Rotation Operators

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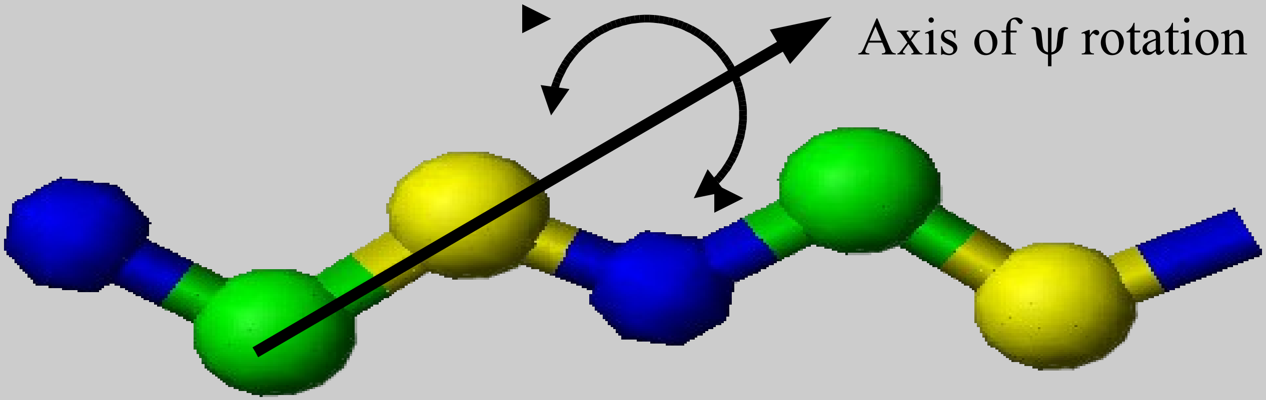
Rotation in Structural Biology

- Rotation about bonds is the most prevalent contributor to conformational changes in Structural Biology
- Rotation about the backbone dihedrals is the major contributor to the structural degrees of freedom
- Meaningful comparison of protein structures requires rotation of their structures into a common principal frame
- A well developed understanding of rotation operators is recommended for computational structural biologists



Three Fundamental Rotations

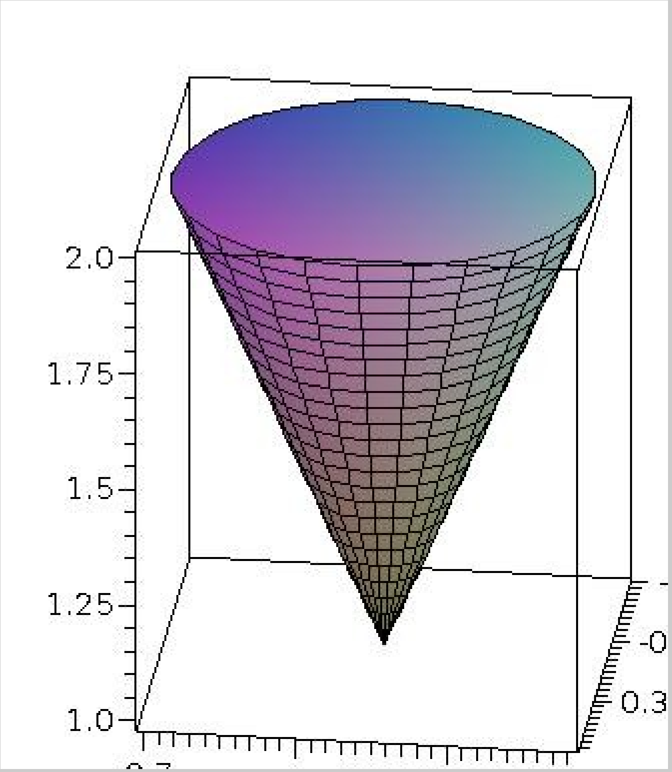
- Three fundamental rotations can be defined in the Cartesian space:
  - $R_x(\alpha)$, $R_y(\alpha)$ and $R_z(\alpha)$ each denotation rotation about x, y and z axes respectively
- Each rotation operator can transform the location/orientation of a single/multiple points/vectors in space

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R_{3\times 3} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Leftrightarrow X' = R \cdot X$$

$$\left(X_1' \, X_2' \cdots X_n' \right) = R \cdot \left(X_1 \, X_2 \cdots X_n \right)$$

Derivation of $R_z(\alpha)$

- Rotation of any vector about z will produce another vector on the surface of a cone
- Rotation about z will not alter the z component of X and X'
- We will utilize the following two trig identities:

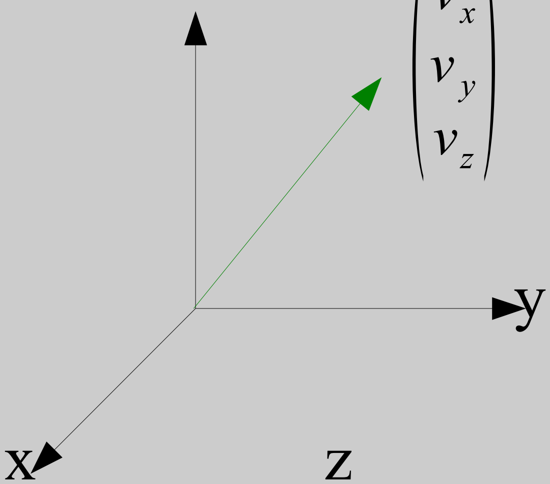


$$\cos(\phi+\alpha)=\cos(\phi)\cos(\alpha)-\sin(\phi)\sin(\alpha)$$

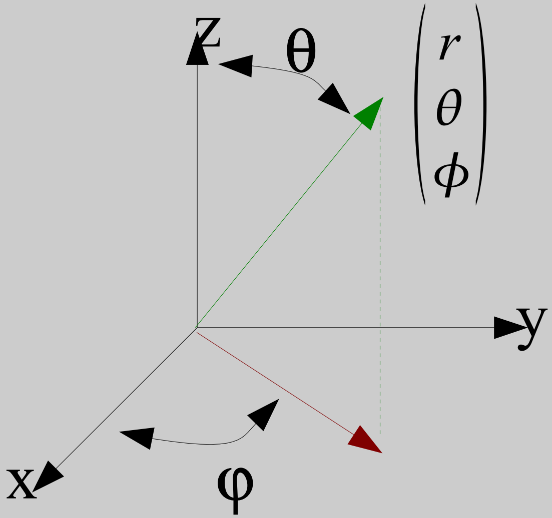
$$\sin(\phi+\alpha)=\sin(\phi)\cos(\alpha)+\cos(\phi)\sin(\alpha)$$

Cartesian versus Spherical Coordinates

- Cartesian Coordinates
- Spherical Coordinates



$$\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}$$

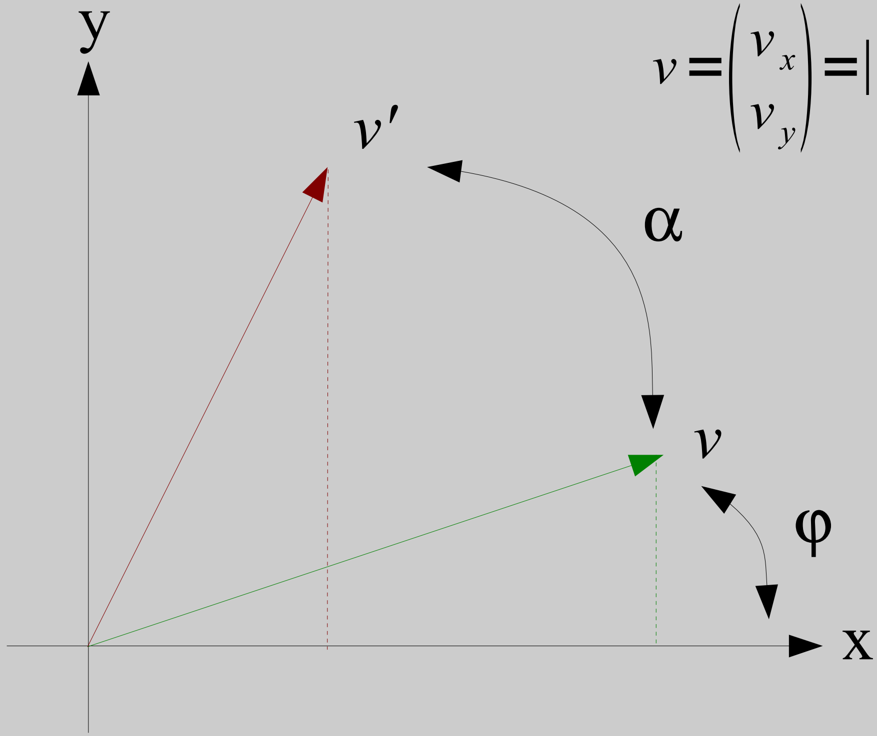


$$\begin{pmatrix} r \\ \theta \\ \phi \end{pmatrix}$$

$$\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} r\,sin(\theta)\cos(\phi) \\ r\,sin(\theta)\,sin(\phi) \\ r\,cos(\theta) \end{pmatrix}$$

$$\begin{pmatrix} r \\ \theta \\ \phi \end{pmatrix} = \begin{pmatrix} \sqrt{(v_x^2+v_y^2+v_z^2)} \\ cos^{-1}(v_z/r) \\ tan^{-1}(v_y, v_x) \end{pmatrix}$$

Derivation of $R_z(\alpha)$



$$v = \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \|v\| \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix} \qquad v' = \begin{pmatrix} v'_x \\ v'_y \end{pmatrix} = \|v\| \begin{pmatrix} \cos(\phi+\alpha) \\ \sin(\phi+\alpha) \end{pmatrix}$$

$$v' = \begin{pmatrix} \cos(\phi)\cos(\alpha) - \sin(\phi)\sin(\alpha) \\ \sin(\phi)\cos(\alpha) + \cos(\phi)\sin(\alpha) \end{pmatrix}$$

$$v' = \begin{pmatrix} v_x \cos(\alpha) - v_y \sin(\alpha) \\ v_y \cos(\alpha) + v_x \sin(\alpha) \end{pmatrix}$$

$$v' = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \end{pmatrix}$$

$$v' = \begin{pmatrix} v'_x \\ v'_y \\ v'_z \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = R_z(\alpha) \cdot v$$

Example

- Rotate vector (0,1,0) by 90º about z

$$v' = R_z(\pi/2)\cdot v = \begin{pmatrix} cos(\pi/2) & -sin(\pi/2) & 0 \\ sin(\pi/2) & cos(\pi/2) & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}$$

- Rotate vector (0,1,0) by -90º about z

$$v' = \begin{pmatrix} cos(-\pi/2) & -sin(-\pi/2) & 0 \\ sin(-\pi/2) & cos(-\pi/2) & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

- Rotate vector (0,0,z) by αº about z

$$v' = \begin{pmatrix} cos(\alpha) & -sin(\alpha) & 0 \\ sin(\alpha) & cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$$

Rotation Operators (Matrices)

- R_x, R_y and R_z denote rotations about X, Y and Z respectively

$$R_x(\alpha)=\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha) & -\sin(\alpha) \\ 0 & \sin(\alpha) & \cos(\alpha) \end{bmatrix}$$

$$R_y(\alpha)=\begin{bmatrix} \cos(\alpha) & 0 & \sin(\alpha) \\ 0 & 1 & 0 \\ -\sin(\alpha) & 0 & \cos(\alpha) \end{bmatrix}$$

$$R_z(\alpha)=\begin{bmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Euler Rotation

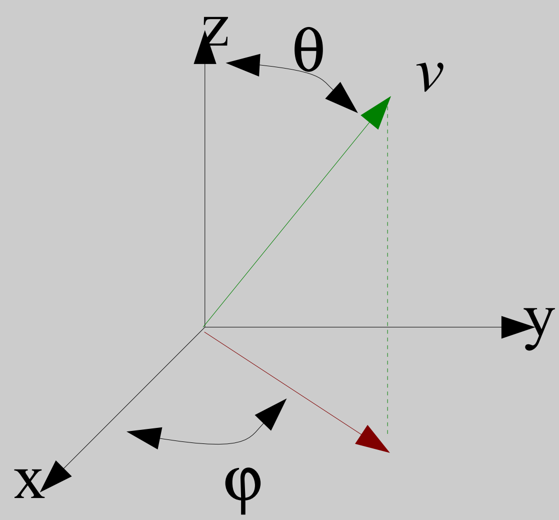
- A total of twelve valid combinations
  - Valid: XYX, ZYZ, ZYX, …
  - Invalid: XXY, ZYY, …
- Normally use ZYZ

$$\xi(\gamma,\beta,\alpha)\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = R_z(\gamma)\cdot R_y(\beta)\cdot R_z(\alpha)\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}$$

$$\xi(\gamma,\beta,\alpha)=\begin{bmatrix} \cos(\gamma) & -\sin(\gamma) & 0 \\ \sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 1 \end{bmatrix}\times\begin{bmatrix} \cos(\beta) & 0 & \sin(\beta) \\ 0 & 1 & 0 \\ -\sin(\beta) & 0 & \cos(\beta) \end{bmatrix}\times\begin{bmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation About any Arbitrary Axis

- Can represent the arbitrary axis of rotation in its spherical coordinates (θ,ϕ)



Put v in its original place

Put v on z-x plane where it was

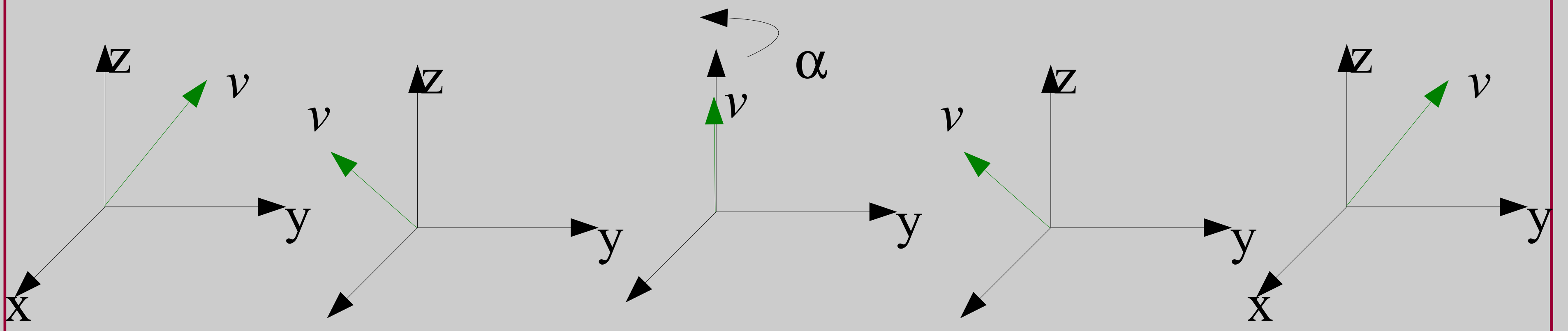
Rotate about z or v

v on z axis

$$R_{\vec{v}}(\alpha) = R_z(\phi)\,R_y(\theta)\,R_z(\alpha)\,R_y(-\theta)\,R_z(-\phi)$$

v on z-x plane

Rotation About any Arbitrary Axis



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v on z axis

$$R_{\vec{v}}(\alpha) = R_z(\phi)\, R_y(\theta)\, R_z(\alpha)\, R_y(-\theta)\, R_z(-\phi)$$

v on z-x plane

Properties of Rotation Operators

- Rotation operators are unitary operators:

$$R \cdot R^{*} = R^{*} \cdot R = I \qquad\qquad R \cdot R^{T} = R^{T} \cdot R = I$$

- Rotation operators preserve internal relationship between points

$$R^{T} = R^{-1}$$

$$R_i(\alpha) \cdot R_i(-\alpha) = I \Rightarrow R_i(-\alpha) = R_i(\alpha)^{T} = R_i(\alpha)^{-1}$$

$$\xi(\alpha, \beta, \gamma)^{-1} = \xi(-\gamma, -\beta, -\alpha)$$

$$R_{\vec{v}}(\alpha)^{-1} = R_{\vec{v}}(-\alpha)$$

Z Rotation Operator