

3.7. CLASSIFICATION AND USE OF IMAGE DATA

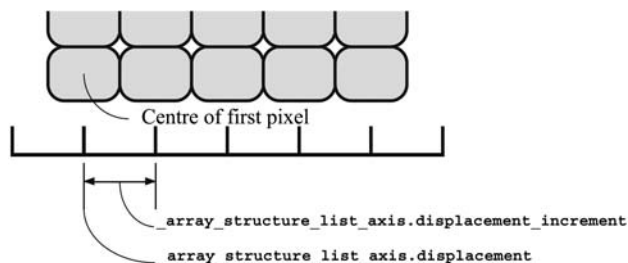


Fig. 3.7.2.1. ARRAY_STRUCTURE_LIST specification of linearly organized image elements.

Note that a spiral scan uses two coupled axes, one for the angular direction and one for the radial direction. This differs from a cylindrical scan for which the two axes are not coupled into one set.

Multiple related axes are gathered together into sets. Each set is identified by the value of the axis set identifier, `_array_structure_list_axis.axis_set_id`, and each axis within a set is identified by the value of `_array_structure_list_axis.axis_id`. Each set given by a value of `*.axis_set_id` is linked to a corresponding value for `_array_structure_list.axis_set_id` to relate settings of the axes in the axis set to particular image elements in ARRAY_STRUCTURE_LIST.

If axes are all independent, no value need be given for `_array_structure_list_axis.axis_set_id`, which is then implicitly given the corresponding value of `_array_structure_list_axis.axis_id`. Each axis given by a value of `_array_structure_list_axis.axis_id` is linked to a corresponding value for `_axis.id` to provide a physical description of the axis. `_array_structure_list_axis.axis_id` and `_array_structure_list_axis.axis_set_id` together uniquely identify a row of data in an ARRAY_STRUCTURE_LIST_AXIS table.

For the remaining data items, there are two important cases to consider: axes that step by Euclidean distance and axes that step by angle. Fig. 3.7.2.1 shows a portion of an array of image elements laid out on a rectangular grid. The starting point of an axis is specified in millimetres by the value of `_array_`

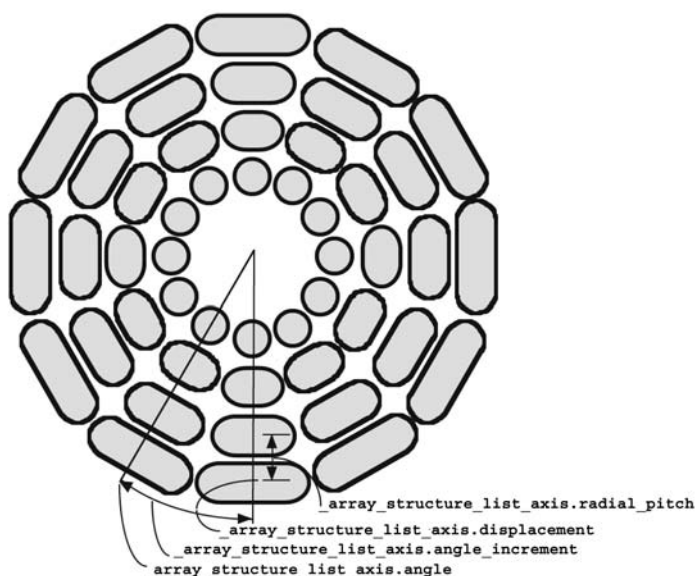


Fig. 3.7.2.2. ARRAY_STRUCTURE_LIST specification of ‘constant-angle’ image elements in a cylindrical scan. The angular and radial axes are independent. Note that outer-zone image elements are further apart, centre-to-centre, than inner-zone image elements.

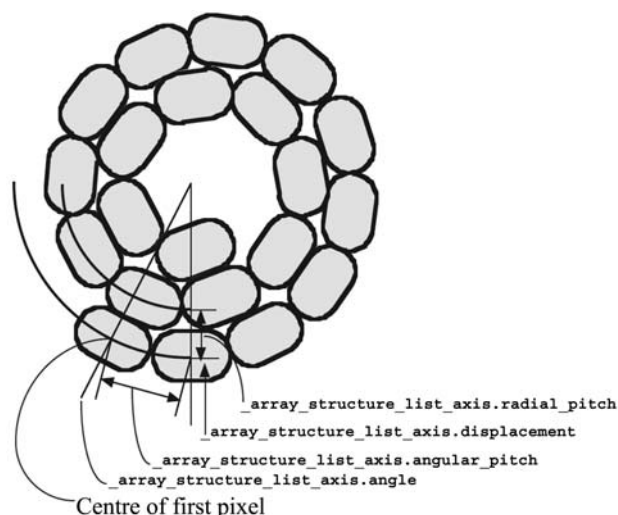


Fig. 3.7.2.3. ARRAY_STRUCTURE_LIST specification of ‘constant-velocity’ image elements in a cylindrical scan. The angular and radial axes are coupled. Note that outer-zone image elements are the same linear distance apart, centre-to-centre, as the inner-zone image elements.

`structure_list_axis.displacement` and the centre-to-centre distance between pixels is specified in millimetres by the value of `_array_structure_list_axis.displacement_increment`.

Fig. 3.7.2.2 shows a portion of an array of image elements laid out in concentric cylinders. The starting point of the angular axis is specified in degrees by the value of `_array_structure_list_axis.angle` and the centre-to-centre angular distance between pixels is specified in degrees by the value of `_array_structure_list_axis.angle_increment`. The starting point of the radial axis is specified by the value of `_array_structure_list_axis.displacement` and the radial distance between cylinders of pixels is specified in millimetres by the value of `_array_structure_list_axis.radial_pitch`. Note that the image elements further from the centre are larger than the image elements closer to the centre.

Fig. 3.7.2.3 shows a portion of a spiral scan array in which the angular and radial axes are coupled. This example represents a ‘constant-velocity’ scan, in which the size of the image elements does not depend on the distance from the centre. The starting point of the angular axis is again specified in degrees by the value of `_array_structure_list_axis.angle`, but the centre-to-centre distance between pixels is specified in millimetres by the value of `_array_structure_list_axis.angular_pitch`. The coupled radial axis is handled in much the same way as for the uncoupled radial axis in the cylindrical array.

These examples show some of the more common two-dimensional data structures. By coupling an additional axis not in the plane of the first two, regular three-dimensional arrays of data can be represented without additional tags. The categories in the DIFFRN group allow arrays of data to be associated with frames and thereby with time and/or wavelength. More general data structures, for example ones based on dope vectors or hash tables, would require the definition of additional tags, but any data structure (see Aho *et al.*, 1987) that can be handled by a modern computer should be manageable within this framework.

3.7.3. Axes

The category describing the axes required to specify the data collection is as follows:

```

AXIS group
  AXIS
    
```

3. CIF DATA DEFINITION AND CLASSIFICATION

Data items in this category are as follows:

```
AXIS
• _axis.equipment
• _axis.id
  _axis.depends_on
    → _axis.id
  _axis.offset[1]
  _axis.offset[2]
  _axis.offset[3]
  _axis.type
  _axis.vector[1]
  _axis.vector[2]
  _axis.vector[3]
```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item.

Data items in the `AXIS` category record the information required to describe the goniometer, detector, source and other axes needed to specify a data collection. The location of each axis is specified by two vectors: the axis itself, given as a unit vector, and an offset to the base of the unit vector. These vectors are referenced to a right-handed laboratory coordinate system with its origin in the specimen, as shown in Fig. 3.7.3.1.

The `X` axis is aligned to the mechanical axis pointing from the specimen along the principal axis of the goniometer.

The `Z` axis is defined next. The `Z` axis is derived from the source axis (the axis running from the sample to the source). If the source axis is orthogonal to the `X` axis, the source axis is the `Z` axis. If the source axis is not orthogonal to the `X` axis, the `Z` axis is the component of the source axis orthogonal to the `X` axis. The direction is chosen to form an acute angle with the source axis.

The `Y` axis is defined last. The `Y` axis completes an orthogonal right-handed system defined by the `X` axis and the `Z` axis (see below).

These axes are based on the goniometer, not on the orientation of the detector, gravity *etc.* The vectors necessary to specify all other axes are given by sets of three components in the order (`X`, `Y`, `Z`). If the axis involved is a rotation axis, it is right-handed, *i.e.* as one views the object to be rotated from the origin (the tail) of the unit vector, the rotation is clockwise. If a translation axis is specified, the direction of the unit vector specifies the sense of positive translation.

Note: This choice of coordinate system is similar to but significantly different from the choice in *MOSFLM* (Lesley & Powell, 2003), in which `X` is along the X-ray beam (our `Z` axis) and `Z` is along the rotation axis.

All rotations are given in degrees and all translations are given in millimetres.

Axes may be dependent on one another. The `X` axis is the only axis that is strictly connected to the hardware. All other axes are specified by the positions they would assume when the axes upon which they depend are at their zero points.

When specifying detector axes, each axis is specified relative to the beam centre. The location of the beam centre on the detector should be given in the `DIFFRN_DETECTOR` category in millimetres from the (0, 0) corner of the detector and should be corrected for distortion.

It should be noted that many different origins arise in the definition of an experiment. In particular, as noted above, we need to specify the location of the beam centre on the detector in terms of the origin of the detector, which is, of course, not coincident with the centre of the sample.

Each axis is uniquely identified by the values of `_axis.id` and of `_axis.equipment`. An axis may be a translation axis, a rotation axis or an axis for which the mode of motion is not relevant. The

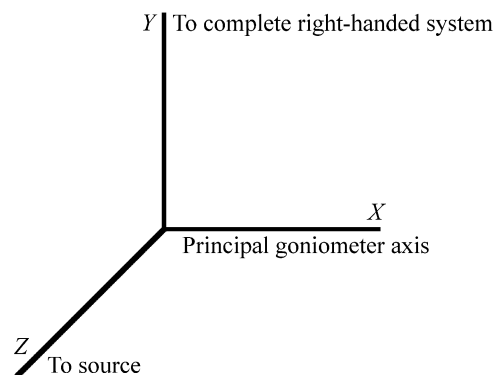


Fig. 3.7.3.1. `AXIS` laboratory coordinate system. The origin is centred in the specimen.

type of axis is specified by the value of `_axis.type`. The base of the axis is specified by the point in the laboratory coordinate system given by the values of `_axis.offset[1]`, `_axis.offset[2]` and `_axis.offset[3]`, and the direction of the axis from that base, as a dimensionless unit vector, is given by `_axis.vector[1]`, `_axis.vector[2]` and `_axis.vector[3]`.

3.7.4. The diffraction experiment

The categories relating to the diffraction experiment are as follows:

`DIFFRN` group

Frames of data (§3.7.4.1)

`DIFFRN_DATA_FRAME`

The detector apparatus (§3.7.4.2)

`DIFFRN_DETECTOR`

`DIFFRN_DETECTOR_AXIS`

`DIFFRN_DETECTOR_ELEMENT`

Apparatus and instrumentation at the crystal (§3.7.4.3)

`DIFFRN_MEASUREMENT`

`DIFFRN_MEASUREMENT_AXIS`

The radiation source (§3.7.4.4)

`DIFFRN_RADIATION`

Intensity measurements (§3.7.4.5)

`DIFFRN_REFLN`

Diffraction scans (§3.7.4.6)

`DIFFRN_SCAN`

`DIFFRN_SCAN_AXIS`

`DIFFRN_SCAN_FRAME`

`DIFFRN_SCAN_FRAME_AXIS`

The `CBF/imgCIF` dictionary extends the `mmCIF` categories in the `DIFFRN` group, which are very similar to their corresponding categories in the core CIF dictionary. The `DIFFRN` group is introduced in the description of the core CIF dictionary in Section 3.2.2.2. Its use in the `mmCIF` dictionary is described in Section 3.6.5.2, from which we quote: ‘The categories in the `DIFFRN` category group describe the diffraction experiment. Data items in the `DIFFRN` category itself can be used to give overall information about the experiment, such as the temperature and pressure. Examples of the other categories are `DIFFRN_DETECTOR`, which is used for describing the detector used for data collection, and `DIFFRN_SOURCE`, which is used to give details of the source of the radiation used in the experiment. Data items in the `DIFFRN_REFLN` category can be used to give information about the raw data and data items in the `DIFFRN_REFLNS` category can be used to give information about all the reflection data collectively.’ In this chapter we focus on the `CBF/imgCIF` extensions.