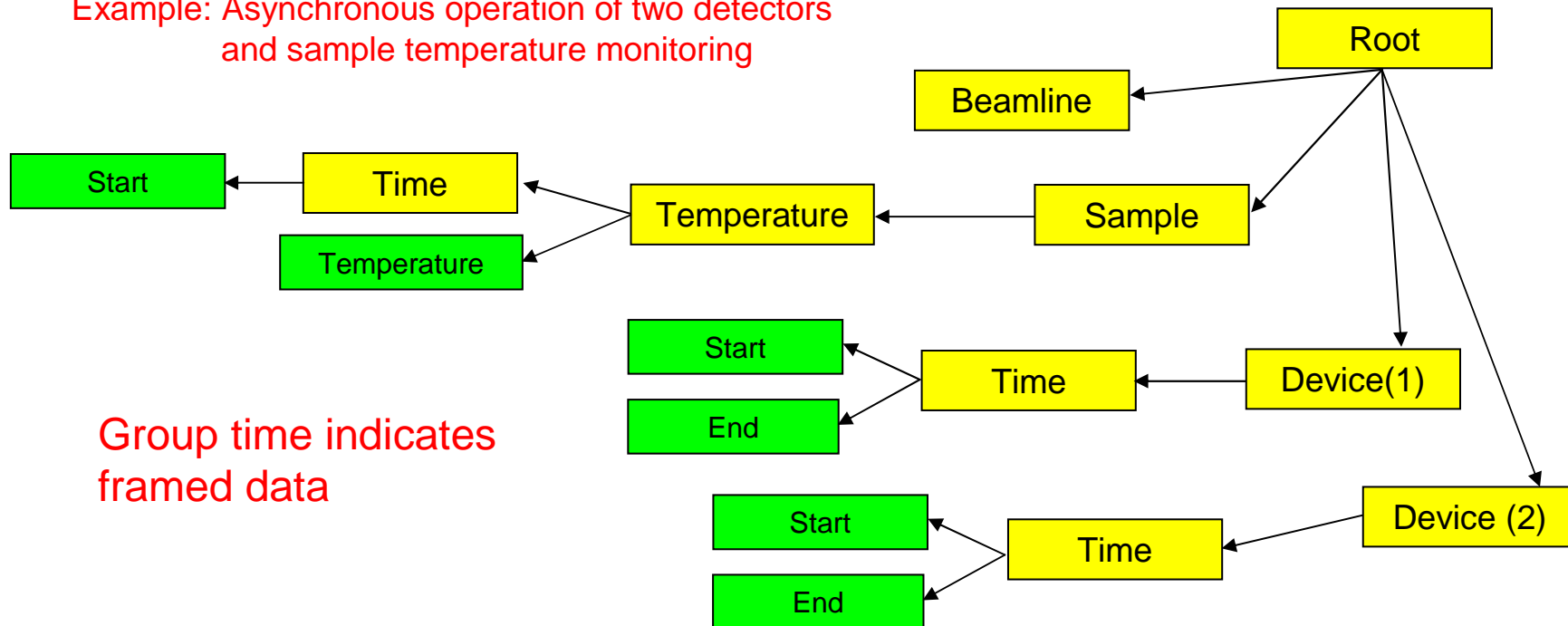
`../sample_pos_x(i)`

`../sample_pos_y(i)`

`../device(k)/time/start(i)`

`../device(k)/time/stop(i)`

Example: Asynchronous operation of two detectors and sample temperature monitoring



Group time indicates framed data

- Each framed data array corresponds to a **start-timestamp** array
- For devices it marks the start of a data acquisition
- For devices a **stop-timestamp** array marks the end of acquisition
- **This allows for asynchronous change of parameters and device operation**
- Synchronous groups share their timestamps, i.e. one element holds the timestamp array(s), the others link to it



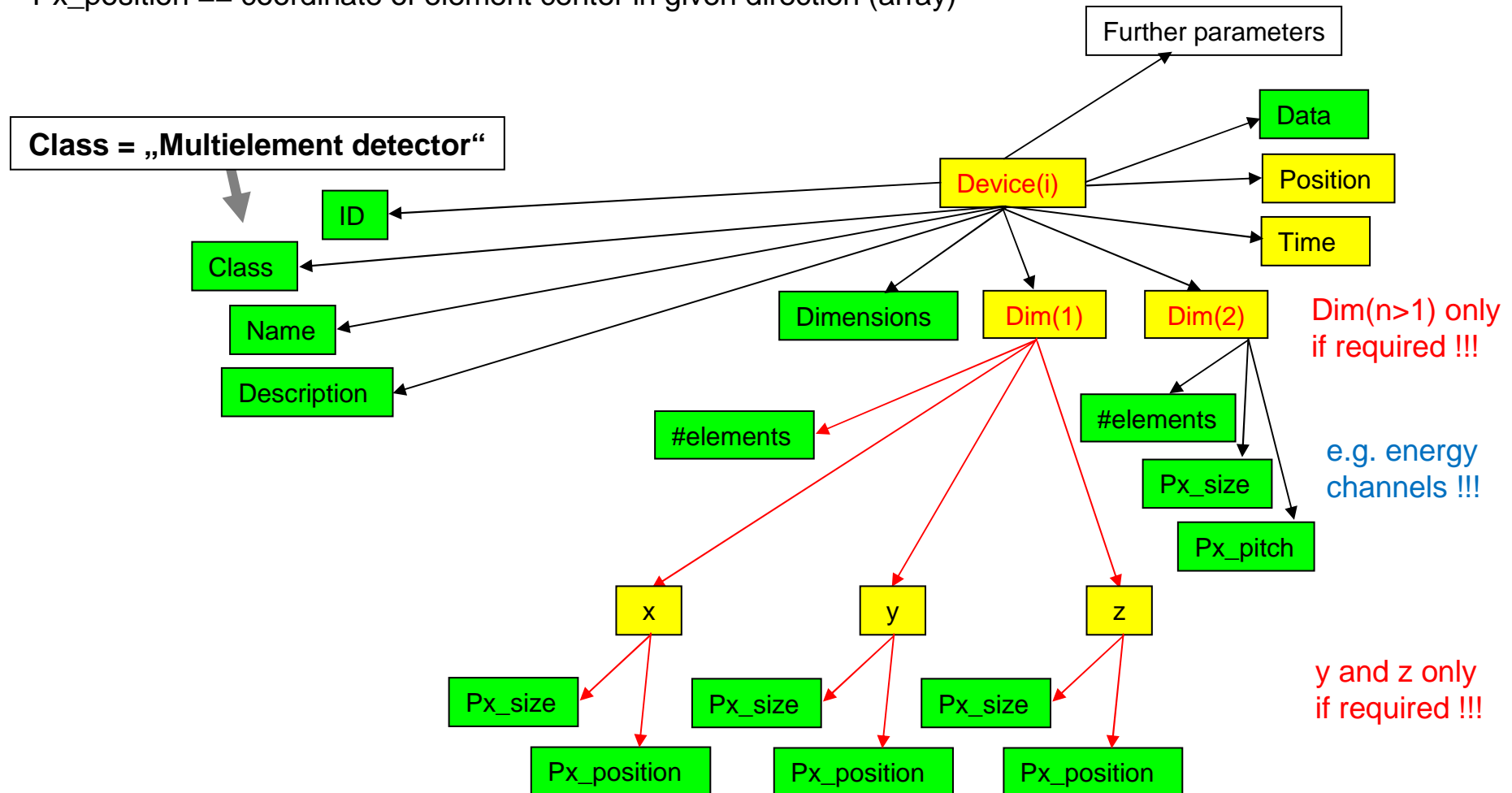
Device Description (general multielement detector)

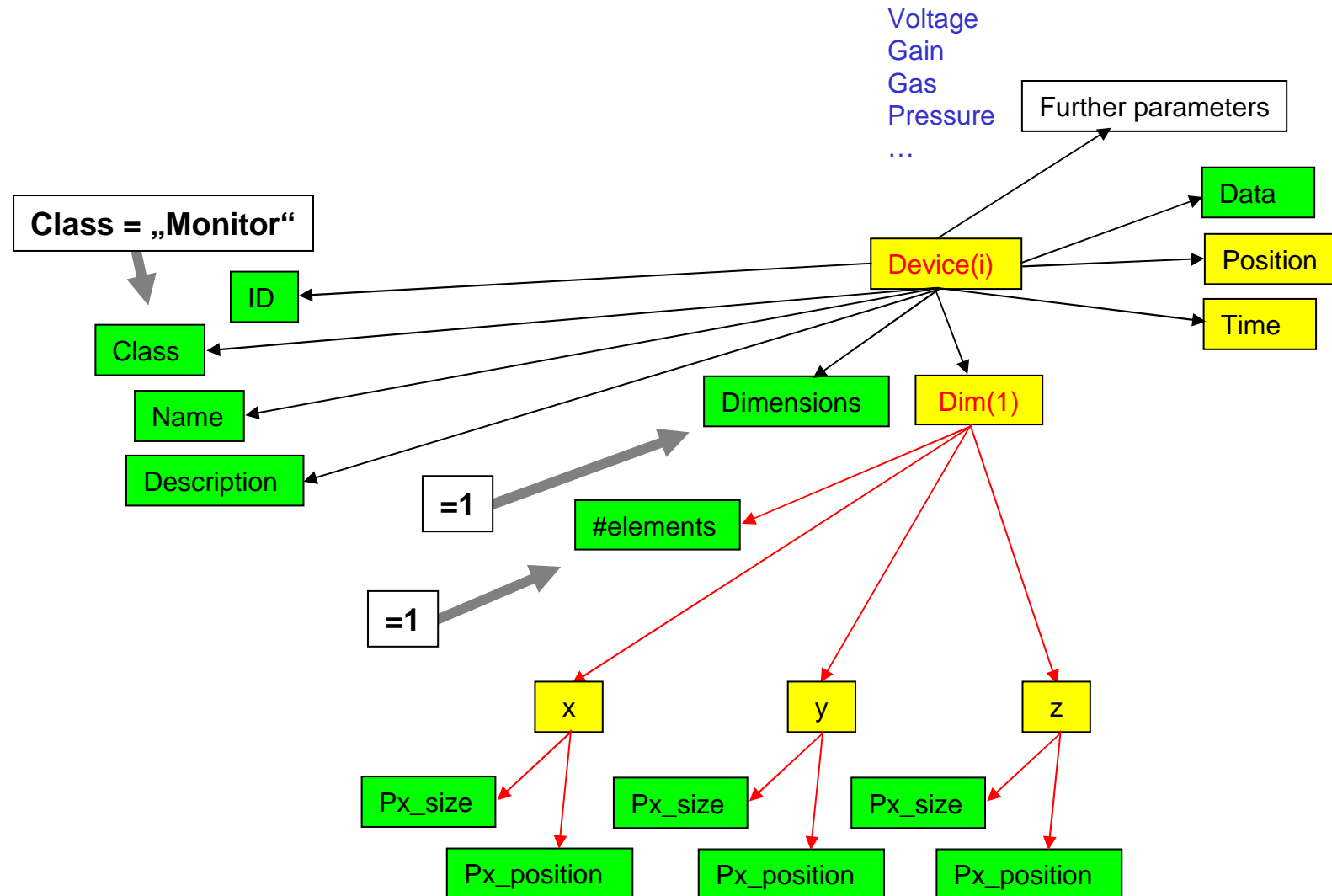


#elements == total number of elements

Px_size == Size of elements in given direction (array)

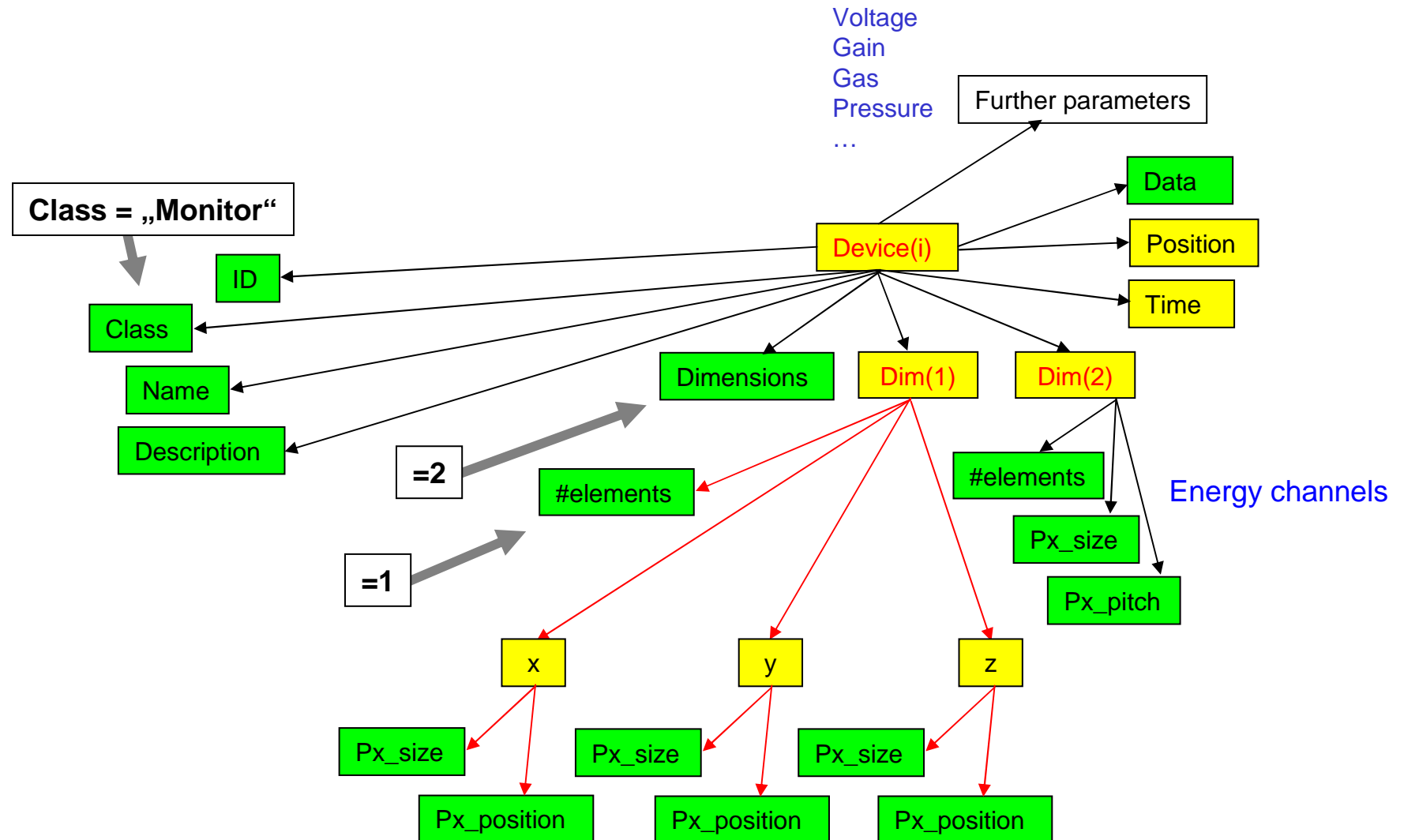
Px_position == coordinate of element center in given direction (array)







Device Description (Example energy resolving point detector)



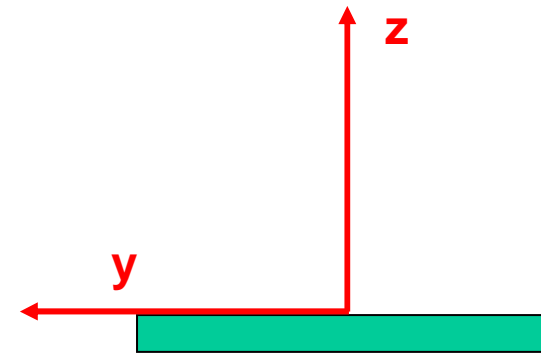
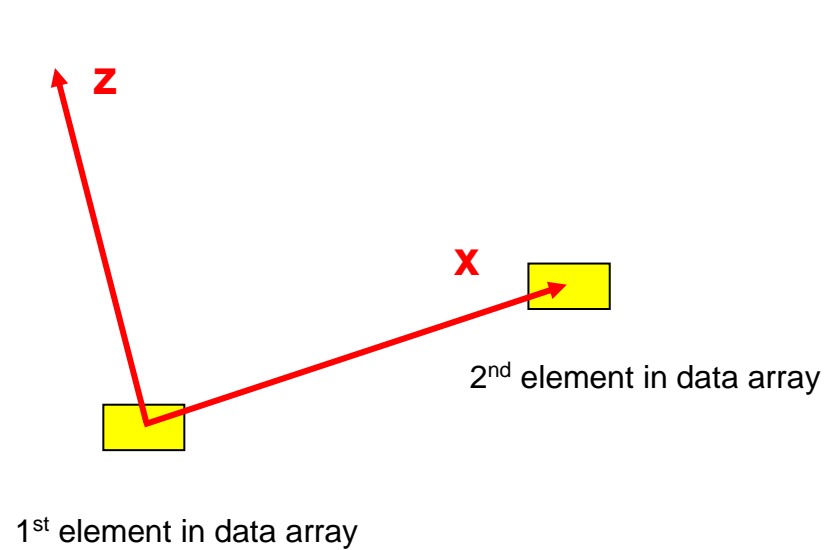


Device and Sample Reference Systems



Device

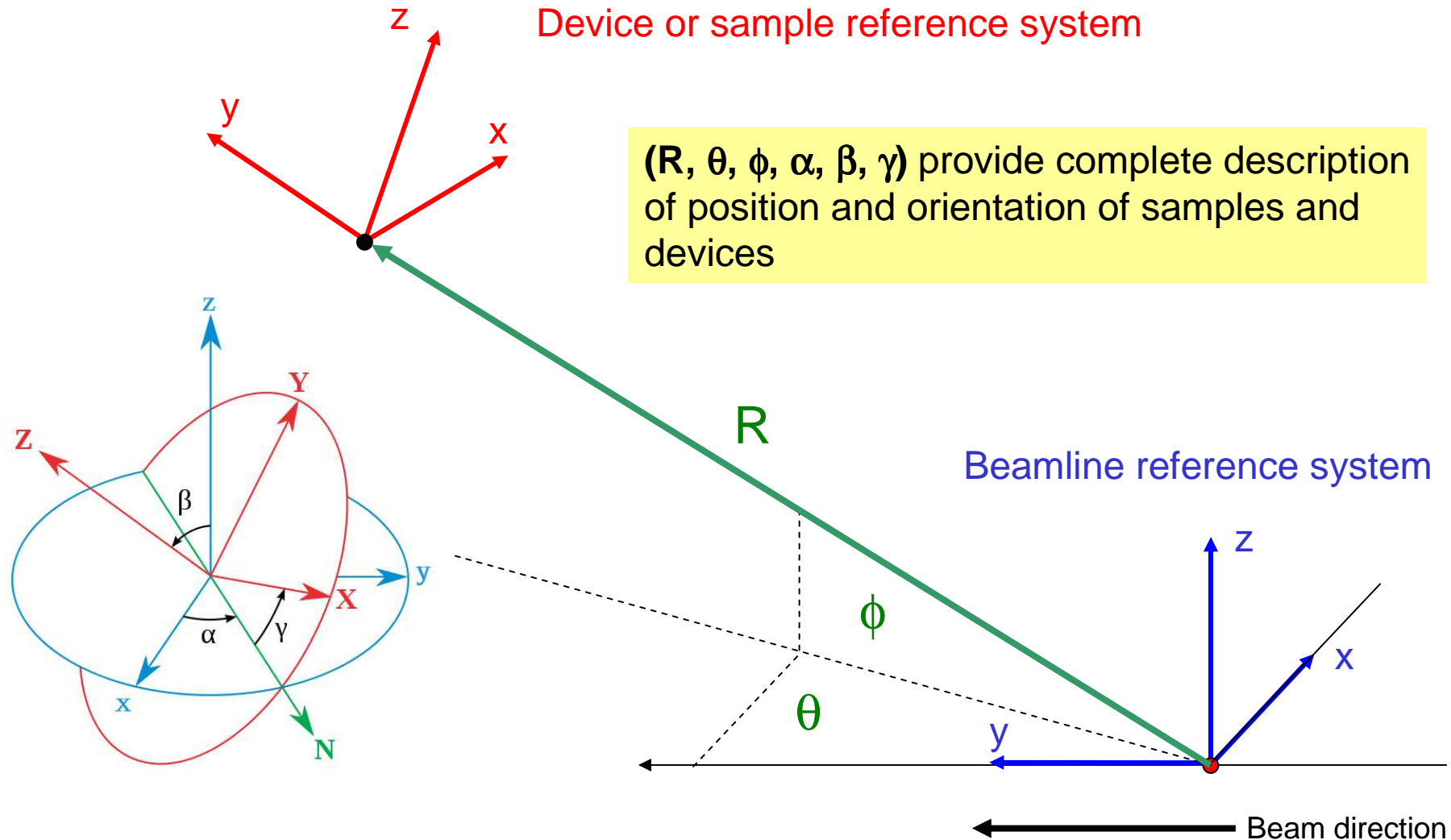
Sample



X-direction is defined by the first two elements
In the first dimension of the data array

Works for samples with defined surface
and shape

Groups „device“ and „sample“ include subgroups „position“



$(R, \theta, \phi, \alpha, \beta, \gamma)$ provide complete description of position and orientation of samples and devices



Positions and orientations



$(R, \theta, \phi, \alpha, \beta, \gamma)$ provide complete description of position and orientation of samples and devices

Pro: **Unified** description of all positions and orientations
(no need to further specify the chosen coordinates)

Con: Simple device or sample movements mostly involve complicated changes of many of the six parameters

Examples: - Change of incident angle in a surface scattering experiment
- Movement of a point detector along different scattering angles
- horizontal sample shift



Sample Description



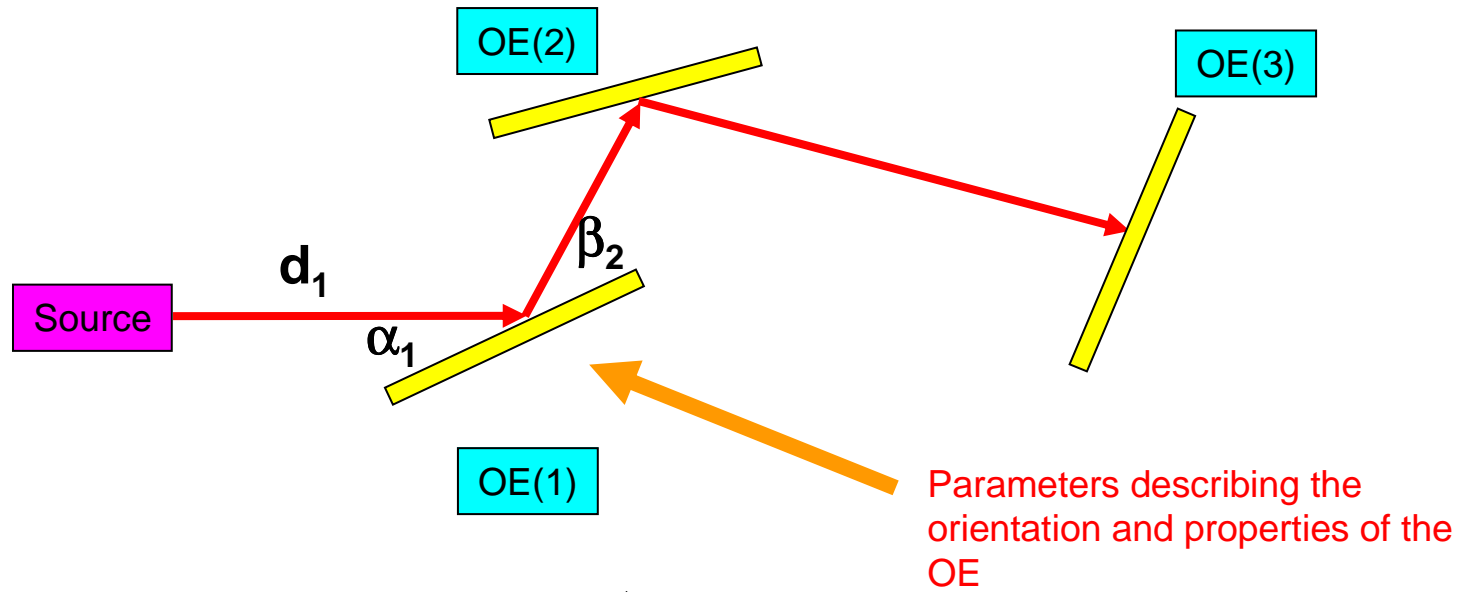
- Position and Orientation (proper coordinate system)
- Description (free text)
- External parameters (e.g. sample temperature, elongation, etc.)
- Flags indicating reference measurements (reference, background)
- Sample changers



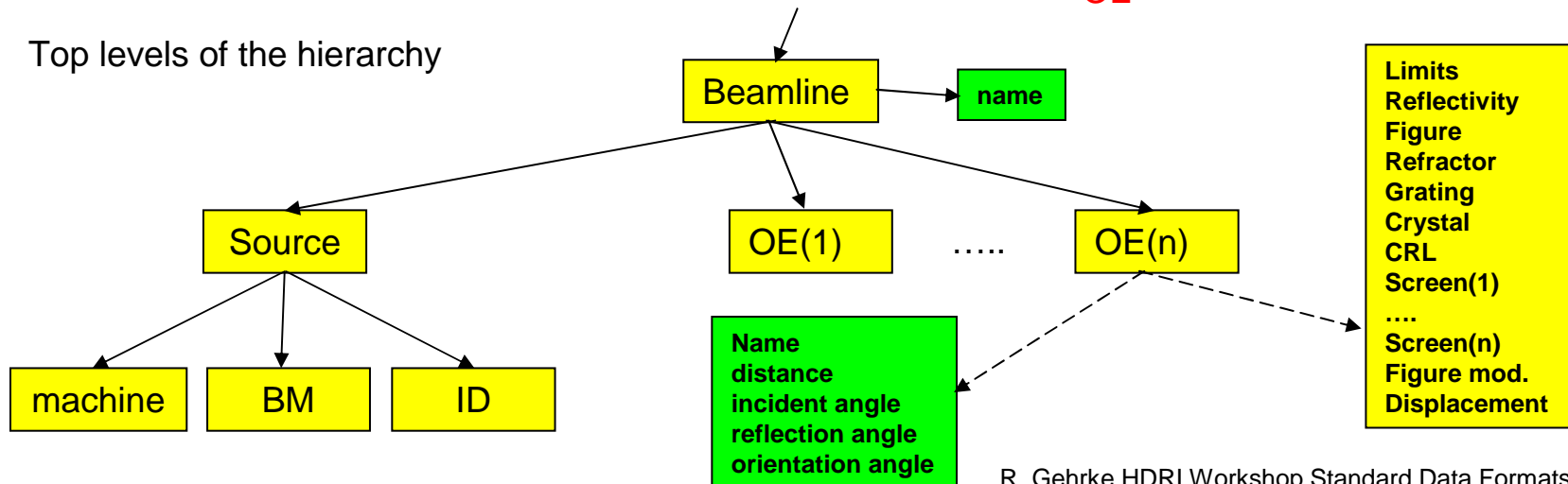
Beamline Description



Based on construction according to raytracing program „Shadow“

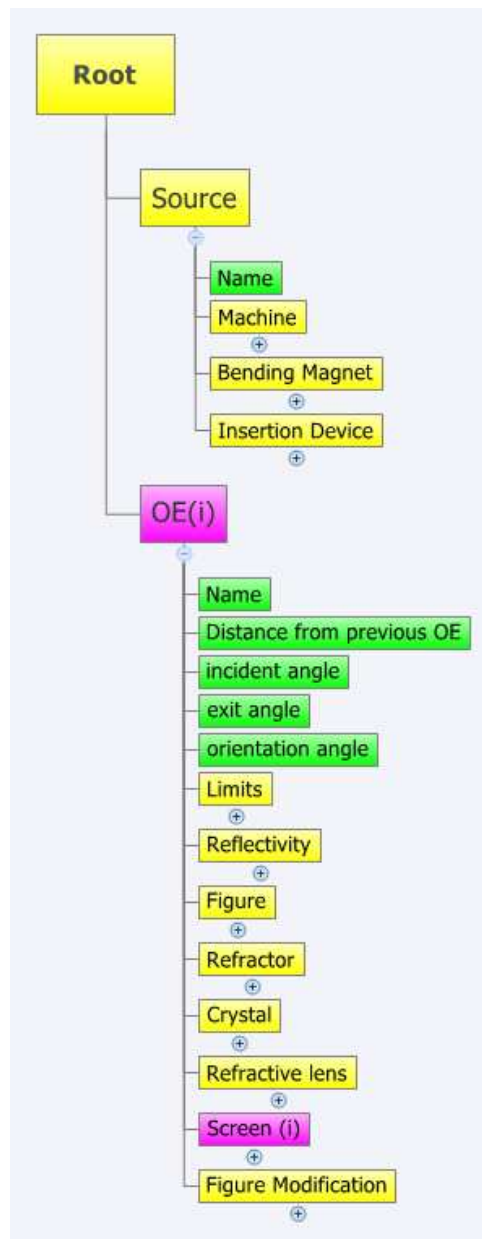


Top levels of the hierarchy





The Instrument Subtree





Data item specification



Name: *Wavelength*

Description: *The center wavelength or Energy of the incident beam*

Type 1: (**mandatory**, optional, user defined)

Type 2: (character, string, **float**,.....)

..

Attribute 1: unit (nm, eV, keV)

Attribute 2:

..

1. **API: Application Programming Interface** → HDF5 (NeXuS?)

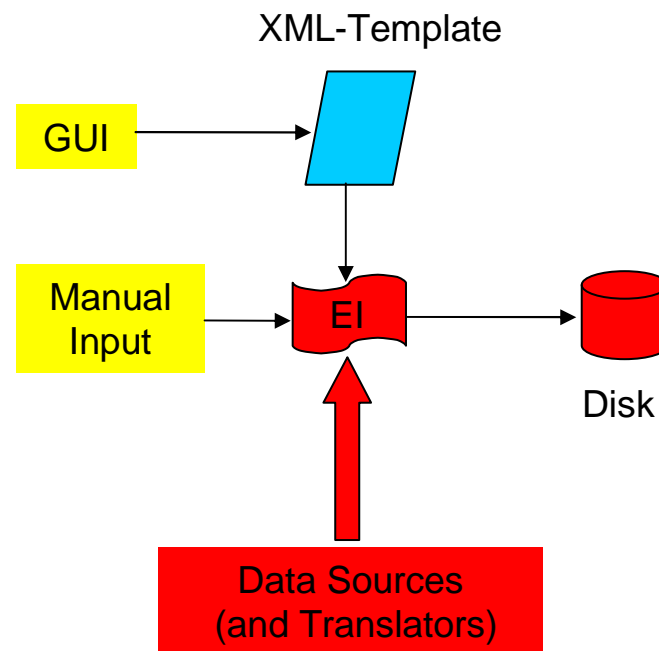
2. **Utilities:** **Content Browser** to list and visualize the content

to extract contents

to manually edit meta data

Validation Tool

3. **Experiment Interface:**



Other features

- Lossless compression
- Change log
- Meta data management



Wiki



<https://hdri-sdf.desy.de/index.php/>

(MediaWiki)

Login:	Password:
FLUO_user	
PX_user	hdri123
SAXS_user	
TOMO_user	

*Everyone can create account
but editor role has to be given by admin*

Links: `[[title]]` link to page **title**
 `[[title|text]]` link to page **title**, display **text**

To create new page: Type URL <https://hdri-sdf.desy.de/index.php/title> in Browser
or in existing page: Create link `[[title]]` and jump to it

To create new category: Type URL <https://hdri-sdf.desy.de/index.php/category:title>
or in existing page: Create link `[[category:title]]` and jump to it

Other Links: `[URL]` Link to external **URL**
 `[[File:filename.ext]]` Link to uploaded file (**ext**=png,gif,jpg,jpeg)

Force line break: `
`



Proposed structure of a Wiki entry



Group/data item

Mandatory/Optional/User defined



Mandatory: Element must be in structure
Optional: If used, must be according to definition
User defined: nobody relies on it

Name

Description

Attributes



List of all attributes to the element with description

Links to ...



Subgroups and data items to this group, list of items with Wiki-Links to corresponding pages

Categories



Wiki categories

Discussion goes to discussion topics

```
Group <br/>
Mandatory

Name: Root

Description: This is where the tree starts

Attributes: none

Links to <br/>
[[Static]] <br/>
[[Framed]] <br/>

[[category: all]] [[category:groups]]
```




XMind



Download

<http://www.xmind.net/xmind/downloads/xmind-win-3.2.0.201009142023.exe>

Java RTE or SDK required