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TECHNICAL NOTE

Detector Alignment at European XFEL: Concepts and Responsibilities

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Contents

Introduction

The analysis of the data from the detectors at the European XFEL will require knowledge of the detector position with respect to both the beam and the sample. A summary of the parameters needed for position determination as well as who is responsible for the summary and when the parameters are to be measured are outlined in this document.

1 Coordinate system

A common coordinate system based on the European XFEL photon distribution coordinate system(s) and therefrom derived systems as described in [1] is to be used. The coordinate system is right-handed with its z-axis horizontal within the experiment hall, extending along the beam direction. Derived systems for each SASE exist—their origins are at the centres of the first undulator segments in each SASE. These coordinate systems will be used for undulator positioning. Additional coordinate systems are implemented for the instruments. These are at a constant offset from the previous coordinate systems and have z=0 at the centres of the third to last undulator segments for SASE1 and SASE2 and the second to last segment for SASE3.

For detector alignment purposes, coordinate systems at a constant z-offset from the last previously mentioned coordinate systems, i.e. the instrument systems, are deemed suitable (Figure 1). They are referred to the instrument reference point in the following. This allows for a trivial transformation to the beamline coordinate system, while limiting the magnitude of the detector z-position.

For the detector coordinate system, z=0 is located on the detector plane, i.e. sensor surface, when the detector is mounted such that the plane normal is parallel to the coordinate system z-axis. For segmented detectors, i.e. detectors with moveable quadrants, the plane of a specified and documented quadrant is to be used. For retractable detectors, i.e. detectors that allow movement along the z-axis while integrated into an experimental station, the fully retracted position is to be used. For detectors mounted flanged to bellows or with variable length tubing in between the detector and the sample chamber, the detector is to be placed (in its fully retracted state) at the minimum sample distance position as determined by the instrument design (Figure 2).

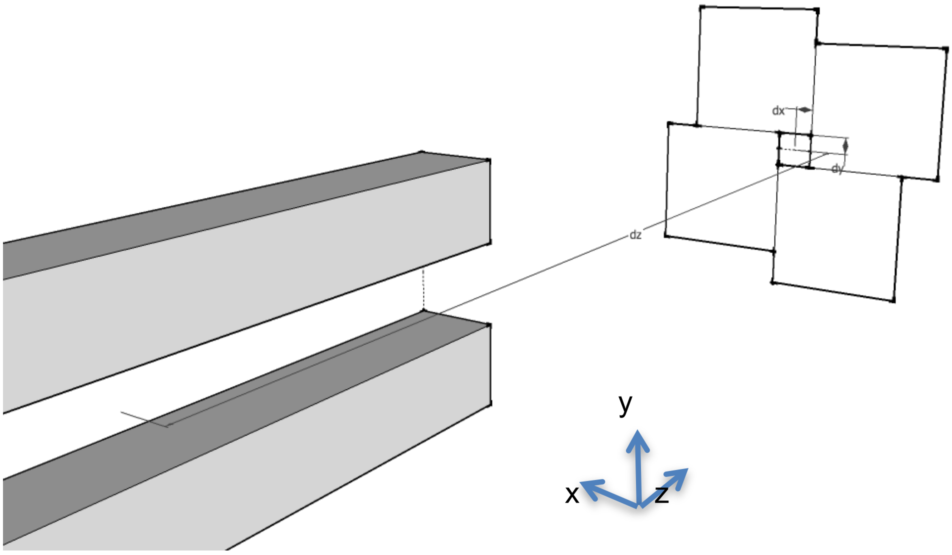

Figure 1: *Sketch of the detector reference coordinate system, which is at a constant z-offset to the photon beamline coordinate system, centred in the middle of a SASE undulator*

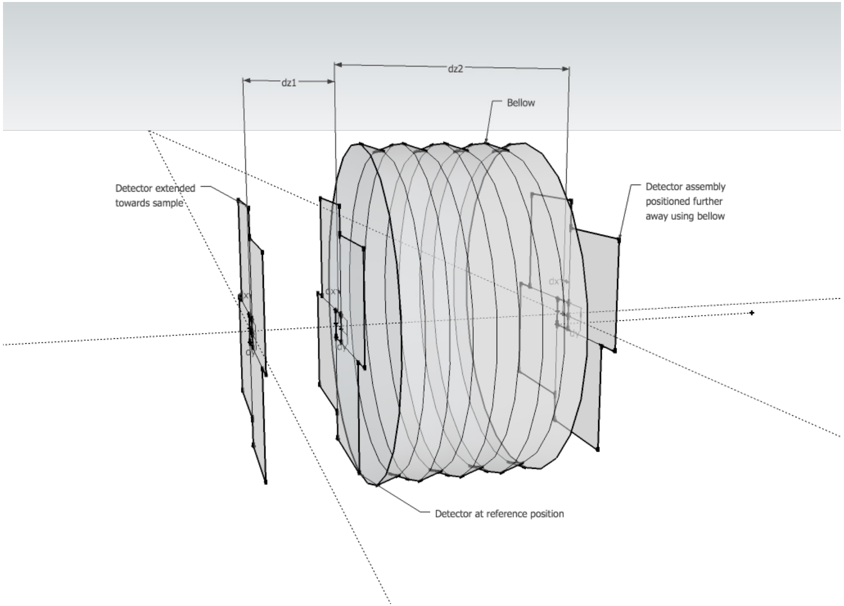

Figure 2: *Examples of the detector in two positions offset along the z-axis from the detector coordinate system origin. The left-most detector is at a negative z-position, which is the case for an extended detector. The right-most detector is at a positive z-position, e.g. when a bellow is used to move the detector further away from the sample. The centre detector is located at the z=0 position.*

The x- and y-axis origins are kept centred on the beam, i.e. no additional transformation will be done. In order to provide these coordinates in terms of stepper motor values alone, a position for the “centred” detector must be defined. This is given as the centre of the hole for the segmented detectors in their most closed position or as the geometric centre of non-segmented detectors.

If the detector is to be rotated off-axis, as is shown in Figure 3, alignment should first occur on-axis, so that a single theta/phi-rotation is sufficient to determine the rotated detector coordinates. In such cases, the instrument has to provide the precise location of the pivot point in reference to the instrument reference point and an accurate measurement of the rotational angle(s).

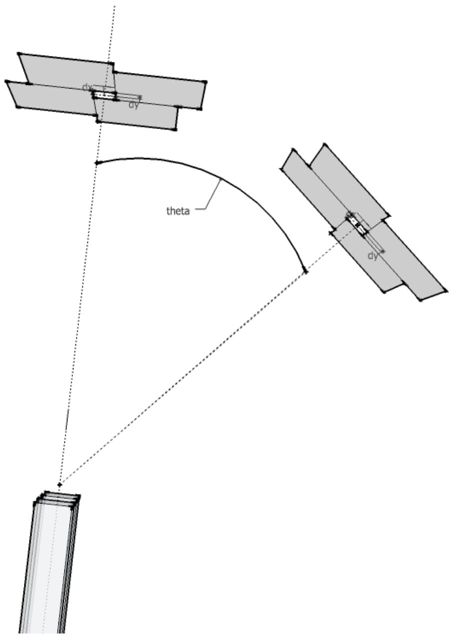

Figure 3: *Example of a detector, which has been rotated by an angle theta away from the z-axis*

The definition of the instrument reference point is instrument-specific. Accordingly, the instrument groups shall provide the means to facilitate the measurement the constant z-offset of the detector coordinate system from it. The Detector Development group (WP75) will provide detector-specific tools to determine the respective detector plane. Coordinate transformations, which determine absolute positions relative to the sample or the beam focal point, should be defined by the instruments in terms of a transformation relative to the fixed reference point for the detector coordinate system.

For standard visualization purposes, e.g. in the Karabo GUI or plots produced by WP75, the detector will always be shown as if one would look onto it in beam direction.

2 Hierarchical alignment concept

In general, a detector can be divided into a hierarchical set of components, which have measureable positions relative to each other. By setting an absolute reference position for the top-level component, i.e. the complete detector, the position of any other component, down to the pixel level, can be deduced. Currently, the following hierarchy is foreseen.

Detector: The complete detector setup as it is integrated into the instrument, including e.g. vacuum vessel and connecting flanges. The detector can be moved along the x-, y-, and z-direction with respect to an absolute reference point for the experiment, given e.g. by the standardized beamline coordinate system defined in [1] or a suitable origin at a constant offset from this system.

Additionally, the detector may be tilted and rotated with respect to the beam axis. This is describable either by a set of angles or by giving the direction of the surface normal of the detector. A minimal set of two times three coordinates plus a rotational angle (position, tilt, rotation) thus needs to be stored for alignment information on the detector level (Figure 4).

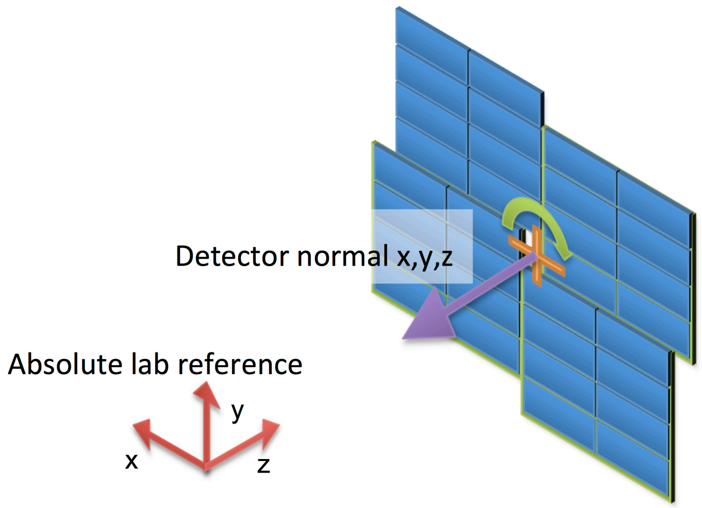

Figure 4: *Schematic representation of the detector positioned relative to a reference coordinate system, with tilt and rotation defined by a normal vector*

Panel/Quadrant: The detector consists of 1...n panels, which in turn hold 1…n modules. For the fast 1 megapixel (Mpx) detectors, a panel corresponds to a quadrant. Panels may be repositioned for each run, and their positions are e.g. determined from the settings of the stepper motors driving them. Each stepper motor setting can thus be attributed to an x, y (and z) position of the panel. For each panel information on its x, y, and z coordinates in relation to the detector coordinate system, as well as the direction of its normal in x,y,z and rotation, have to be stored. This yields 7 values per panel, or 2 per panel if the z-position, rotation, and tilt can be derived from the stepper motor position alone (Figure 5) by means of a deterministic dependency.

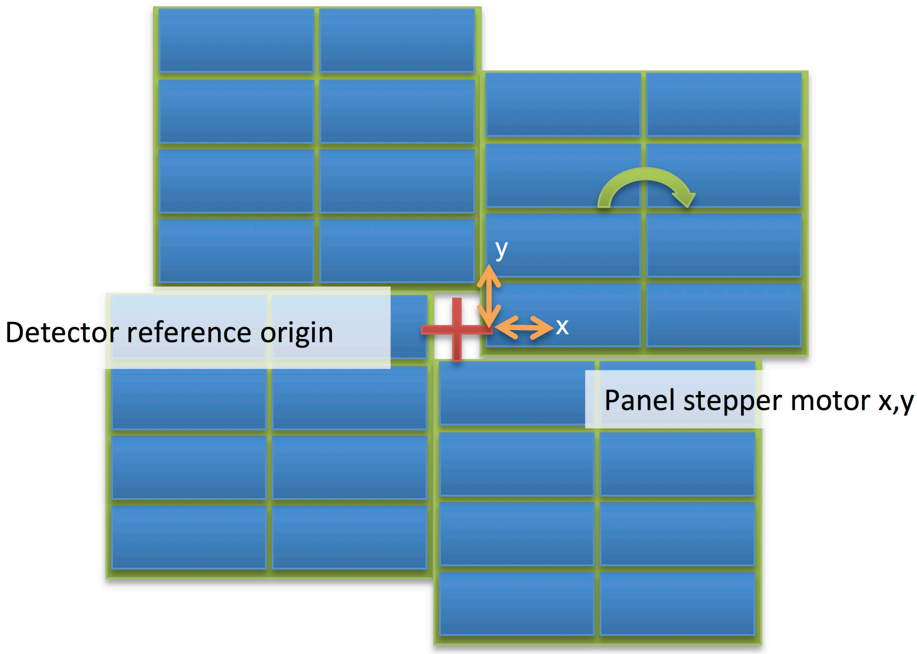

Figure 5: *Example of panels/quadrants that are positioned relative to the detector reference coordinates*

Especially for the startup phase, panel positions given through stepper-motor positions shall be cross-checked by an independent means of measurement. One possible method, which has been suggested by the instrument groups, is to use reference samples, which produce well-characterized diffraction patterns when illuminated by the X-ray beam. These can then be evaluated to give the precise pixel positions and tilt.

Additionally, the feasibility of using an infrared (IR) laser to illuminate the detector is being investigated and will be reported on in a later version of this report.

Module: A module (or tile) is the smallest individually exchangeable block of a detector and consists of 1...n sensitive cells (pixels). Modules are fixed in position and orientation after integration into panels. Accordingly, these parameters are measured by the Large Pixel Detector (LPD) Consortium and WP75 during integration and only need to be re-determined if modules are exchanged. For each module on a panel, a set of 7 coordinates defining position and orientation as well as a rotational vector thus needs to be stored (Figure 6).

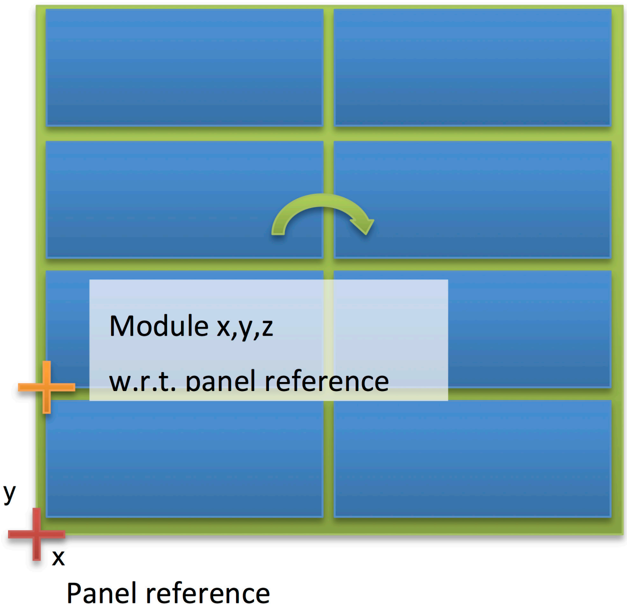

Figure 6: *Module level hierarchy showing the module/tile positions relative to panels/quadrants*

In the context of the LPD, an additional super-module hierarchy level with similar parameters exists. Super-modules thus need to be realigned after exchanging.

Pixels: Due to lithographic manufacturing process of sensor modules, it is assumed that the pixel positions across the module are absolutely determined by the module design. Nevertheless, the complete pixel matrix may be slightly shifted on a module-by-module basis with respect to the module reference point. Similar to the module positions, these coordinates are determined once for each individual module and are valid throughout the module lifetime. For the pixel matrix position, one coordinate set consisting of three parameters (x,y,z) needs to be stored, if the module itself is assumed plane and with negligible warping.

2.1 Alignment accuracy

Three major factors contribute to alignment accuracy: for the X- and Y-coordinates, which extend parallel to the detector plane, the achievable accuracy is limited by the (absolute) repositioning accuracy of the detector's translational stages if no additional cross-checks using an IR laser or standardized diffraction samples are implemented. If such measures are implemented, the accuracy depends on how the pixel size influences the obtainable accuracy in the analysis of the data collected for the cross-checking method.

It is reasonable to assume that the positional reproducibility of 10–20 μm is achievable for the translational motion stages. This accuracy has been demonstrated for the Adaptive Gain Integrating Pixel Detector (AGIPD) motion system. Analysis methods used for diffraction ring data, or reconstruction of charge cloud centres, can typically super-sample the position to approx. one tenth of a pixel size. For the fast Mhz detectors, this translates to approx. 20 μm accuracy as well.

For Z-axis alignment, and also the x–y axis alignment with respect to the beam, the accuracy of determining the detector coordinate system's origin critically limits the overall alignment accuracy.

A summary of the methods needed for obtaining alignment information alongside their accuracy and limiting factors is given in Table 1. The accuracy requirements for each instrument are summarized in Table 2.

For the HED instrument, a concept better matching the experimental scenarios will be prepared, but the general choice of hierarchical coordinate systems, defined relative to each other, as well as divided responsibilities, will be maintained.

Table 1: *Methods used for obtaining alignment information and their respective reasonably achievable accuracies. IR-laser alignment is still under investigation.*

Parameter	**Achievable accuracy (µm)**	**Limited by**	**Responsibility**
X-axis plane (motor encoding, relative to the detector centre)	10–20	Absolute reproducibility given by stage	WP75 / Detector Consortia
Y-axis plane (motor encoding, relative to the detector centre)	10–20	Absolute reproducibility given by stage	WP75 / Detector Consortia
X-axis plane (diffraction sample, w.r.t. sample)	20	Pixel size and analysis method, sample positioning and alignment accuracy	Instrument groups
Y-axis plane (diffraction sample, w.r.t. sample)	20	Pixel size and analysis method, sample positioning and alignment accuracy	Instrument groups
X-axis plane (IR laser, relative to the laser position)	20	Pixel size and analysis method, laser positional and alignment accuracy	WP75
Y-axis plane (IR laser, relative to the laser position)	20	Pixel size and analysis method, laser positional and alignment accuracy	WP75
Determination of detector coordinate system origin relative to the instrument fixed reference system	20	—	Instrument groups
X-axis plane (combined, relative to the origin)	20	Aforementioned methods, accuracy determining origin	Instrument groups / WP75
X-axis plane (combined, relative to the origin)	20	Aforementioned methods, accuracy determining origin	WP75
Z-axis plane (relative to the detector panel)	50	—	WP75
Z-axis plane (relative to the photon coordinate system)	500–1000	—	Instrument groups

Table 2: *Required alignment accuracies for the Mpx detectors with Mhz readout rate with respect to each instrument (relative to fixed reference). For SQS, the alignment precision for the micro-channel plate (MCP) detector is shown.*

Instrument	SPB	FXE	SQS	MID	SCS
X-axis (μm)	20	50	50	50	50
Y-axis (μm)	20	50	50	50	50
Z-axis (μm)	100	100	100	100	100
Tilt (deg)	1	1	1	1	1
Roll (deg)	Less than a pixel width over the half width of the detector				

2.2 Alignment data requirements

Alignment data can be stored either in a database or in a Hierarchical Data Format 5 (HDF5) file. A combination of both is foreseen. The alignment data will be injected into the calibration database in order to have a consistent representation of alignment information evolution during the detector lifetime.

Additionally, a HDF5 file containing alignment information is distributed alongside each set of image data. Within this file, the HDF5 structure allows for direct mapping to the alignment concept. Tools will be provided to apply this information to the image data within the Karabo toolchain.

3 Responsibilities

The production of alignment data is to be shared amongst the Detector Development group (WP75) and the instrument groups. The following responsibilities are defined.

3.1 Detector Development group

The Detector Development group is responsible for the following:

- Provide alignment information up to the movable quadrant or panel level, i.e. for all detector components, which cannot be repositioned by users or instrument scientists.
- Define the alignment information to be stored. Coordinate with Control and Analysis Software (CAS) and IT and Data Management (ITDM) storage concepts (DB, HDF5) for this data.
- Coordinate with the CAS group the implementation of tools to apply alignment information to transform detector coordinates (i.e. pixels) into the Cartesian X-ray free-electron laser (FEL) beamline coordinate system.
- Support the instrument groups in implementing alignment data production with respect to the aforementioned concepts.
- Perform an initial investigation on whether an IR laser–based in-hutch alignment system is feasible.
- Maintain alignment data in the calibration database for the duration of X-ray FEL operation
- Provide quality and release management of the alignment data through a detector support scientist liaison with the instruments.

3.2 Instrument groups

The instrument groups are responsible for the following:

- Determine the position of the detector coordinate system reference point matching the criteria stated in Section 2, “Hierarchical alignment ”, together with WP75.
- Investigate and implement means of producing alignment information independent of the quadrant stepper motor positions, e.g. by using standardized samples, in coordination with WP75.
- Implement additional coordinate transformations as required into the alignment application tools.

A References

[1] H. Sinn: "Coordinate Systems for the Beam Distribution Systems", XFEL.EU TN 2012-003-02 (2013)