CARNEGIE MELLON UNIVERSITY

DEPARTMENT OF
MATERIALS SCIENCE AND ENGINEERING

Rodrigues vectors and unit Quaternions

27-750

Texture, Microstructure & Anisotropy

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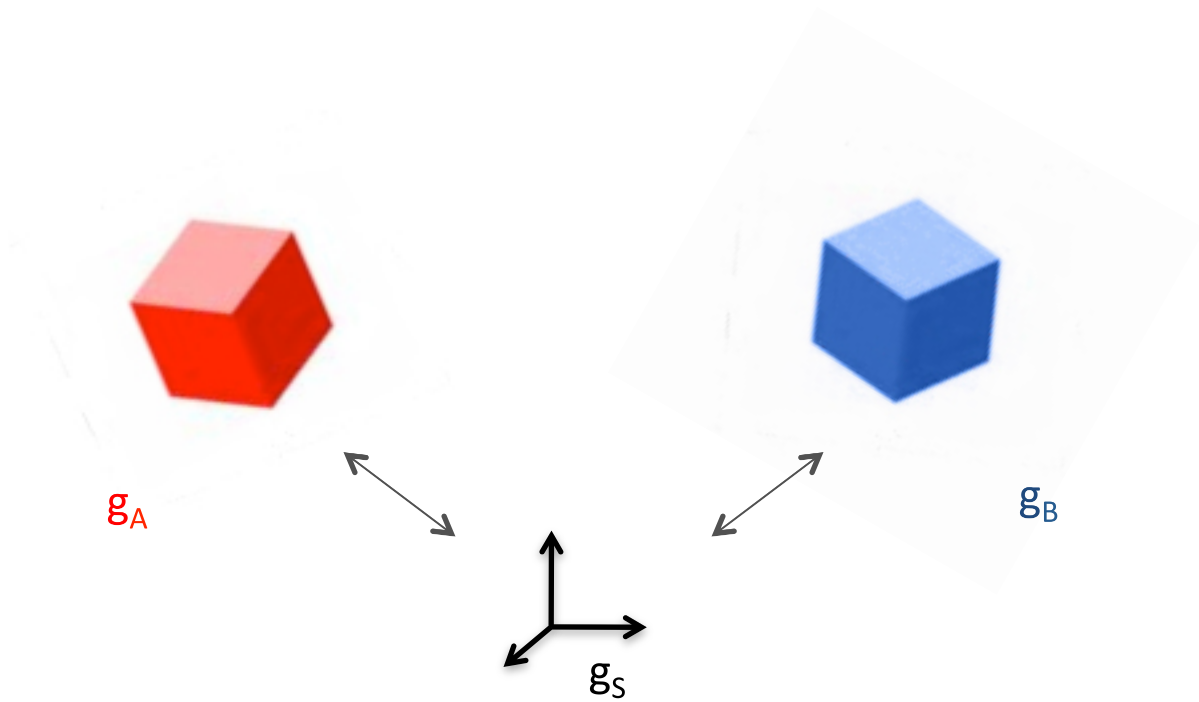
Last revised: 21st Mar. 2014

Objectives

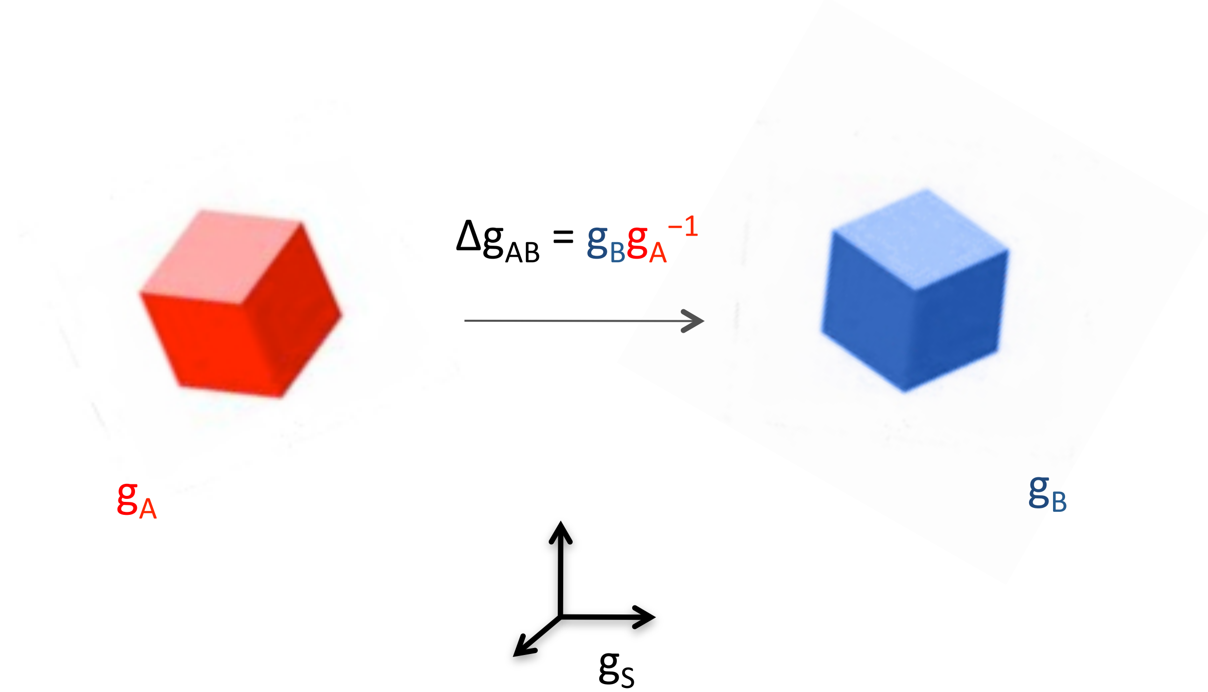
- Briefly describe rotations/orientations
- Introduce Rodrigues-Frank vectors
- Introduce quaternions
- Learn how to manipulate and use quaternions as rotation operators
- Discuss conversions between Euler angles, rotation matrices, RF vectors, and (unit) quaternions

Why do we need to learn about orientations and rotations?



Orientation distributions: Define single-grain orientations relative sample reference frame, and take symmetry into account (both sample and crystal).

Why do we need to learn about orientations and rotations?



Misorientation distributions: Compare orientations on either side of grain boundaries to determine boundary character.

MISORIENTATION : The rotation required to transform from the coordinate system of grain A to grain B

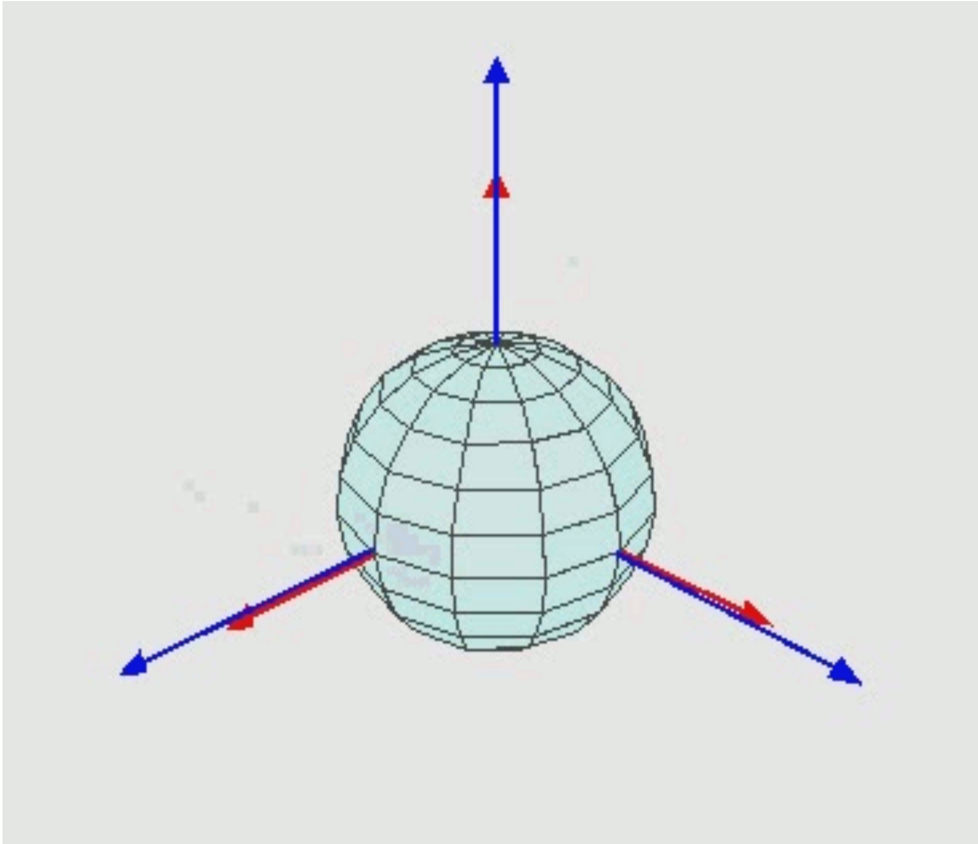
Review: Euler angles

Euler angles:

- ANY rotation can be written as the composition of at most 3 very simple rotations.

$$\mathcal{R}(\varphi_1,\Phi,\varphi_2) = \mathcal{R}(\varphi_2)\mathcal{R}(\Phi)\mathcal{R}(\varphi_1)$$

- Once the Euler angles are known, rotation matrices for any rotation are therefore straight-forward to compute.



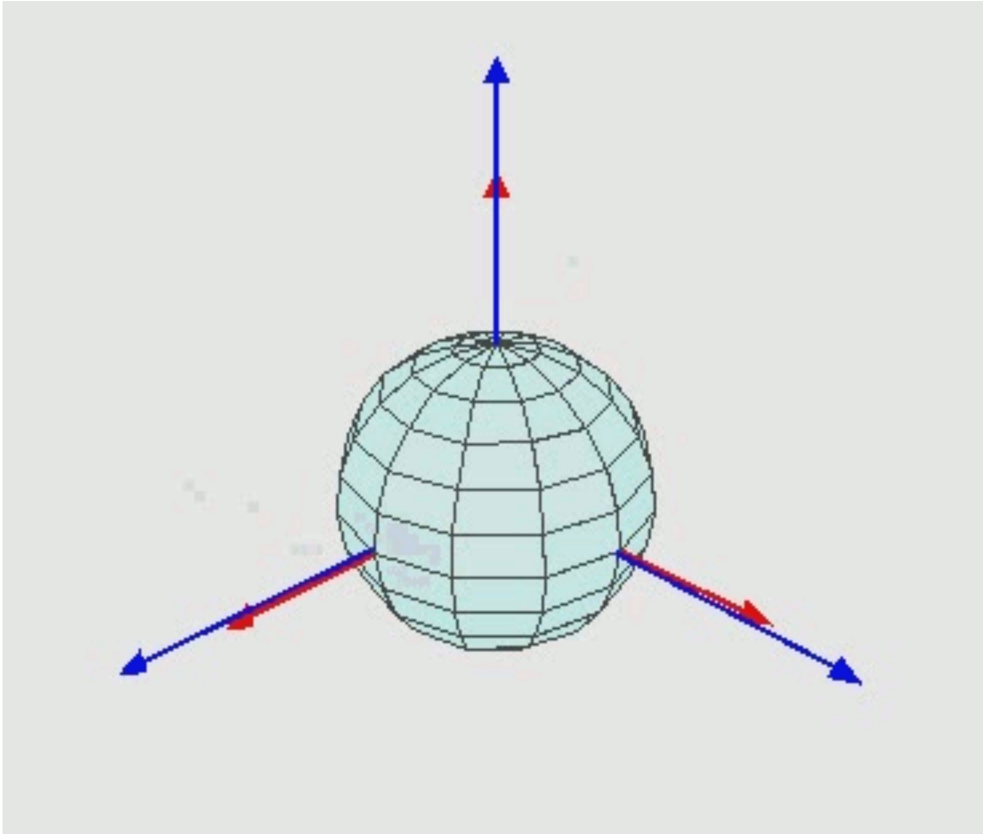
z-x-z rotation sequence

Movie credit: Wikipedia

Review: Euler angles

Difficulties with Euler angles:

- Non-intuitive, difficult to visualize.
- There are 12 different possible axis-angle sequences. The "standard" sequence varies from field to field, and even within fields.
- Every rotation sequence contains at least one artificial singularity, where Euler angles do not make sense, and which can lead to numerical instability in nearby regions.
- Operations involving rotation matricies derived from Euler angles are not nearly as efficient as quaternions.



z-x-z rotation sequence

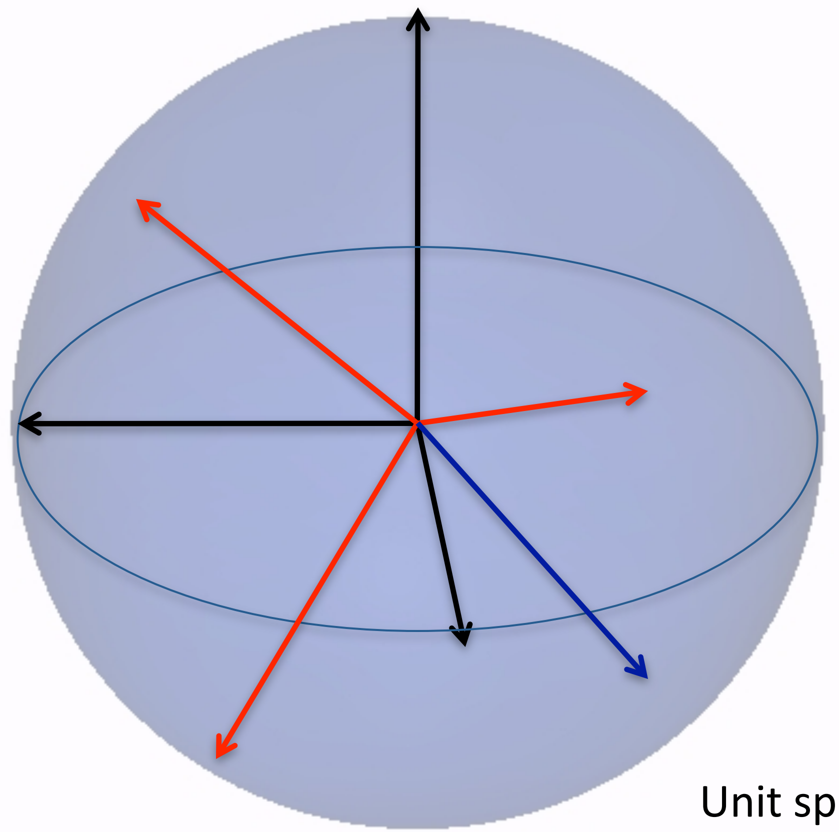
Movie credit: Wikipedia

Passive rotations

We want to be able to quantify transformations between coordinate systems

"Passive" rotations:

Given the coordinates (v_x, v_y, v_z) of vector **v** in the **black** coordinate system, what are its coordinates (v_x, v_y, v_z) in the **red** system?



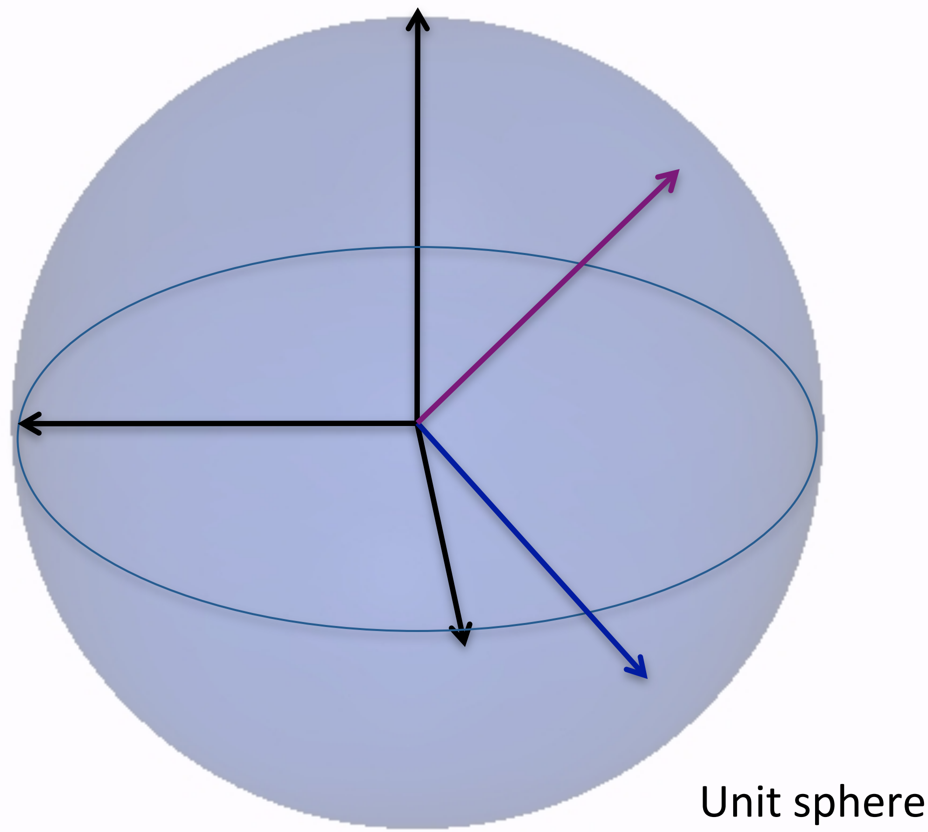
Unit sphere

Active rotations

We want to be able to quantify transformations between coordinate systems

"Active" rotations:

Given the coordinates (v_x, v_y, v_z) of vector **v** in the **black** coordinate system, what are the coordinates (w_x, w_y, w_z) of the rotated vector **w** in the **black** system?

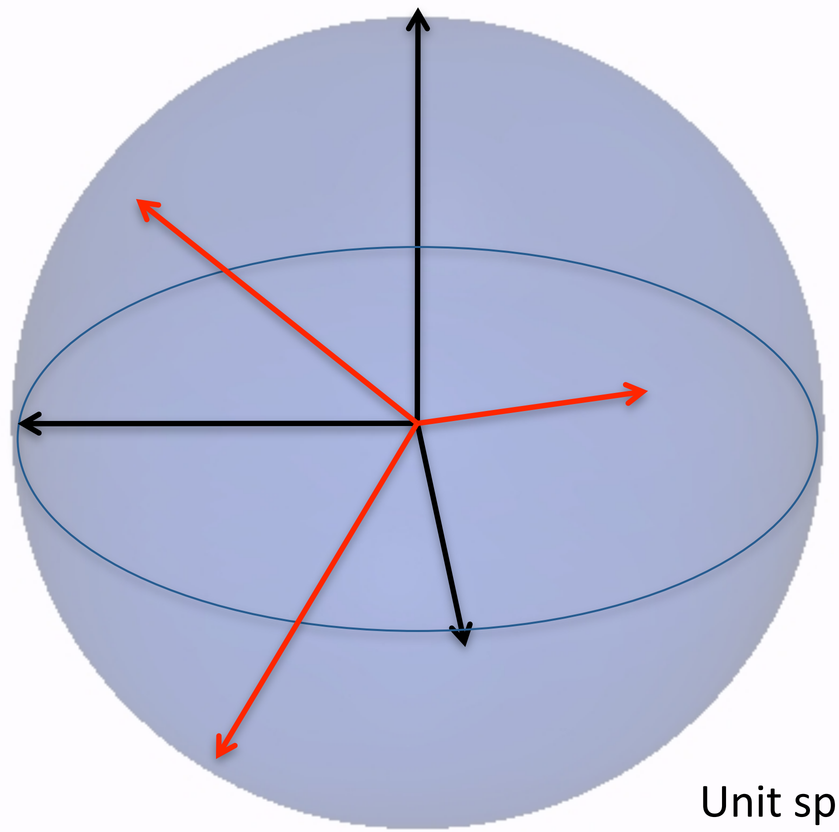


Passive / Active : "only a minus sign" difference, but it is <u>very important</u>

Basics, reviewed

We also need to describe how to quantify and represent the rotation that relates any two orientations

An orientation may be represented by the rotation required to transform from a specified reference orientation (sample axes)



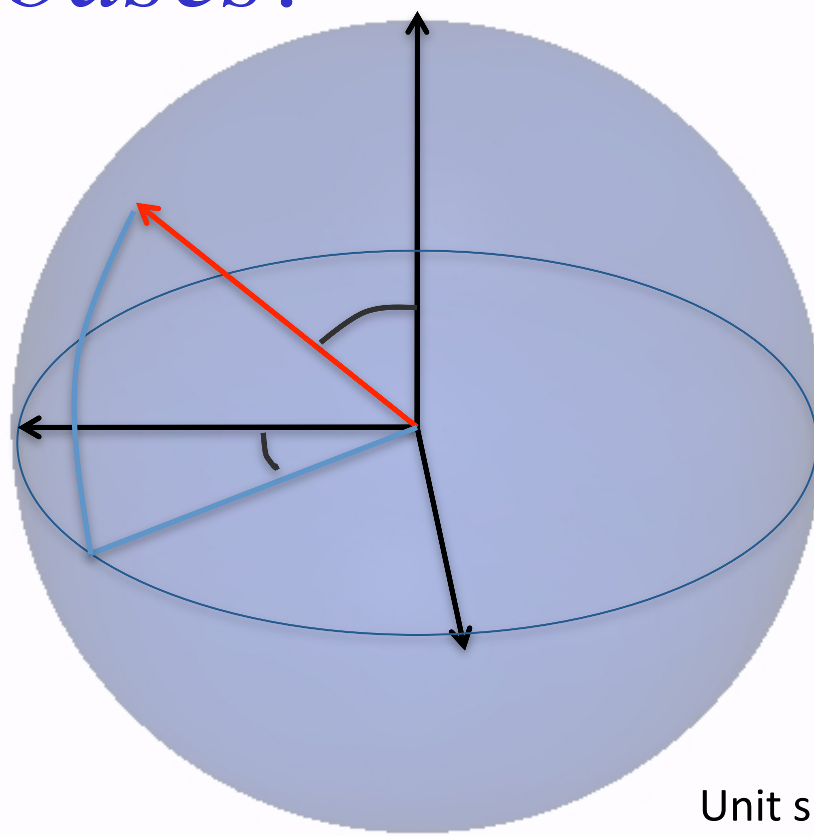
Unit sphere

We need to be able to ***quantitatively*** represent and manipulate 3D rotations in order to deal with orientations

How to relate two orthonormal bases?

First pick a direction represented by a unit normal **r**

Two numbers related to the black system are needed to determine **r**



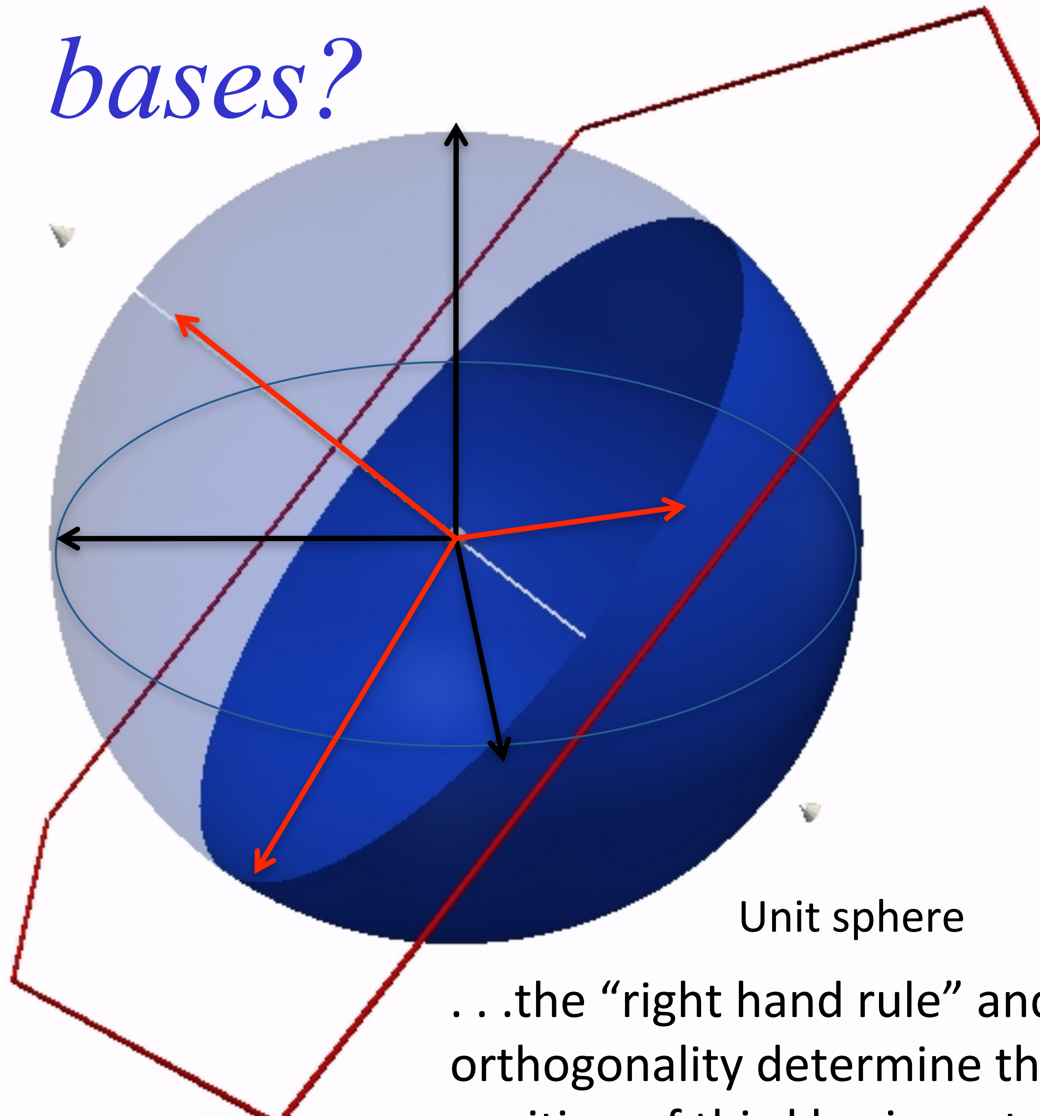
Unit sphere

(i.e. r_x and r_y, or latitude and longitude, or azimuthal and polar angles)

How to relate two orthonormal bases?

To specify an orthonormal basis, one more number is needed (such as an angle in the plane perpendicular to **r**)

Three numbers are required to describe a transformation from the black basis to the red basis



. . .the “right hand rule” and orthogonality determine the position of third basis vector.

Rodrigues vectors

Any rotation may therefore be characterized by an axis $\boldsymbol{r}$ and a rotation angle α about this axis

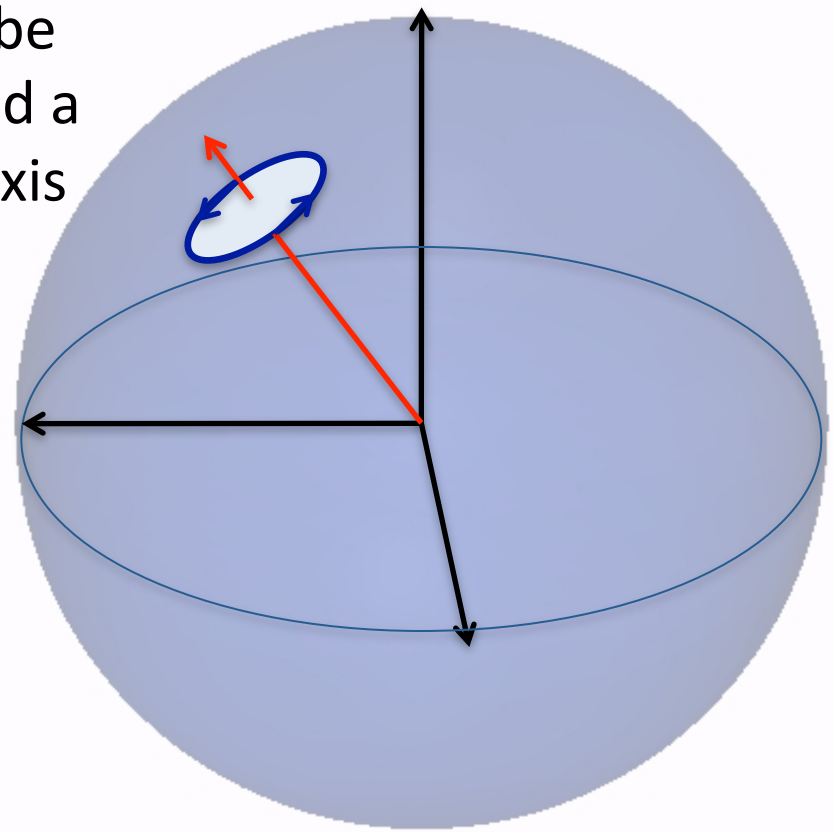
$$\mathcal{R}(\boldsymbol{r}, \alpha)$$

"axis-angle" representation

The RF representation instead scales $\boldsymbol{r}$ by the tangent of $\alpha/2$

$$\boxed{\rho = \hat{r}\tan(\alpha/2)}$$

Note semi-angle



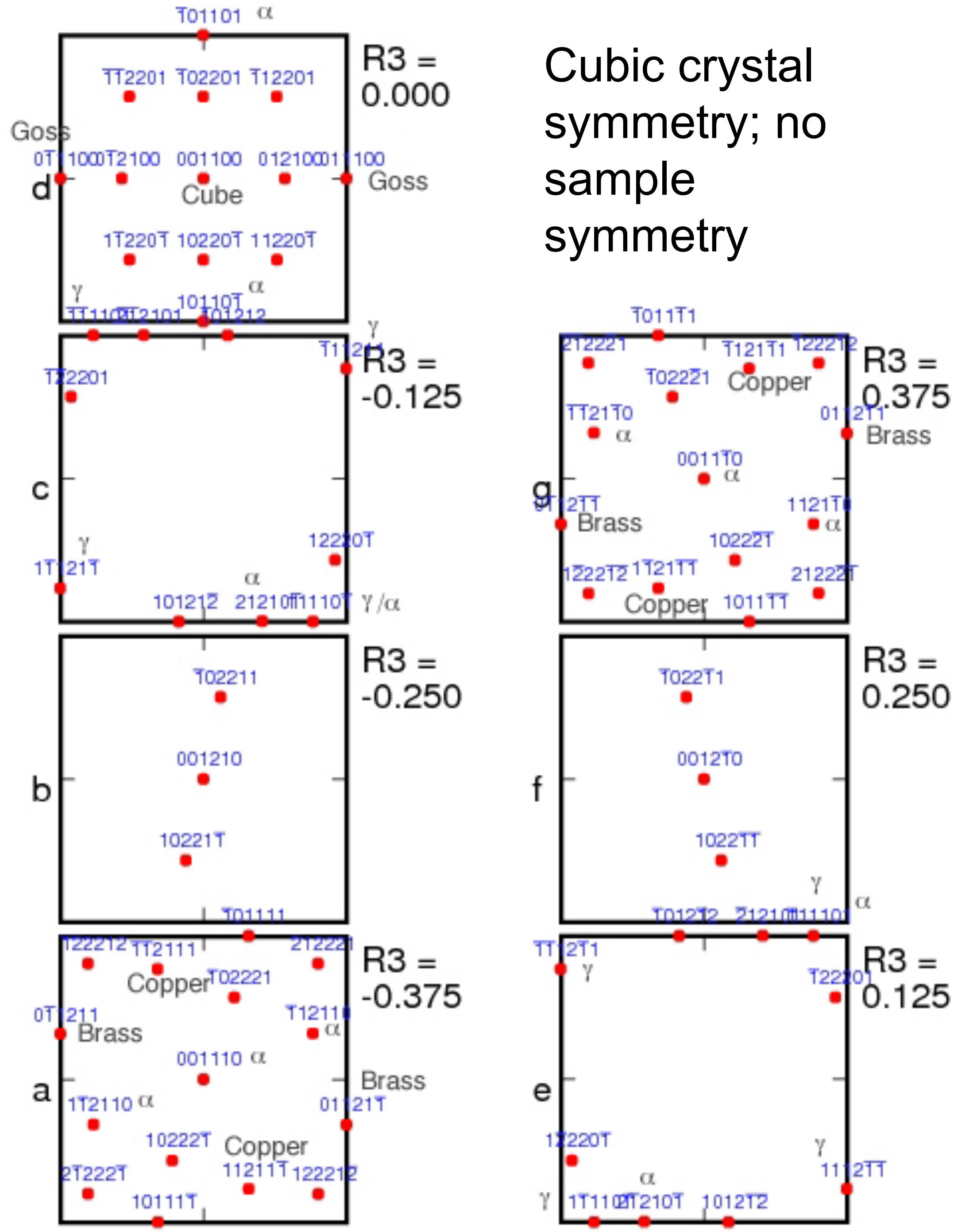
BEWARE: Rodrigues vectors do NOT obey the parallelogram rule (because rotations are NOT commutative!) See slide 16…

Rodrigues vectors

- Rodrigues vectors were popularized by Frank ["Orientation mapping." *Metall. Trans.* **19A**: 403-408 (1988)], hence the term Rodrigues-Frank space for the set of vectors.
- Most useful for representation of *misorientations*, i.e. grain boundary character; also useful for orientations (texture components).
- Application to misorientations is popular because the Rodrigues vector is so closely linked to the rotation axis, which is meaningful for the crystallography of grain boundaries.

Miller Index Map in RF-space

Cubic crystal symmetry; no sample symmetry



- The map shows the location of texture components, identified as (hkl)[uvw], up to order 2.
- Note that many of the low index points lie on the boundary of the cubic-triclinic fundamental zone.
- If the component has a name, or belongs to a fiber, that is noted next to the point.

Generated by RFpoints_HKLUVW_1Jun07.f

Transformation Matrix from Axis-Angle Pair

Written out as a complete 3x3 matrix:

$$
\begin{aligned}
g_{ij} &= \delta_{ij}\cos\theta + r_i r_j(1-\cos\theta) \\
&\qquad + \sum_{k=1,3} \varepsilon_{ijk} r_k \sin\theta \\
&= \begin{pmatrix}
\cos\theta + u^2(1-\cos\theta) & uv(1-\cos\theta) + w\sin\theta & uw(1-\cos\theta) - v\sin\theta \\
uv(1-\cos\theta) - w\sin\theta & \cos\theta + v^2(1-\cos\theta) & vw(1-\cos\theta) + u\sin\theta \\
uw(1-\cos\theta) + v\sin\theta & vw(1-\cos\theta) - u\sin\theta & \cos\theta + w^2(1-\cos\theta)
\end{pmatrix}
\end{aligned}
$$

Note the "+" sign before the third term (with permutation tensor), signifying a passive rotation.

Axis-Angle from Matrix

The rotation axis, **r**, is obtained from the skew-symmetric part of the matrix:

$$\hat{r} = \frac{(a_{23} - a_{32}),(a_{31} - a_{13}),(a_{12} - a_{21})}{\sqrt{(a_{23} - a_{32})^2 + (a_{31} - a_{13})^2 + (a_{12} - a_{21})^2}}$$

Another useful relation gives us the magnitude of the rotation, θ, in terms of the *trace* of the matrix, a_{ii}:

$$a_{ii} = 3\cos\theta + (1 - \cos\theta)n_i^2 = 1 + 2\cos\theta$$

, therefore,

$$\cos\,\theta = 0.5\ (\mathrm{trace}(a) - 1).$$

See the slides on Rotation_matrices for what to do when you have small angles, or if you want to use the full range of 0-360° and deal with switching the sign of the rotation axis. Also, be careful that the argument to arc-cosine is in the range -1 to +1 : round-off in the computer can result in a value outside this range.

Symmetry Operator examples

- Diad on z: [uvw] = [001], θ = 180° - substitute the values of *uvw* and angle into the formula

$$g_{ij} = \begin{pmatrix} \cos 180 + 0^2(1-\cos 180) & 0*0(1-\cos 180)+1*\sin 180 & 0*1(1-\cos 180)-0\sin 180 \\ 0*0(1-\cos 180) - w\sin 180 & \cos 180 + 0^2(1-\cos 180) & 0*1(1-\cos 180)+0\sin 180 \\ 0*1(1-\cos 180)+0\sin 180 & 0*1(1-\cos 180)-0\sin 180 & \cos 180 + 1^2(1-\cos 180) \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- 4-fold on *x*:
  [uvw] = [100]
  θ = 90°

$$g_{ij} = \begin{pmatrix} \cos 90 + 1^2(1-\cos 90) & 1*0(1-\cos 90)+w\sin 90 & 0*1(1-\cos 90)-0\sin 90 \\ 0*1(1-\cos 90) - 0\sin 90 & \cos 90 + 0^2(1-\cos 90) & 1*0(1-\cos 90)+1\sin 90 \\ 0*1(1-\cos 90)+0\sin 90 & 0*0(1-\cos 90)-1\sin 90 & \cos 90 + 0^2(1-\cos 90) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

Matrix representation of the *rotation point groups*

What is a *group*? A group is a set of objects that form a closed set: if you combine any two of them together, the result is simply a different member of that same group of objects. Rotations in a given point group form closed sets - try it for yourself!

Table II. Symmetry operators of rotation groups

tetragonal branch	hexagonal branch	cubic branch	
$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$ 1	$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&0&-1\\0&-1&0\\-1&0&0\end{matrix}$
$\begin{matrix}-1&0&0\\0&1&0\\0&0&-1\end{matrix}$ 2	$\begin{matrix}-.5&a&0\\-a&-.5&0\\0&0&1\end{matrix}$	$\begin{matrix}0&0&1\\1&0&0\\0&1&0\end{matrix}$	$\begin{matrix}0&0&1\\0&-1&0\\1&0&0\end{matrix}$
$\begin{matrix}1&0&0\\0&-1&0\\0&0&-1\end{matrix}$	$\begin{matrix}-.5&-a&0\\a&-.5&0\\0&0&1\end{matrix}$ 3	$\begin{matrix}0&1&0\\0&0&1\\1&0&0\end{matrix}$	$\begin{matrix}0&0&1\\0&1&0\\-1&0&0\end{matrix}$
$\begin{matrix}-1&0&0\\0&-1&0\\0&0&1\end{matrix}$ 222	$\begin{matrix}.5&a&0\\-a&.5&0\\0&0&1\end{matrix}$	$\begin{matrix}0&-1&0\\0&0&1\\-1&0&0\end{matrix}$	$\begin{matrix}0&0&-1\\0&1&0\\1&0&0\end{matrix}$
$\begin{matrix}0&1&0\\-1&0&0\\0&0&1\end{matrix}$	$\begin{matrix}-1&0&0\\0&-1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&-1&0\\0&0&-1\\1&0&0\end{matrix}$	$\begin{matrix}-1&0&0\\0&0&-1\\0&-1&0\end{matrix}$
$\begin{matrix}0&-1&0\\1&0&0\\0&0&1\end{matrix}$	$\begin{matrix}.5&-a&0\\a&.5&0\\0&0&1\end{matrix}$ 6	$\begin{matrix}0&1&0\\0&0&-1\\-1&0&0\end{matrix}$	$\begin{matrix}1&0&0\\0&0&-1\\0&1&0\end{matrix}$
$\begin{matrix}0&1&0\\1&0&0\\0&0&-1\end{matrix}$	$\begin{matrix}-.5&-a&0\\-a&.5&0\\0&0&-1\end{matrix}$	$\begin{matrix}0&0&-1\\1&0&0\\0&-1&0\end{matrix}$	$\begin{matrix}1&0&0\\0&0&1\\0&-1&0\end{matrix}$
$\begin{matrix}0&-1&0\\-1&0&0\\0&0&-1\end{matrix}$ 42	$\begin{matrix}1&0&0\\0&-1&0\\0&0&-1\end{matrix}$	$\begin{matrix}0&0&-1\\-1&0&0\\0&1&0\end{matrix}$	$\begin{matrix}-1&0&0\\0&0&1\\0&1&0\end{matrix}$
	$\begin{matrix}-.5&a&0\\a&.5&0\\0&0&-1\end{matrix}$	$\begin{matrix}0&0&1\\-1&0&0\\0&-1&0\end{matrix}$	$\begin{matrix}0&-1&0\\-1&0&0\\0&0&-1\end{matrix}$
	$\begin{matrix}.5&a&0\\a&-.5&0\\0&0&-1\end{matrix}$	$\begin{matrix}-1&0&0\\0&1&0\\0&0&-1\end{matrix}$	$\begin{matrix}0&1&0\\-1&0&0\\0&0&1\end{matrix}$
	$\begin{matrix}-1&0&0\\0&1&0\\0&0&-1\end{matrix}$	$\begin{matrix}-1&0&0\\0&-1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&1&0\\1&0&0\\0&0&-1\end{matrix}$
	$\begin{matrix}.5&-a&0\\-a&-.5&0\\0&0&-1\end{matrix}$ 622	$\begin{matrix}1&0&0\\0&-1&0\\0&0&-1\end{matrix}$ 23	$\begin{matrix}0&-1&0\\1&0&0\\0&0&1\end{matrix}$ 432

$a \equiv \sqrt{3}/2$

The dashed boxes in this column make up group 4.

The dashed boxes in this column make up group 32.

The dashed box in this column comprises the 3-fold axes only.

Kocks, Tomé, Wenk: Ch. 1 Table II

The 4 operators enclosed in orange boxes are also the 222 point group, appropriate to orthorhombic symmetry

Note: the 3rd matrix in the 1st column (x-diad) is missing a "-" on the 33 element; this is corrected in this slide. Also, in the 2nd from the bottom, last column: the 33 element should be +1, not -1. In some versions of the book, in the last matrix (bottom right corner) the 33 element is incorrectly given as -1; here the +1 is correct.

Cubic Crystal Symmetry Operators

Symmetry Operator		Rodrigues Vector	Unit Quaternion
2-fold on <100>	L_{100}^{2}	∞(1,0,0) ∞(0,1,0) ∞(0,0,1)	±(1,0,0,0), ±(0,1,0,0) ±(0,0,1,0)
4-fold on <100>	L_{100}^{4}	±(1,0,0) ±(0,1,0) ±(0,0,1)	±1/√2(±1,0,0,1), ±1/√2 (0, ±1,0,1) ±1/√2 (0,0, ±1,1)
2-fold on <110>	L_{110}^{2}	∞(1, ±1,0) ∞(1,0, ±1) ∞(0,1, ±1)	±1/√2 (±1,1,0,0), ±1/√2 (0,1, ±1,0) ±1/√2 (±1,0,1,0)
3-fold on <111>	L_{111}^{3}	±(1,1,1) ±(1,-1,1) ±(1,1,-1) ±(-1,-1,1)	±1/2 (±1,1,1,1), ±1/2 (1, –1, 1,1), ±1/2 (1,1,–1,1), ±1/2 (-1,–1, 1,1) ±1/2 (-1,1,–1,1), ±1/2 (1,–1,–1,1) ±1/2 (-1,-1,–1,1))

The numerical values of these symmetry operators can be found at:
http://neon.materials.cmu.edu/texture_subroutines: quat.cubic.symm etc.

(432) in unit quaternions

```
quat.symm.cubic        file with 24 proper rotations in quaternion form
24
   0     0     0     1
   1     0     0     0
   0     1     0     0
   0     0     1     0
   0.707107     0     0     0.707107
    0    0.707107     0     0.707107
    0     0    0.707107     0.707107
   -0.707107     0     0     0.707107
    0    -0.707107     0     0.707107
    0     0    -0.707107     0.707107
   0.707107     0.707107     0     0
  -0.707107     0.707107     0     0
    0    0.707107     0.707107     0
    0   -0.707107     0.707107     0
    0.707107     0     0.707107     0
   -0.707107     0     0.707107     0
    0.5   0.5   0.5   0.5
   -0.5  -0.5  -0.5   0.5
    0.5  -0.5   0.5   0.5
   -0.5   0.5  -0.5   0.5
    -0.5   0.5   0.5   0.5
    0.5  -0.5  -0.5   0.5
    -0.5  -0.5   0.5   0.5
     0.5   0.5  -0.5   0.5
```

Cubic point group; proper rotations expressed as quaternions; the first four lines/elements/ operators are equivalent to (222) and represent orthorhombic symmetry; the next 12 lines are 90° rotations about <100> or 180° rotations about <110>; the last 8 lines are 120° rotations.

Conversions: matrix→RF vector

- Conversion from rotation (misorientation) matrix, due to Morawiec, with

$\Delta g_{AB} = g_B g_A^{-1}$:

$$\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} = \begin{bmatrix} [\Delta g(2,3) - \Delta g(3,2)] / [1 + tr(\Delta g)] \\ [\Delta g(3,1) - \Delta g(1,3)] / [1 + tr(\Delta g)] \\ [\Delta g(1,2) - \Delta g(2,1)] / [1 + tr(\Delta g)] \end{bmatrix}$$

Conversion from Bunge Euler Angles

- $\tan(\alpha/2) = \sqrt{}\{(1/[\cos(\Phi/2)\cos\{(\phi_1 + \phi_2)/2\}]^2 - 1\}$
- $\rho_1 = \tan(\Phi/2)\ [\cos\{(\phi_1 - \phi_2)/2\}/\cos\{(\phi_1 + \phi_2)/2\}]$
- $\rho_2 = \tan(\Phi/2)\ [\sin\{(\phi_1 - \phi_2)/2\}/[\cos\{(\phi_1 + \phi_2)/2\}]$
- $\rho_3 = \tan\{(\phi_1 + \phi_2)/2\}$

P. Neumann (1991). "Representation of orientations of symmetrical objects by Rodrigues vectors."
Textures and Microstructures **14-18**: 53-58.

Conversion from Rodrigues to Bunge Euler angles:

sum = atan(R_3) ; diff = atan (R_2/R_1)

ϕ_1 = sum + diff; Φ = 2. * atan(R2 * cos(sum) / sin(diff)); ϕ_2 = sum - diff

Conversion Rodrigues vector to axis transformation matrix

- Due to Morawiec:

$$a_{ij} = \frac{1}{1+\rho_l\rho_l}\left([1-\rho_l\rho_l]\delta_{ij} + 2\rho_i\rho_j + 2\epsilon_{ijk}\rho_k\right)$$

Example for the 12 entry:

$$a_{12} = \frac{1}{1+\rho_l\rho_l}\left([1-\rho_l\rho_l]\delta_{12} + 2\rho_1\rho_2 + 2\rho_3\right)$$

$$= \frac{2(\rho_1\rho_2+\rho_3)}{1+\rho_l\rho_l}$$

NB Morawiec's Eq on p22 has a minus sign in front of the last term; this will give an active rotation matrix, rather than the passive rotation matrix seen here.

Combining Rotations as RF vectors

- Two Rodrigues vectors combine to form a third, ρ_C, as follows, where ρ_B follows *after* ρ_A. Note that this is *not* the parallelogram law for vectors!

$$\rho_C = (\rho_A, \rho_B) =$$
$$\{\rho_A + \rho_B - \rho_A \times \rho_B\}/\{1 - \rho_A \bullet \rho_B\}$$

addition

vector product

scalar product

Combining Rotations as RF vectors: component form

$$\left(\rho_1^C, \rho_2^C, \rho_3^C\right) = \frac{\begin{pmatrix} \rho_1^A + \rho_1^B - \left[\rho_2^A \rho_3^B - \rho_3^A \rho_2^B\right], \\ \rho_2^A + \rho_2^B - \left[\rho_3^A \rho_1^B - \rho_1^A \rho_3^B\right], \\ \rho_3^A + \rho_3^B - \left[\rho_1^A \rho_2^B - \rho_2^A \rho_1^B\right] \end{pmatrix}}{1 - \left(\rho_1^A \rho_1^B + \rho_2^A \rho_2^B + \rho_3^A \rho_3^B\right)}$$

Quaternions: Yet another representation of rotations

What is a quaternion?

A quaternion is first of all an ordered set of four real numbers q_0, q_1, q_2, and q_3, (sometimes q_1, q_2 q_3, and q_4) . Here, **i, j, k** are the familiar unit vectors that correspond to the x-, y-, and z-axes, resp.

$$
\begin{aligned}
q &= q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3 \\
&= (q_0, q_1, q_2, q_3) \\
&= q_0 + \mathbf{q}
\end{aligned}
$$

Scalar part Vector part

Addition of two quaternions and multiplication of a quaternion by a real number are as would be expected of normal four-component vectors.

$$p + q = (p_0 + q_0) + \mathbf{i}\,(p_1 + q_1) + \mathbf{j}\,(p_2 + q_2) + \mathbf{k}\,(p_3 + q_3)$$

Magnitude of a quaternion:

$$|q|^2 = q^* q = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

Conjugate of a quaternion:

$$
\begin{aligned}
q^* &= q_0 - \mathbf{q} \\
&= q_0 - \mathbf{i}q_1 - \mathbf{j}q_2 - \mathbf{k}q_3
\end{aligned}
$$

On a New Species of Imaginary Quantities Connected with a Theory of Quaternions, by William Rowan Hamilton, *Proceedings of the Royal Irish Academy*, **2** (1844), 424–434.

Multiplication of two quaternions

However, quaternion multiplication is ingeniously defined in such a way so as to reproduce **rotation composition**.

$$q = q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3 \\ = (q_0, q_1, q_2, q_3) \\ = q_0 + \mathbf{q}$$

Multiplication of the basis quaternions is *defined* as follows:

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$$

$$\mathbf{ij} = \mathbf{k} = -\mathbf{ji}$$

$$\mathbf{ki} = \mathbf{j} = -\mathbf{ik}$$

$$\mathbf{jk} = \mathbf{i} = -\mathbf{kj}$$

[1] Quaternion multiplication is non-commutative ($pq \neq qp$).
[2] There are similarities to complex numbers (which correspond to rotations in 2D).

From these rules it can be shown that the product of two arbitrary quaternions *p,q* is given by:

$$pq = p_0 q_0 - (p_1 q_1 + p_2 q_2 + p_3 q_3) \\ p_0 (\mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3) + q_0 (\mathbf{i}p_1 + \mathbf{j}p_2 + \mathbf{k}p_3) \\ + \mathbf{i}(p_2 q_3 - p_3 q_2) + \mathbf{j}(p_3 q_1 - p_1 q_3) + \mathbf{k}(p_1 q_2 - p_2 q_1)$$

Using more compact notation:

$$pq = \underbrace{[p_0 q_0 - \mathbf{p} \cdot \mathbf{q}]}_{\text{Scalar part}} + \underbrace{[p_0 \mathbf{q} + q_0 \mathbf{p} + \mathbf{p} \times \mathbf{q}]}_{\text{Vector part}}$$

On a New Species of Imaginary Quantities Connected with a Theory of Quaternions,
by William Rowan Hamilton, *Proceedings of the Royal Irish Academy*, **2** (1844), 424–434.

Unit quaternions as rotations

We state without proof that a rotation of α degrees about the (normalized) axis **r** may be represented by the following unit quaternion:

$$\boxed{q = \cos(\alpha/2) + \mathbf{r}\sin(\alpha/2)}$$

It is easy to see that this is a unit quaternion, i.e. that $q_0^2 + |\mathbf{q}|^2 = 1$
Note the similarity to Rodrigues vectors, except with a different scaling.

For two rotations q and p that share a single axis $\mathbf{r}$, note what happens when q and p are multiplied:

$$\begin{aligned} pq &= [p_0 q_0 - \mathbf{p}\cdot\mathbf{q}] + [p_0\mathbf{q} + q_0\mathbf{p} + \mathbf{p}\times\mathbf{q}] \\ &= \cos\alpha\cos\beta - \sin\alpha\sin\beta + \mathbf{r}(\sin\alpha\cos\beta + \cos\alpha\sin\beta) \\ &= \cos(\alpha+\beta) + \mathbf{r}\sin(\alpha+\beta) \end{aligned}$$

Multiplication of a quaternion and a 3-D vector

It is useful to define the multiplication of vectors and quaternions as well. Vectors have three components, and quaternions have four. How to proceed?

Every vector $\mathbf{v}$ corresponds to a "pure" quaternion whose 0^{th} component is zero.

$$\mathbf{v} = 0 + \mathbf{i}v_x + \mathbf{j}v_y + \mathbf{k}v_z$$

…and proceed as with two quaternions:

$$pq = [p_0 q_0 - \mathbf{p} \cdot \mathbf{q}] + [p_0 \mathbf{q} + q_0 \mathbf{p} + \mathbf{p} \times \mathbf{q}]$$

Note that in general that the product of a quaternion and a vector can result in a non-pure quaternion with non-zero scalar component.

Rotation of a vector by a unit quaternion

Although the quantity $q\mathbf{v}$ may not be a vector, it can be shown that the triple products $q^*\mathbf{v}q$ and $q\mathbf{v}q^*$ are.

In fact, these vectors are the images of $\mathbf{v}$ by passive and active rotations corresponding to quaternion q.

$\mathbf{w} = q^*\mathbf{v}q$	Passive rotation
$\mathbf{s} = q\mathbf{v}q^*$	Active rotation

Rotation of a vector by a unit quaternion

Expanding these expressions yields

$$\mathbf{w} = \left(2q_0^2 - 1\right)\mathbf{v} + 2\left(\mathbf{v}\cdot\mathbf{q}\right)\mathbf{q} + 2q_0\left(\mathbf{v}\times\mathbf{q}\right)$$ Passive rotation

$$\mathbf{s} = \left(q_0^2 - |\mathbf{q}|^2\right)\mathbf{v} + 2\left(\mathbf{v}\cdot\mathbf{q}\right)\mathbf{q} + 2q_0\left(\mathbf{q}\times\mathbf{v}\right)$$ Active rotation

Moreover, the composition of two rotations (one rotation following another) is equivalent to quaternion multiplication.

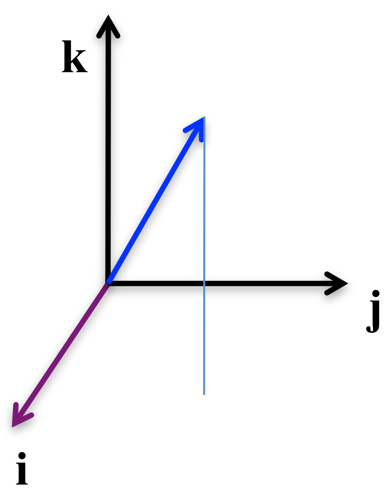
$$\begin{aligned}\mathbf{w} &= q^*\left(p^*\mathbf{v}p\right)q \\ &= (pq)^*\,\mathbf{v}\,(pq)\end{aligned}$$

since

$$(pq)^* = q^*p^*$$

Example: Rotation of a Vector by Quaternion-Vector Multiplication

Consider rotating the vector ***i*** by an angle of α = $2\pi/3$ about the <111> direction.



Rotation axis: $\mathbf{r} = \left(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}\right)$

$$\begin{aligned} q &= \cos(\alpha/2) + \mathbf{r}\sin(\alpha/2) \\ &= \frac{1}{2} + \left(\mathbf{i}\frac{1}{\sqrt{3}} + \mathbf{j}\frac{1}{\sqrt{3}} + \mathbf{k}\frac{1}{\sqrt{3}}\right)\frac{\sqrt{3}}{2} \end{aligned}$$

$$q_0 = \frac{1}{2} \qquad \mathbf{q} = \frac{1}{2}\mathbf{i} + \frac{1}{2}\mathbf{j} + \frac{1}{2}\mathbf{k}$$

$$\mathbf{q}\cdot\mathbf{i} = \frac{1}{2} \qquad \mathbf{q}\times\mathbf{i} = \frac{1}{2}\mathbf{j} - \frac{1}{2}\mathbf{k}$$

For an active rotation:

$$\begin{aligned} \mathbf{s} &= q\mathbf{i}q^* \\ &= \left(\frac{1}{4} - \frac{3}{4}\right)\mathbf{i} + 2\left(\frac{1}{2}\right)\mathbf{q} + 2\left(\frac{1}{2}\right)\left(\frac{1}{2}\mathbf{j} - \frac{1}{2}\mathbf{k}\right) \\ &= -\frac{1}{2}\mathbf{i} + \frac{1}{2}\mathbf{i} + \frac{1}{2}\mathbf{j} + \frac{1}{2}\mathbf{k} + \frac{1}{2}\mathbf{j} - \frac{1}{2}\mathbf{k} \\ &= \mathbf{j} \end{aligned}$$

For a passive rotation:

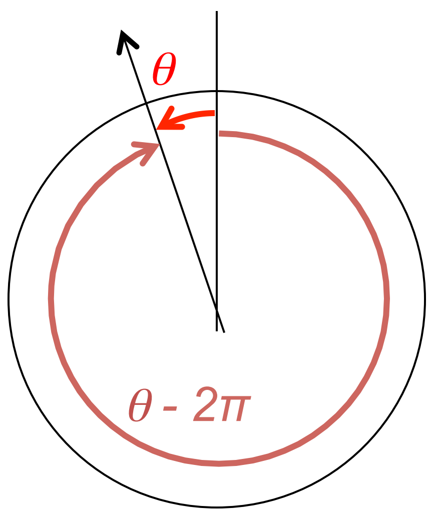
$$\begin{aligned} \mathbf{w} &= q^*\mathbf{i}q \\ &= \mathbf{k} \end{aligned}$$

Positive vs Negative Rotations

- One curious feature of quaternions that is not obvious from the definition is that they allow positive and negative rotations to be distinguished. This is more commonly described in terms of requiring a rotation of 4π to retrieve the same quaternion as you started out with but for visualization, it is more helpful to think in terms of a difference in the sign of rotation.

Positive vs Negative Rotations

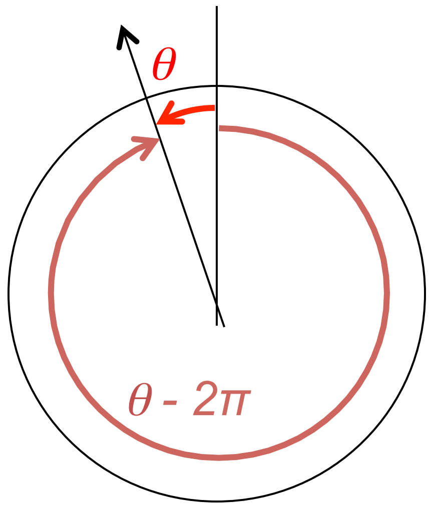
- Let's start with considering a positive rotation of θ about an arbitrary axis, **r**. From the point of view of the result one obtains the same thing if one rotates *backwards* by the complementary angle, θ - 2π (also about **r**). Expressed in terms of quaternions, however, the representation is different! Setting $\mathbf{r} = [u,v,w]$ again,



- $\mathbf{q}(\mathbf{r},\theta) =$
  $q(u \sin\theta/2, v \sin\theta/2, w \sin\theta/2, \cos\theta/2)$

Positive vs Negative Rotations

- $\mathbf{q}(\mathbf{r},\theta\text{-}2\pi)$ =
  $q(u\ \sin(\theta\text{-}2\pi)/2,\ v\ \sin(\theta\text{-}2\pi)/2,$
  $w\ \sin(\theta\text{-}2\pi)/2,\ \cos(\theta\text{-}2\pi)/2)$
  =
  $q(-u\ \sin\theta/2,\ -v\ \sin\theta/2,$
  $-w\ \sin\theta/2,\ -\cos\theta/2) = -\mathbf{q}(\mathbf{r},\theta)$



Positive vs Negative Rotations

- The result, then is that the quaternion representing the negative rotation is the negative of the original (positive) rotation. This has some significance for treating dynamic problems and rotation: angular momentum, for example, depends on the sense of rotation. For static rotations, however, the positive and negative quaternions are equivalent or, more to the point, physically indistinguishable, $\mathbf{q} \equiv -\mathbf{q}$.
- Caution! By "negative rotation" we mean the position arrived at by rotating in the opposite direction. This is **not** the same as taking the same axis but rotating in the opposite sense.

Conversions: matrix→quaternion

Formulae, due to Morawiec:

$$\cos\theta/2 = 1/2\sqrt{1+tr(\Delta g)} \equiv q_4 = \pm\frac{\sqrt{1+tr(\Delta g)}}{2}$$

Note: passive rotation/ axis transformation (axis changes sign for for active rotation)

$$q_i = \pm\frac{\varepsilon_{ijk}\Delta g_{jk}}{4\sqrt{1+tr(\Delta g)}}$$

$$\begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix} = \begin{bmatrix} \pm[\Delta g(2,3)-\Delta g(3,2)]/2\sqrt{1+tr(\Delta g)} \\ \pm[\Delta g(3,1)-\Delta g(1,3)]/2\sqrt{1+tr(\Delta g)} \\ \pm[\Delta g(1,2)-\Delta g(2,1)]/2\sqrt{1+tr(\Delta g)} \\ \pm\sqrt{1+tr(\Delta g)}/2 \end{bmatrix}$$

Note the coordination of choice of sign!

Bunge angles → quaternion

- $[q_1, q_2, q_3, q_4] =$

  $$[\sin \Phi/2 \cos\{(\phi_1 - \phi_2)/2\},$$
  $$\sin \Phi/2 \sin\{(\phi_1 - \phi_2)/2\},$$
  $$\cos \Phi/2 \sin\{\phi_1 + \phi_2)/2\},$$
  $$\cos \Phi/2 \cos\{(\phi_1 + \phi_2)/2\}]$$

Note the occurrence of sums and differences of the 1st and 3rd Euler angles (that eliminate the degeneracy at the origin of Euler space)!

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