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AND MATERIALS SCIENCE
Polish Academy of Sciences

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An introduction to computations in crystallographic textures

A.Morawiec

Polish Academy of Sciences

Institute of Metallurgy and Materials Science

Interdisciplinary PhD Studies in Materials Engineering with English as the language of instruction
Institute of Metallurgy and Materials Science
Polish Academy of Sciences
Reymonta 25, 30-059 Krakow, tel. +48 12 295 28 00, fax +48 12 295 28 04
www.imim-phd.edu.pl
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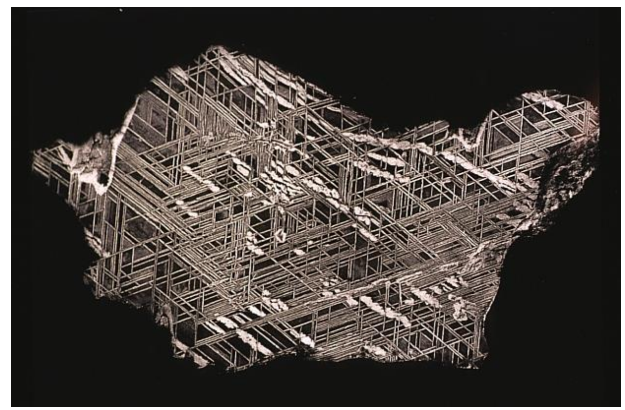
Motivation

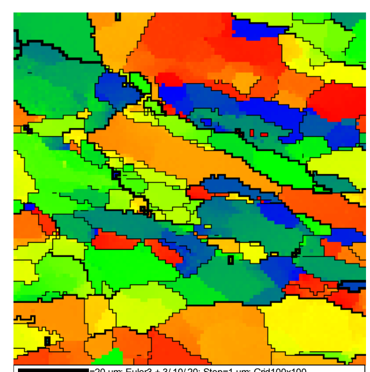
Comprehensive understanding of description of orientations
is crucial for research on polycrystalline materials.

Examples:

- Orientation relationships
- Crystal deformation mechanisms
- Some phase transformation mechanisms
- Orientation mapping



http://www.museumwales.ac.uk



Outline

- Rotations and rotation parameterizations
- Crystal orientation and crystal symmetry
- Statistics in the orientation space
- Standard (mis)orientation distributions
- Example of texture application: effective elastic properties of polycrystals

Suggested reading

- H.J. Bunge,
Texture Analysis in Materials Science,
Butterworths, London, 1982.

- U. F. Kocks, C. N. Tome, H.R. Wenk,
Texture and Anisotropy,
Preferred Orientations in Polycrystals and their Effect on Materials Properties,
Cambridge University Press, Cambridge, 1998.

- A. Morawiec,
Orientations and Rotations,
Computations in Crystallographic Textures,
Springer Verlag, Berlin, 2004.

Rotations and rotation parameterizations

A.Morawiec

Polish Academy of Sciences

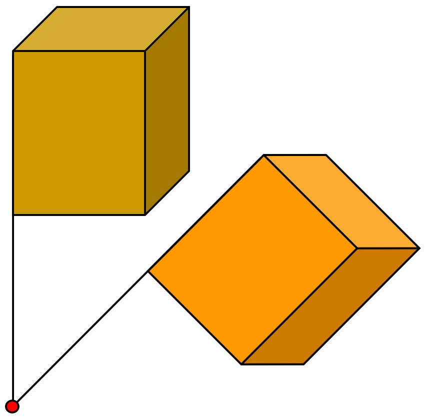
Institute of Metallurgy and Materials Science

Outline

- Basics: orientations vs. rotations
- Numerical representation of rotations and orientations
- Composition of rotations
- Parameterizations of rotations and orientations

Basics

Basics

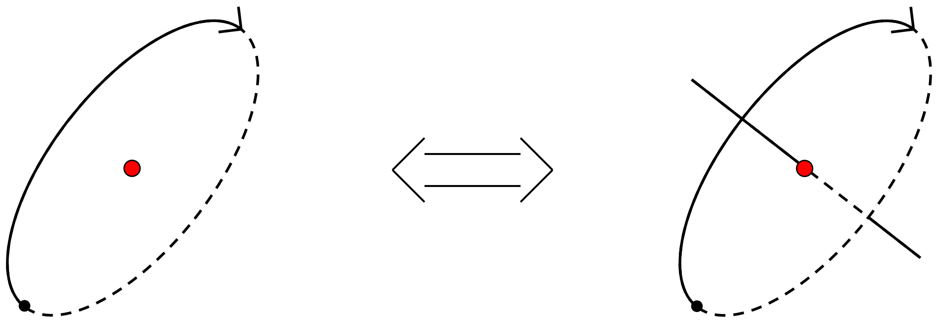


Rotation about a point – a displacement in which the location of the point is not changed.

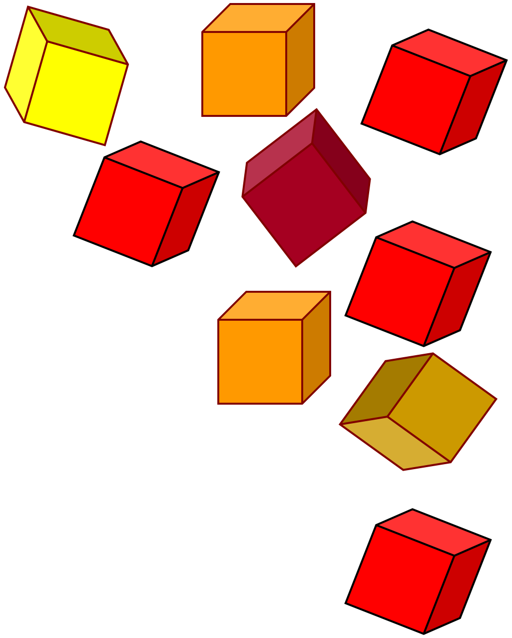
Rotation about a line – a displacement in which points of a line retain their locations.

Euler theorem:

Rotation about a point is equivalent to a rotation about a line



Basics



An orientation – the equivalence class
of all displacements which differ by a translation.

With a universal reference orientation,
an *orientation* of an object is determined by the *rotation*
from the reference orientation to that orientation.

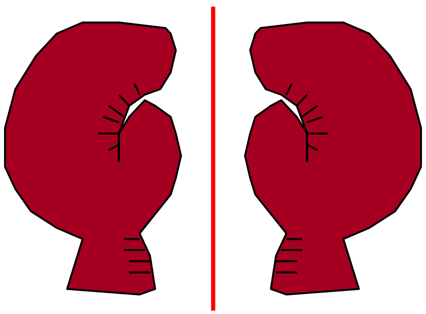
object's orientations ⟷ rotations about an axis

one-to-one correspondence

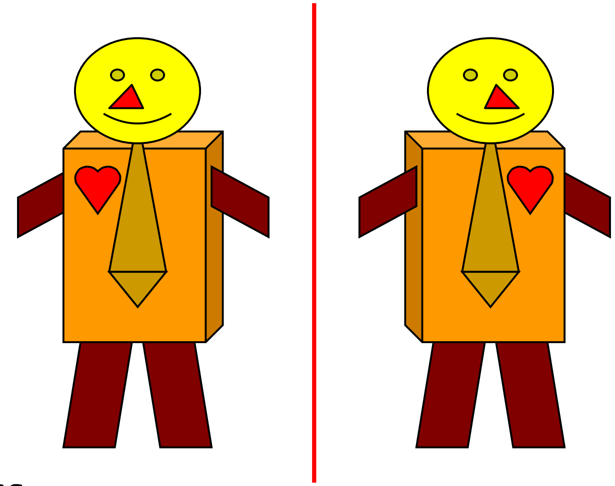
Orientation – state || Rotation – process (displacement)

Basics

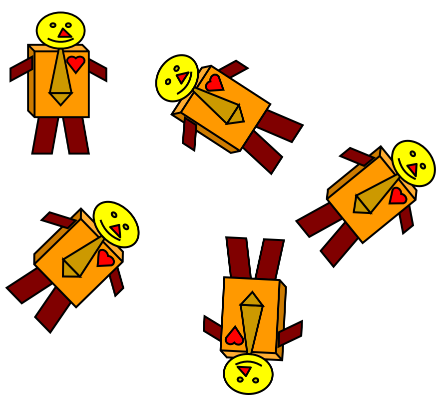
‘Mirror’ transformation with a fixed point = improper rotation



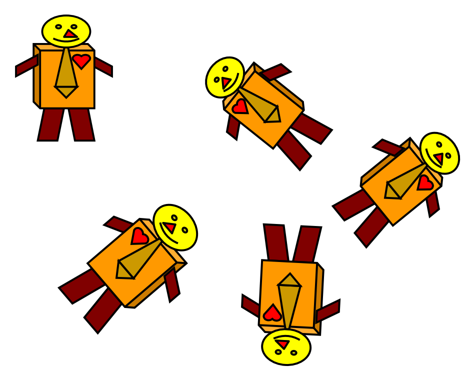
Improper rotations change handedness



Mirror images



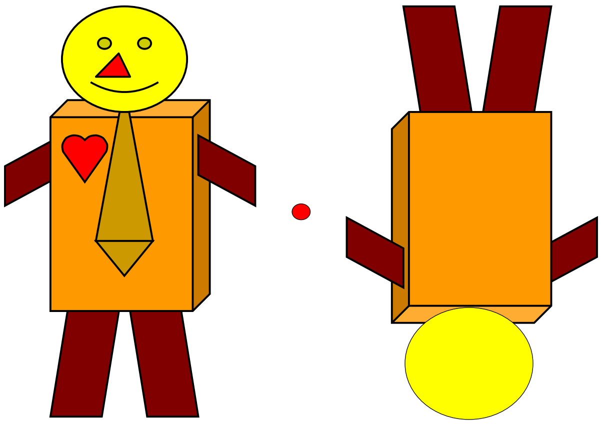
Effects of proper rotations



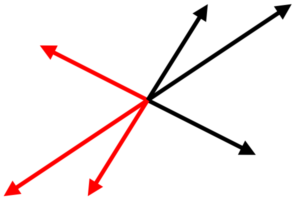
Effects of proper and improper rotations

Basics

Inversion



Inversion = half-turn about a line followed by reflection
with respect to a plane perpendicular to the line.



improper rotation = proper rotation composed with inversion

Numerical representation of rotations and orientations

To refresh memory …

Matrix – an array of $m \times n$ numbers

A_{ij} $\quad i = 1,2,\ldots,m \quad j = 1,2,\ldots,n$

$$A = \begin{bmatrix} A_{11} & A_{12} & \ldots & A_{1n} \\ A_{21} & A_{22} & \ldots & A_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ A_{m1} & A_{m2} & \ldots & A_{mn} \end{bmatrix}$$

An $m \times n$ matrix A is:
- square matrix if $m = n$
- zero if $A_{ij} = 0$
- transpose of $B = A^T$ if $A_{ij} = B_{ji}$

$$\delta_{ij} = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}$$

A square matrix A is:
- unit if $A_{ij} = I_{ij} = \delta_{ij}$
- anti-symmetric if $A_{ij} = -A_{ji}$
- symmetric if $A_{ij} = A_{ji}$

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } (ijk) \text{ even permutation of } (123) \\ -1 & \text{if } (ijk) \text{ odd permutation of } (123) \\ 0 & \text{in other cases} \end{cases}$$

Matrix algebra

Matrix product: $C = AB$ $\qquad C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj} = A_{i1} B_{1j} + A_{i2} B_{2j} + \ldots + A_{in} B_{nj} = A_{ik} B_{kj}$

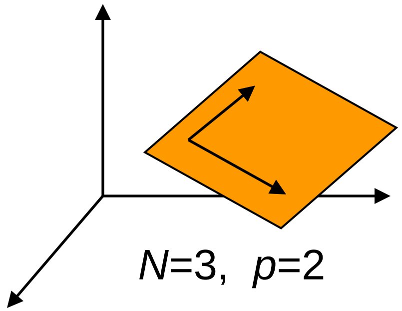
Trace of square matrix A_{ij}: $\mathrm{Tr}(A) = A_{ii} = A_{11} + A_{22} + \ldots + A_{nn}$

Det of 3×3 matrix A_{ij}: $\det(A) = \varepsilon_{ijk} A_{i1} A_{j2} A_{k3}$

Square matrix A is invertable if $\det(A)$ is non-zero; $AA^{-1} = I$

Matrix representation of orientations

p dim object immersed in *N* dim Euclidean space



Orientation is determined by *p* linearly independent vectors

$$a = [a_1 \quad a_2 \quad a_3]$$
$$b = [b_1 \quad b_2 \quad b_3] \Rightarrow \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} = O$$

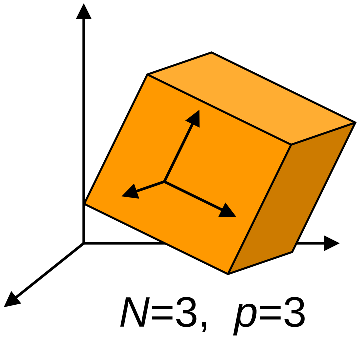
With orthonormal bases $OO^T = \begin{bmatrix} a \cdot a & a \cdot b \\ b \cdot a & b \cdot b \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

$$\boxed{OO^T = I_p}$$

An orientation of a *p* dim object immersed in *N* dim Euclidean space can be represented numerically by a $p \times N$ matrix O satisfying $OO^T=I$.

Matrix representation of orientations

$N = p = 3$



$$OO^T = I_3$$

O – an orthogonal matrix

Arbitrary rotations (including improper rotations)

$$(\det O)^2 = 1$$

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

$$OO^T = I_3 \qquad \det O = +1$$

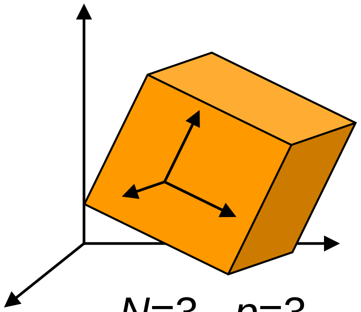
O – a special orthogonal matrix

Proper rotations

Matrix representation of orientations

N=p = 3

Example (special) orthogonal matrix



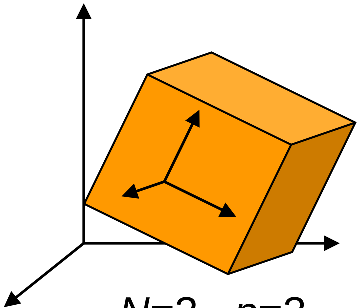
$$O=\begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix}$$

$$OO^T=\begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix}\begin{bmatrix} 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \end{bmatrix}=\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}=I_3$$

$$\det O=+1$$

Matrix representation of orientations

$N = p = 3$



$$OO^T = I_3$$

O – an orthogonal matrix

Arbitrary rotations (including improper rotations)

$$(\det O)^2 = 1$$

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O – a special orthogonal matrix

Proper rotations

Groups of
- orthogonal matrices – $O(3)$
- special orthogonal matrices – $SO(3)$

Composition of rotations

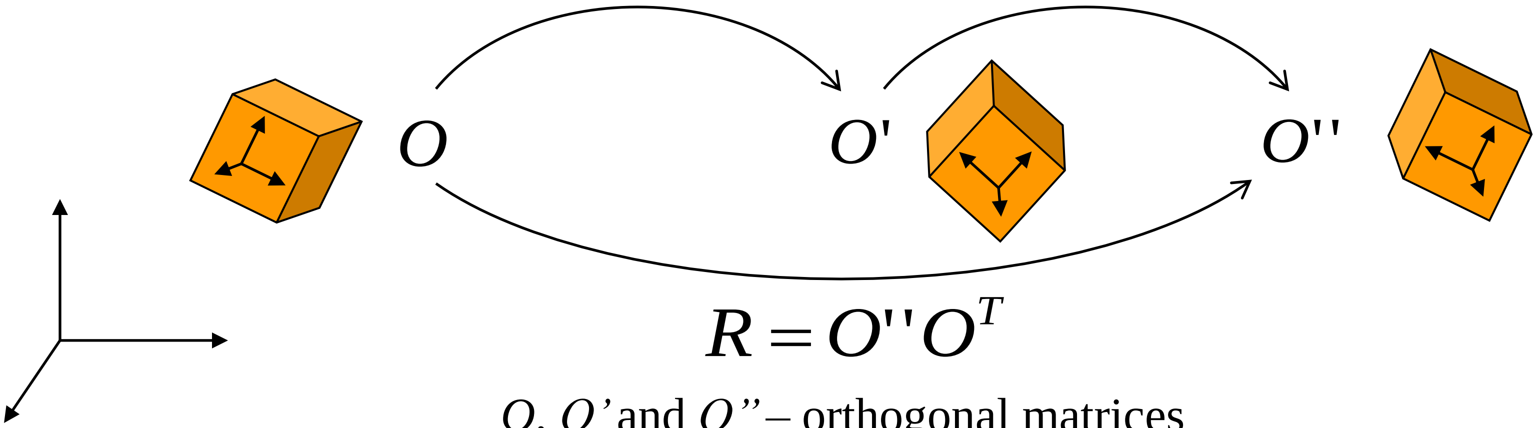
Groups $\left\{ \begin{array}{l} O(3) \\ \\ SO(3) \end{array} \right.$ one-to-one correspondence to – all rotations / – proper rotations

$O(3)$ – all rotations

$SO(3)$ – proper rotations

Composition of rotations

$$R' = O'O^T \qquad R'' = O''O'^T$$



$$R = O''O^T$$

O, *O'* and *O''* – orthogonal matrices

$$R = O''O^T = O''IO^T = O''(O'^T O')O^T = (O''O'^T)(O'O^T) = R''R'$$

$$\boxed{R = R''R'}$$

Composition of rotations corresponds to multiplication of representing them orthogonal matrices.

Composition of rotations

$$R' = \begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix} \qquad R'' = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$R''R' = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix} = \begin{bmatrix} 2/3 & 2/3 & -1/3 \\ 2/3 & -1/3 & 2/3 \\ 1/3 & -2/3 & -2/3 \end{bmatrix} = R$$

$$\boxed{R = R''R'}$$

Composition of rotations corresponds to multiplication of representing them orthogonal matrices.

Composition of rotations − algebra of quaternions

e_μ - basis of a 4 dimensional vector space, $\mu = 0,1,2,3$ $i, j, k = 1,2,3$

$$x = x_\mu e_\mu = x_0 e_0 + x_1 e_1 + x_2 e_2 + x_3 e_3$$

Standard multiplication plus the quaternion multiplication rule

$$\begin{cases} e_\mu e_0 = e_0 e_\mu = e_\mu \\ e_i e_j = \varepsilon_{ijk} e_k - \delta_{ij} e_0 \end{cases}$$

$$x = x_\mu e_\mu \qquad y = y_\mu e_\mu$$

$$xy = \left(x_0 y_0 - x_i y_i\right) e_0 + \left(x_0 y_k + x_k y_0 + \varepsilon_{ijk} x_i y_j\right) e_k$$

$$xy \neq yx$$

Unit quaternions and rotations

$i, j, k = 1,2,3$
$\mu = 0,1,2,3$

q_μ - components of a unit quaternion

$$q_\mu q_\mu = q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$$

$$A_{ij} = \left((q_0)^2 - q_k q_k\right) \delta_{ij} + 2q_i q_j - 2\varepsilon_{ijk} q_k q_0$$

A is a special orthogonal matrix

$$q = [\ q_0,\ q_1,\ q_2,\ q_3\ ] = [\ 1/2,\ 1/2,\ 1/2,\ 1/2\ ]$$

$$A = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Unit quaternions and rotations

q, q' – unit quaternions

O, O' – special orthogonal matrices

$$q \to O \qquad q' \to O'$$

$$qq' \to OO'$$

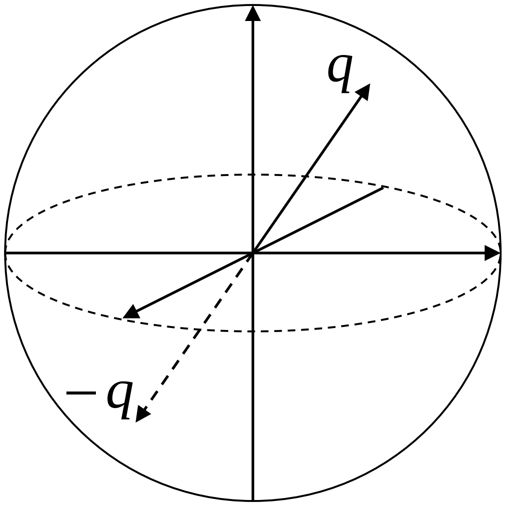
There is a two-to-one corespondence between unit quaternions and special orthogonal matrices.

There is a two-to-one corespondence between unit quaternions and proper rotations.

Unit quaternions and rotations

Unit quaternion sphere in 4D

$$q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$$



Quaternions q and $-q$ represent the same orientations

$$O_{ij}(q) = \left((q_0)^2 - q_k q_k\right)\delta_{ij} + 2q_i q_j - 2\varepsilon_{ijk} q_k q_0 = O_{ij}(-q)$$

Summary

Euler theorem.

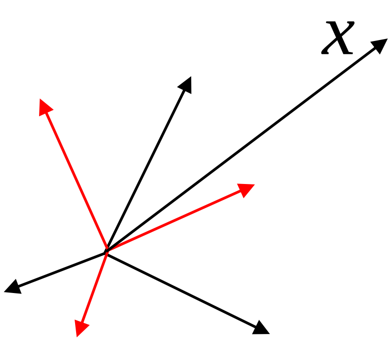
(Proper) rotations can be represented (special) orthogonal matrices.

Composition of rotations is represented by the product of orthogonal matrices.

There is two-to-one correspondence between unit quaternions
and special orthogonal matrices.

Composition of rotations is represented by the product of unit quaternions.

Transformation of vector components



$$a_i \cdot a_j = \delta_{ij} \quad \text{and} \quad a'_i \cdot a'_j = \delta_{ij}$$

$$x = x^j a_j = x'^k a'_k \quad \Big\| \quad \cdot a'_i$$

$$x'^i = x^j a_j \cdot a'_i = R_{ij} x^j \qquad a'_i \cdot a_j = R_{ij}$$

$$\boxed{x' = Rx}$$

Parameterizations

- Rodrigues parameters
- Axis and angle
- Rotation vector
- Euler angles
- Miller indices

Independent orientation parameters

Special orthogonal matrix – **9** parameters $\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$

Unit quaternion – **4** parameters $\begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix}$

Number of <u>independent</u> parameters - **3**

Is it possible to have a „nice" global parameterization (one-to-one, continuous, with continuous inverse), which would map rotations into the 3 dimensional Euclidean space?

No!

Cayley transformation

O - special orthogonal matrix such that

$(I + O)$ non-singular

$$R = (I + O)^{-1}(I - O)$$

$$O = (I - R)(I + R)^{-1}$$ $(I + R)$ non-singular

R - an antisymmetric 3x3 matrix

3 independent parameters

$$R = \begin{bmatrix} 0 & r_3 & -r_2 \\ -r_3 & 0 & r_1 \\ r_2 & -r_1 & 0 \end{bmatrix}$$

Cayley transformation, example

$$O = \begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix}$$

$$R = (I+O)^{-1}(I-O) = \begin{bmatrix} 0 & 1/3 & -1/3 \\ -1/3 & 0 & 1/3 \\ 1/3 & -1/3 & 0 \end{bmatrix} = \begin{bmatrix} 0 & r_3 & -r_2 \\ -r_3 & 0 & r_1 \\ r_2 & -r_1 & 0 \end{bmatrix}$$

$$r = [r_1,\ r_2,\ r_3] = [1/3,\ 1/3,\ 1/3]$$

Rodrigues parameters

$$R=\begin{bmatrix}0 & r_3 & -r_2\\ -r_3 & 0 & r_1\\ r_2 & -r_1 & 0\end{bmatrix}$$

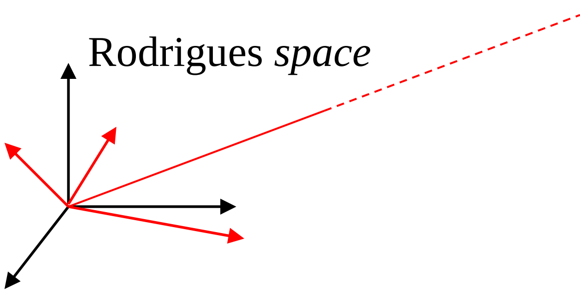
$$r_i=\frac{1}{2}\varepsilon_{ijk}R_{jk}$$

$$R_{ij}=\varepsilon_{ijk}r_k$$

$$r_i=-\frac{1}{1+O_{ll}}\varepsilon_{ijk}O_{jk}$$

$$O_{ij}=\frac{1}{1+r_l r_l}\left(\left(1-r_k r_k\right)\,\delta_{ij}+2r_i r_j-2\varepsilon_{ijk}r_k\right)$$

Rodrigues parameters / unit quaternion: $r_i=\frac{q_i}{q_0}$



$$r\rightarrow O \qquad r'\rightarrow O'$$

$$r\circ r'\rightarrow OO'$$

$$(r\circ r')_i=\frac{r_i+r'_i-\varepsilon_{ijk}r_j r'_k}{1-r_l r'_l}$$

one-to-one corespondence

Axis and angle

Euler theorem → rotation axis

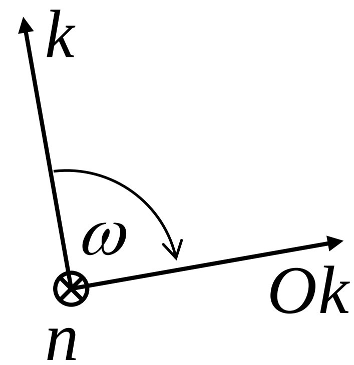
magnitude of rotation – rotation angle

$Or = r$ - Rodrigues vector is parallel to rotation axis

The axis is represented by vector *n* of unit magnitude $\boldsymbol{n} = \boldsymbol{r} / |\boldsymbol{r}|$

$$k \cdot n = 0$$

$$k \cdot k = 1$$



$$(Ok) \cdot k = \cos\omega$$

$$\cos\omega = (O_{ii} - 1)/2$$

Axis and angle

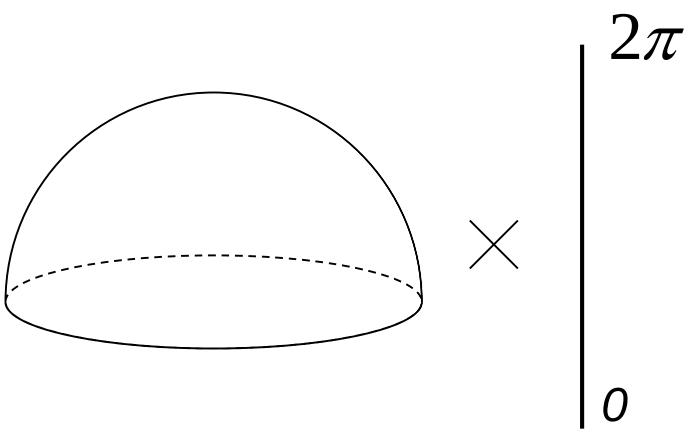
$$r_i = \tan(\omega/2)\ n_i \qquad\qquad q_i = \sin(\omega/2)\ n_i$$

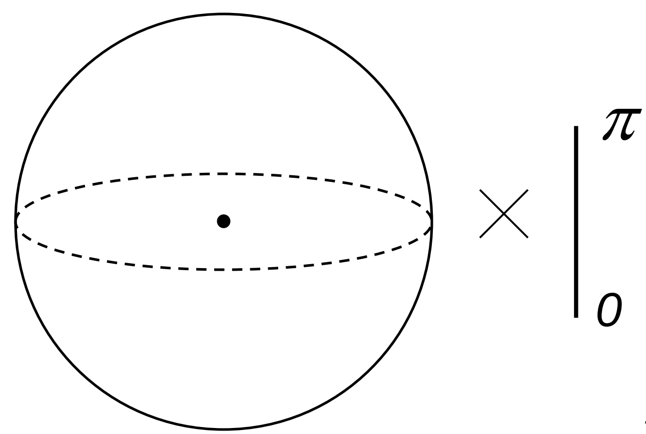
$$O_{ij}(n,\omega) = \delta_{ij}\cos\omega + n_i n_j(1-\cos\omega) - \varepsilon_{ijk} n_k \sin\omega$$

$$O(n,\omega) = O(-n, 2\pi-\omega)$$

$n \in S_+^2$
$0 \le \omega < 2\pi$

$n \in S^2$
$0 \le \omega \le \pi$





Axis and angle, example

$$O=\begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix}$$

$$r=[r_1,\ r_2,\ r_3]=[1/3,\ 1/3,\ 1/3]$$

$$n=\frac{r}{\sqrt{r\cdot r}}=[1/\sqrt{3},\ 1/\sqrt{3},\ 1/\sqrt{3}]=[1,\ 1,\ 1]\ /\sqrt{3}$$

$$\cos\omega=\left(O_{ii}-1\right)/2=1/2 \qquad \omega=\pi/3=60^\circ$$

$$(n,\omega)=\left(\frac{1}{\sqrt{3}}\ [1,\ 1,\ 1],\ \frac{\pi}{3}\right)$$

Rotation vector

$$(n, \omega) = \left(\frac{1}{\sqrt{3}} \ [1,\ 1,\ 1],\ \frac{\pi}{3} \right)$$

$$r = \tan(\omega / 2) \cdot n = \tan(\pi / 6) \left(\frac{1}{\sqrt{3}} [1,\ 1,\ 1] \right) = \frac{1}{3} [1,\ 1,\ 1]$$

$$\rho = \omega \cdot n = \frac{\pi}{3\sqrt{3}} \ [1,\ 1,\ 1]$$

$$\rho_i = f(\omega) \ n_i$$

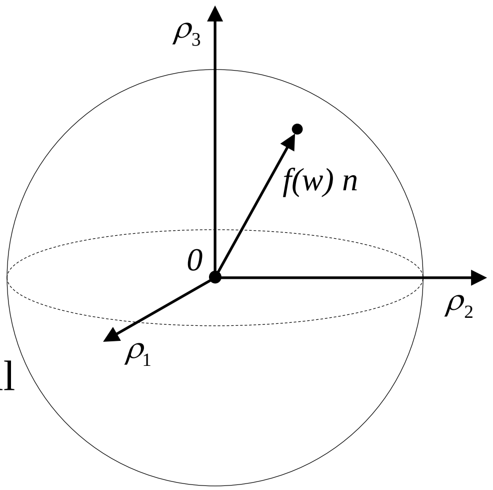
Rotation vector

$$\rho_i = f(\omega)\, n_i$$

$f:[0,\pi]\rightarrow R$ strictly increasing, $\quad f(0)=0$

$\omega=\pi: \quad \{\rho_i\}\equiv\{-\rho_i\}$

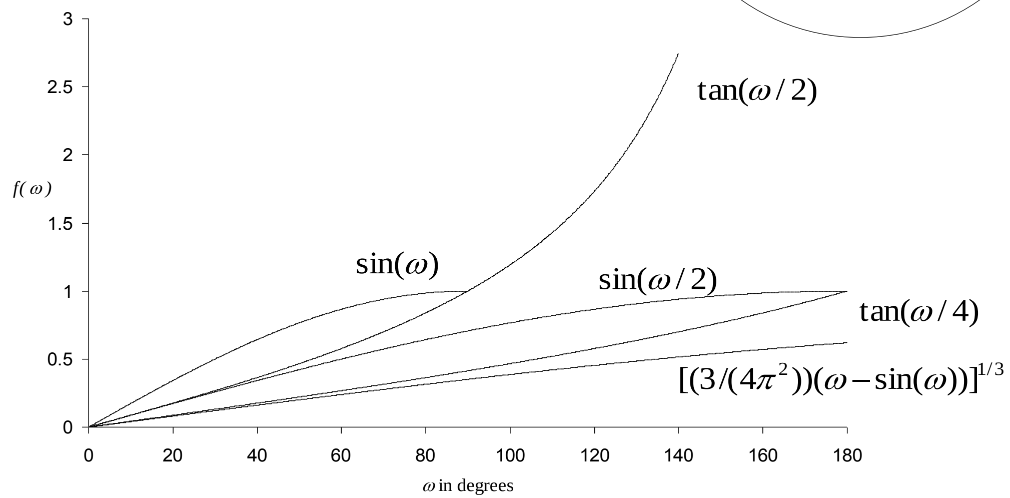
parametric ball



$$f(\omega)=\omega$$

$$f(\omega)=\tan(\omega/2)$$

$$f(\omega)=\sin(\omega/2)$$



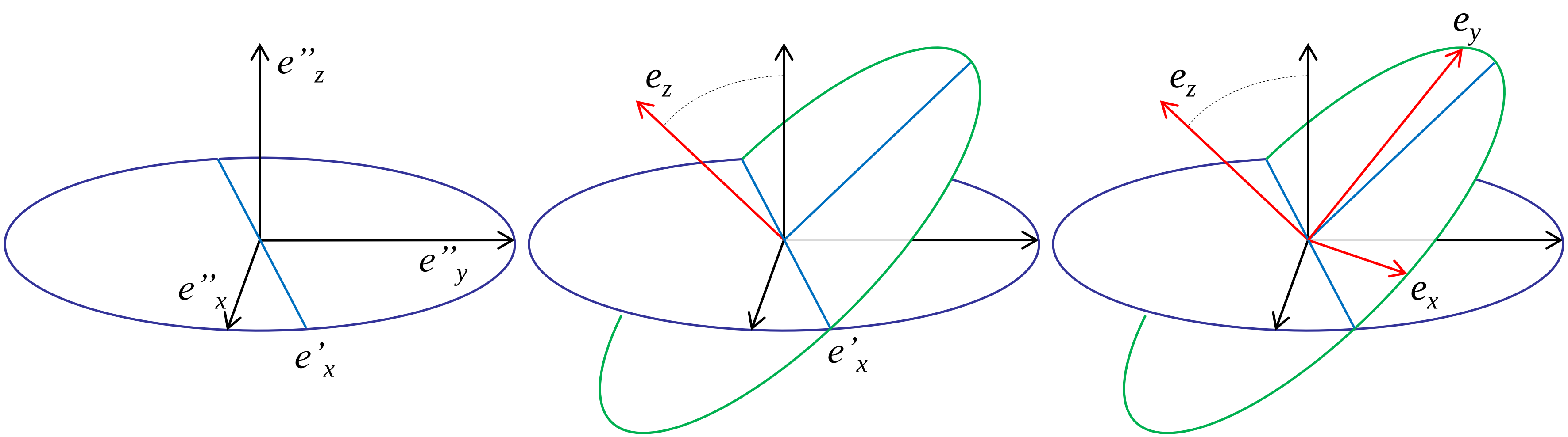
$$f(\omega)=\left(3(\omega-\sin\omega)/\left(4\pi^2\right)\right)^{1/3}$$ – isochoric parameters

Euler angles

$$O = O(n, \omega)$$

x-convention

$$O(\varphi_1, \phi, \varphi_2) = O(e_z, \varphi_1)\ O(e'_x, \phi)\ O(e''_z, \varphi_2)$$



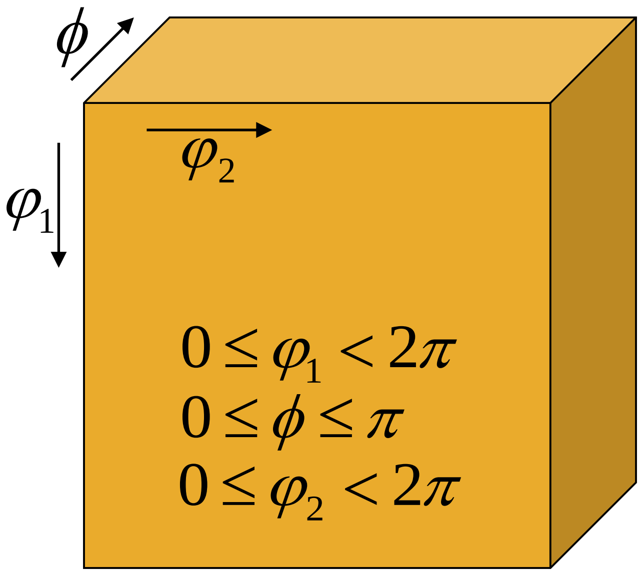
$$O(\varphi_1, \phi, \varphi_2) = O(e_z, \varphi_2)\ O(e_x, \phi)\ O(e_z, \varphi_1)$$

Euler angles

$$O(\varphi_1,\phi,\varphi_2)=O(e_z,\varphi_2)\ O(e_x,\phi)\ O(e_z,\varphi_1)$$

The domain of all proper rotations is covered when

$$0\le\varphi_1<2\pi \qquad 0\le\phi\le\pi \qquad 0\le\varphi_2<2\pi$$



Euler angles, example

$$O = O(n, \omega)$$

$$O(\varphi_1, \phi, \varphi_2) = O(e_z, \varphi_2)\ O(e_x, \phi)\ O(e_z, \varphi_1)$$

$$\varphi_1 = 90° \qquad \phi = 60° \qquad \varphi_2 = 90°$$

$$O(e_z, 90°) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad O(e_x, 60°) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/2 & \sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$O(90°, 60°, 90°) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/2 & \sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & 1/2 \end{bmatrix} \times \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1/2 & 0 & \sqrt{3}/2 \\ 0 & -1 & 0 \\ \sqrt{3}/2 & 0 & 1/2 \end{bmatrix}$$

$$(n, \omega) = \left([1,\ 0,\ \sqrt{3}]/2\ ,\ \pi \right)$$

Euler angles

$$O(\varphi_1, \phi, \varphi_2) = O(e_z, \varphi_2)\ O(e_x, \phi)\ O(e_z, \varphi_1)$$

Singularity:

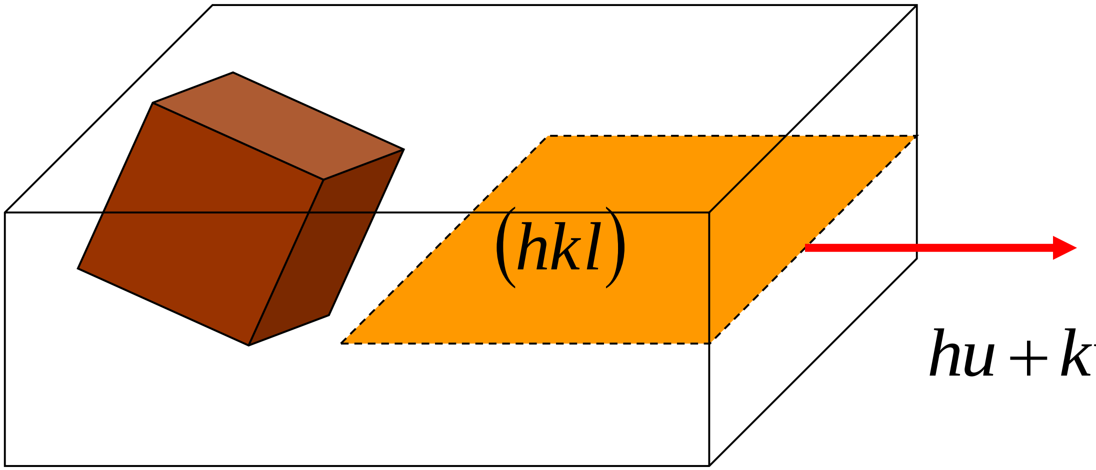
$$O(\varphi_1, 0, \varphi_2) = O(\varphi_1 + \alpha, 0, \varphi_2 - \alpha)$$

$$O(\varphi_1, \pi, \varphi_2) = O(\varphi_1 + \alpha, \pi, \varphi_2 + \alpha)$$

Lattman angles:

$$\varphi^+ = \left(\varphi_1 + \varphi_2\right)/2 \qquad \varphi^- = \left(\varphi_1 - \varphi_2\right)/2$$

Miller indices



$$e.g., (110)[001]$$

$$[uvw]$$

$$hu + kv + lw = 0$$

e_i – i-th external basis vector
a_j – j-th basis vector of crystal direct lattice

$$A_{ij} = e_i \cdot a_j \qquad B = A^{-1}$$

$$(hkl) \propto (A_{i1}O_{i3}, A_{i2}O_{i3}, A_{i3}O_{i3}) \qquad [uvw] \propto [B_{1i}O_{i1}, B_{2i}O_{i1}, B_{3i}O_{i1}]$$

Cubic system $\quad (hkl) \propto (O_{13}O_{23}O_{33}) \quad [uvw] \propto [O_{11}O_{21}O_{31}]$

Miller indices, example

Cubic system

$$(hkl) \propto (O_{13} O_{23} O_{33}) \qquad [uvw] \propto [O_{11} O_{21} O_{31}]$$

$$O = \begin{bmatrix} 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix}$$

First column: $[uvw]$; third column: (hkl)

$$(hkl) \propto (O_{13} O_{23} O_{33}) \propto (2\ \bar{1}\ 2)$$

$$[uvw] \propto [O_{11} O_{21} O_{31}] \propto [2\ 2\ \bar{1}]$$

$$(hkl)\ [uvw] = (2\ \bar{1}\ 2)[2\ 2\ \bar{1}]$$

Summary

Summary

• Euler theorem: Rotation about a point is equivalent to a rotation about a line.

• There is one-to-one correspondence between object's orientations and rotations about a fixed point.

• An orientation of an object can be represented an orthogonal matrix.

(Proper) rotations are represented (special) orthogonal matrices.

Composition of rotations corresponds to multiplication of representing them orthogonal matrices.

• There is two-to-one correspondence between unit quaternions and special orthogonal matrices.

An orientation of an object can be represented a unit quaterion.

Composition of rotations corresponds to multiplication of representing them unit quaternions.

Summary

• There are a number of orientation parameterizations.

„Nice” parameterizations involve more than 3 numbers.

There is a relationship between antisymmetric matrices and special orthogonal matrices (Cayley transformation).

Cayley transformation is a good starting point for deriving 3-number rotation parameterizations.

- Axis and angle
- Euler angles
- Rodrigues parameters
- Rotation vector
- Miller indices

$i, j, k = 1,2,3$
$\mu = 0,1,2,3$

q_μ - components of a unit quaternion

$$q_\mu q_\mu = q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$$

$$O_{ij} = \left((q_0)^2 - q_k q_k \right) \delta_{ij} + 2 q_i q_j - 2 \varepsilon_{ijk} q_k q_0$$

O – special orthogonal matrix

$$q_i = \pm \varepsilon_{ijk} O_{kj} / (2\xi) \qquad q_i = \mp \varepsilon_{ijk} O_{jk} / (2\xi)$$

$$\xi = (1 + O_{ll})^{1/2}$$