

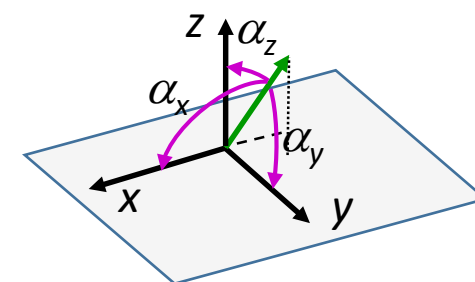
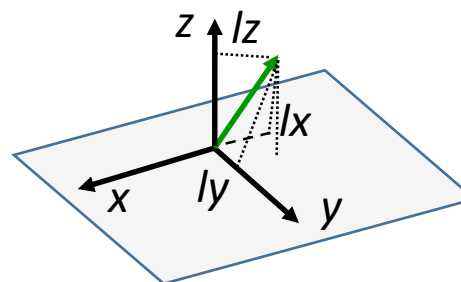
Direction cosines

Rotation axis

$$l_x = \cos(\alpha_x)$$

$$l_y = \cos(\alpha_y)$$

$$l_z = \cos(\alpha_z)$$



Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} = \begin{pmatrix} l_x^2 \cdot (1 - \cos \kappa) + \cos \kappa & l_x \cdot l_y \cdot (1 - \cos \kappa) - l_z \sin \kappa & l_x \cdot l_z \cdot (1 - \cos \kappa) + l_y \sin \kappa \\ l_x \cdot l_y \cdot (1 - \cos \kappa) + l_z \sin \kappa & l_y^2 \cdot (1 - \cos \kappa) + \cos \kappa & l_y \cdot l_z \cdot (1 - \cos \kappa) - l_x \sin \kappa \\ l_x \cdot l_z \cdot (1 - \cos \kappa) - l_y \sin \kappa & l_y \cdot l_z \cdot (1 - \cos \kappa) + l_x \sin \kappa & l^2 \cdot (1 - \cos \kappa) + \cos \kappa \end{pmatrix}$$

Getting angles from the rotation matrix

$$0 \leq \kappa \leq \pi$$

$$-1 \leq l_x \leq 1$$

$$-1 \leq l_y \leq 1$$

$$-1 \leq l_z \leq 1$$

$$\kappa = \arccos(r_{11} + r_{22} + r_{33} - 1)$$

if $\kappa = 0$:

$$l_x = 0$$

$$l_y = 0$$

$$l_z = 1$$

if $0 < \kappa < \pi$:

$$l_x = \arccos(\frac{1}{2}(r_{32} - r_{23})/\sin \kappa)$$

$$l_y = \arccos(\frac{1}{2}(r_{13} - r_{31})/\sin \kappa)$$

$$l_z = \arccos(\frac{1}{2}(r_{21} - r_{12})/\sin \kappa)$$

if $\kappa = \pi$:

$$l_x = \text{sign}(r_{13}) \cos(\frac{1}{2} \arccos(r_{11}))$$

$$l_y = \text{sign}(r_{23}) \cos(\frac{1}{2} \arccos(r_{22}))$$

$$l_z = \cos(\frac{1}{2} \arccos(r_{33}))$$

Equivalent parameters :

$$\kappa' = 2\pi - \kappa ;$$

$$l_x' = -l_x ; l_y' = -l_y ; l_z' = -l_z$$

Relevant programs : CCP4, CNS