

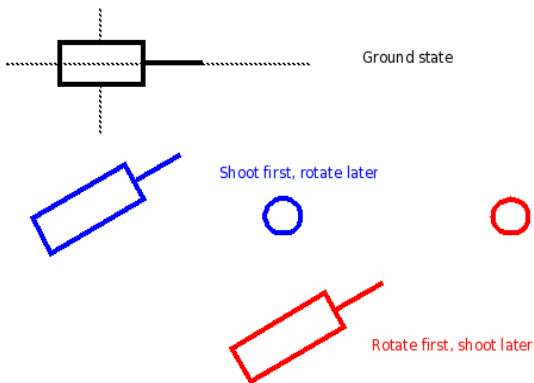
- Finalize
- Hope for endorsement of CIF community
- AIM: provide data necessary to derive positions of components from transformation matrices

$$T = \begin{pmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & z \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$R = \begin{pmatrix} r_{11} & r_{12} & r_{13} & 0 \\ r_{21} & r_{22} & r_{23} & 0 \\ r_{31} & r_{32} & r_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Combining Transformations



- Transformations can be combined by matrix multiplications
- Individual matrices can be derived by looking at the situation when everything else is 0
- Absolute positions can be obtained by multiplying the resulting matrix with its transpose
- Defines new coordinate systems at components
- CIF contains a duplication: vector, offset scheme

- Allows to calculate absolute positions of components in the laboratory coordinate systems
- Can directly convert from a detector coordinate system to vectors in Lab coordinate system
- Calculate things like impact of primary beam on detector, SAS
- Allows arbitray axis to be expressed
- Intuitively describe an instrument with angles and translations and still be able to recover absolute coordinates

- rotation_angle, polar_angle, rotate 0 1 0
- azimuthal_angle, rotate 0 0 1
- distance, translate 0 0 1
- chi, rotate 0 0 1
- phi rotate, 0 1 0
- NeXus polar coordinate system: rotate azimuthal_angle, rotate polar_angle, translate by distance

CIF Dependency Table

axis-id	type	equipment	dependson	vector	offset
gonio_phi	rotation	goniometer	.	1,0,0,	...
det_z	translation	detector	.	0,0,-1	0 0 0
det_y	translation	detector	det_z	0,1,0	0,0,0
det_x	translation	detector	det_y	1,0,0	0,0,0

- Implied: use existing NeXus coordinate system
- depends_on attribute pointing to depending axis
- Create a special container to hold axis dependencies, NXtransformations, to collect the dependencies in one place for easy access. This is what CIF does

sample, NXsample

rotation_angle

chi

phi

transformations, NXtransformations

sample/chi =

sample/rotation_angle

sample/phi =

sample/chi

instrument/detector/x_translation =

instrument/detector/distance

instrument/detector/distance =

instrument/detector/polar_angle

sample, NXsample

rotation_angle (vector 0,1,0)

chi (depends_on rotation_angle, vector 0,0,1)

phi (depends_on chi, vector 0,1,0)

depends_on

phi

- Add offset attribute to fully cover CIF. This is an extra translation
- offset_unit to give units for offset
- The vector attribute becomes mandatory
- This gives us CIF endorsement!