Quaternions

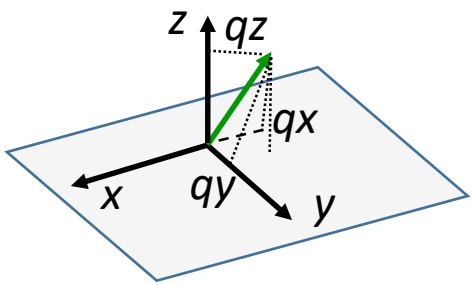
Rotation axis

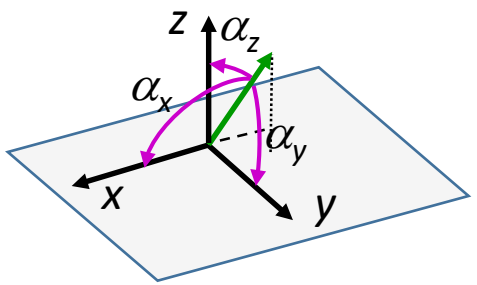
$q0 = \cos(\kappa/2)$

$qx = \cos(\alpha_x) \cdot \sin(\kappa/2)$

$qy = \cos(\alpha_y) \cdot \sin(\kappa/2)$

$qz = \cos(\alpha_z) \cdot \sin(\kappa/2)$





Rotation matrix

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix} = \begin{pmatrix} q0^2 + qx^2 - qy^2 - qz^2 & 2(qx \cdot qy - qz \cdot q0) & 2(qx \cdot qz + qy \cdot q0) \\ 2(qy \cdot qx + qz \cdot q0) & q0^2 + qy^2 - qz^2 - qx^2 & 2(qy \cdot qz - qx \cdot q0) \\ 2(qz \cdot qx - qy \cdot q0) & 2(qz \cdot qy + qx \cdot q0) & q0^2 + qz^2 - qx^2 - qy^2 \end{pmatrix}$$

Getting angles from the rotation matrix

$q0 = \frac{1}{2}\sqrt{(r_{11}+r_{22}+r_{33}+1)}$

if q0 = 0 :

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

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

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

$-1 \le q0 \le 1$
$-1 \le qx \le 1$
$-1 \le qy \le 1$
$-1 \le qz \le 1$

If q0 > 0 :

$qx = (r_{32}-r_{23})/(4 \cdot q0)$

$qy = (r_{13}-r_{31})/(4 \cdot q0)$

$qz = (r_{21}-r_{12})/(4 \cdot q0)$

Equivalent parameters :

$q0' = -q0$;

$qx' = -qx$; $qy' = -qy$; $qz' = -qz$

Relevant programs : CCP4, CNS