Rodrigues vectors, unit Quaternions

27-750

Texture, Microstructure & Anisotropy

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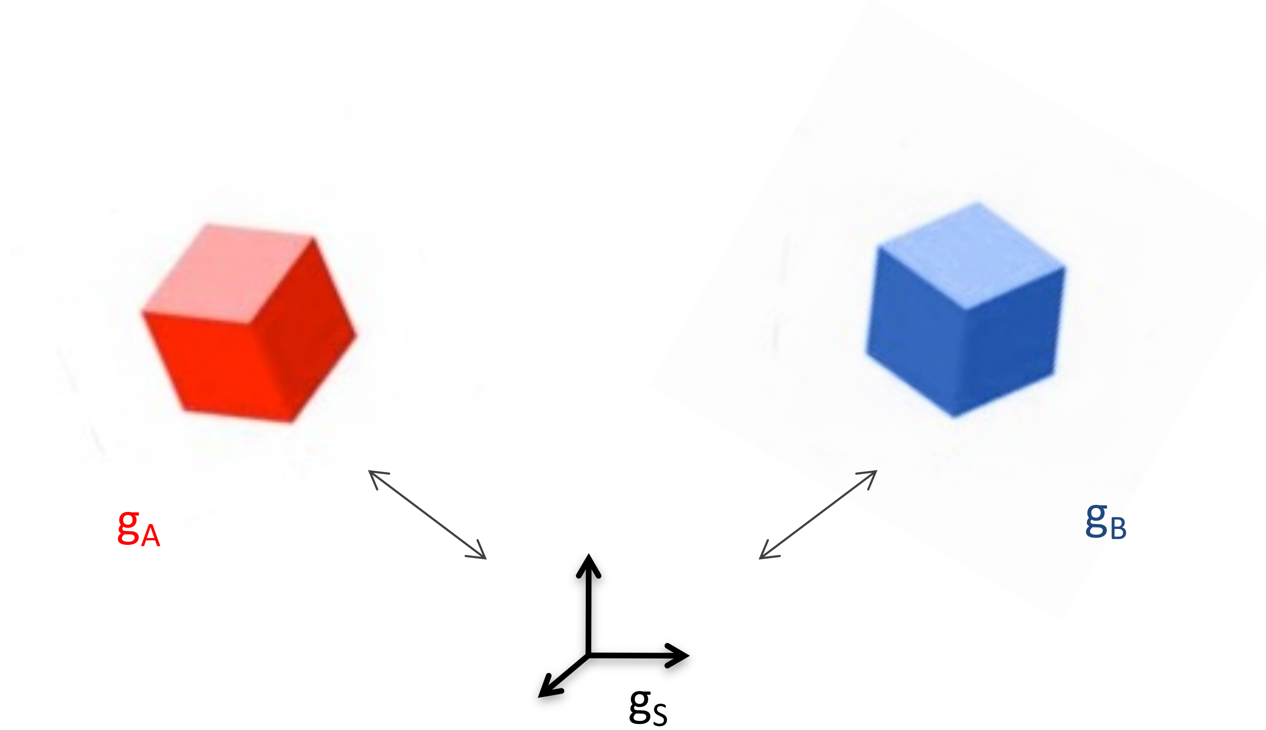
Objectives

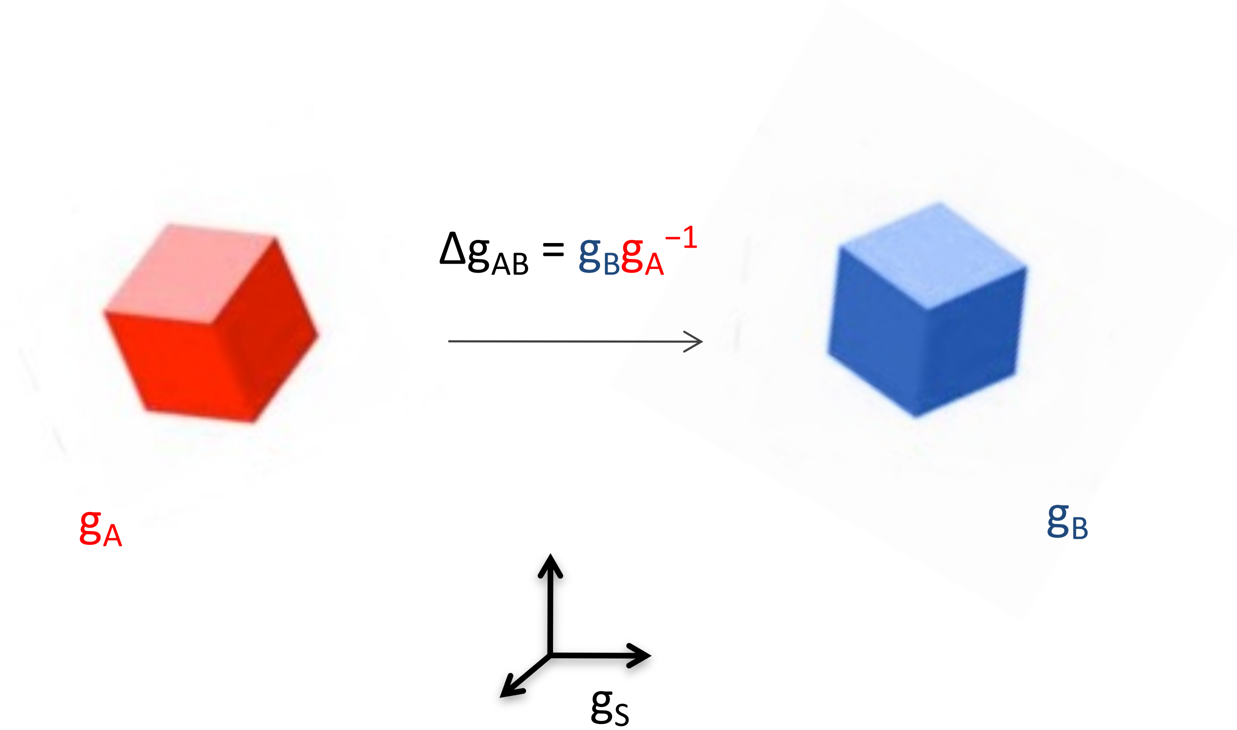
- Briefly describe rotations/orientations
- Introduce Rodrigues-Frank vectors
- Introduce unit quaternions
- Learn how to manipulate and use quaternions as rotation operators
- Discuss conversions between Euler angles, rotation matrices, RF vectors, and quaternions

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.

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

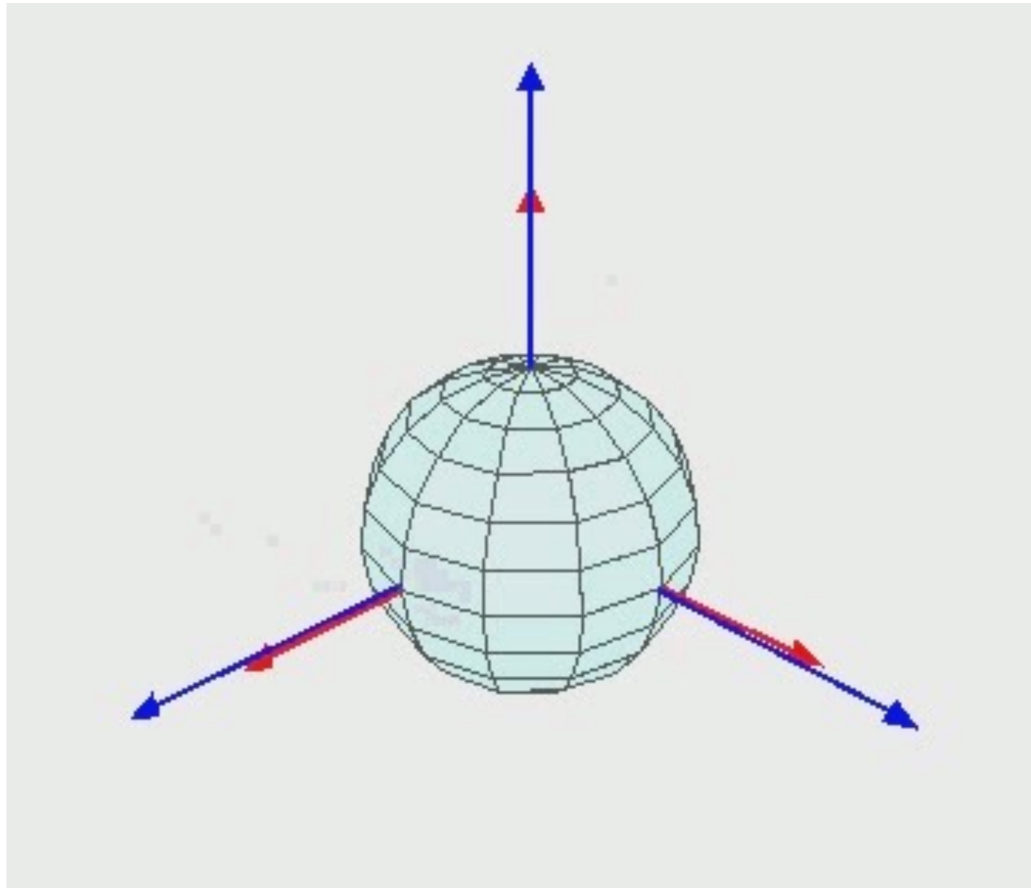
Review: Euler angles

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.
- Note the order in which the rotation sequence is written (for passive rotations): the 1st is on the right, and the last is on the left.



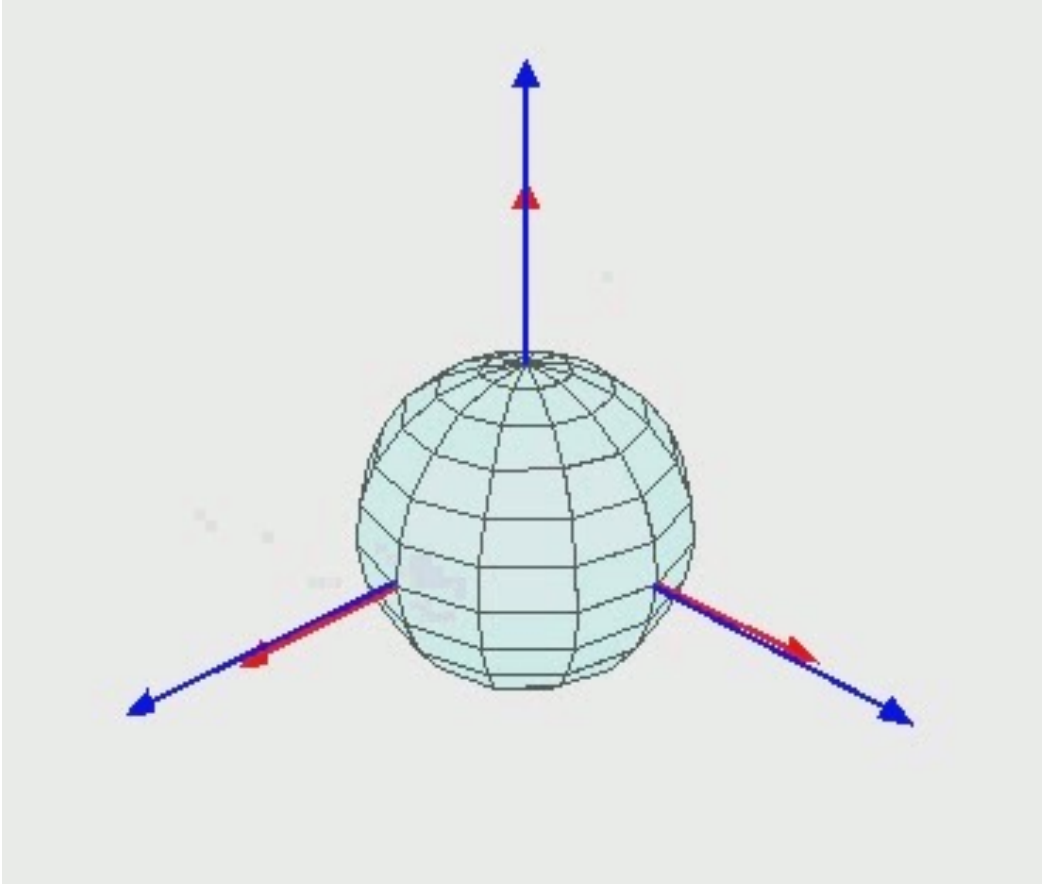
z-x-z rotation sequence

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.
- We use the Bunge convention, as noted on the movie.
- 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 matrices derived from Euler angles are not nearly as efficient as quaternions.

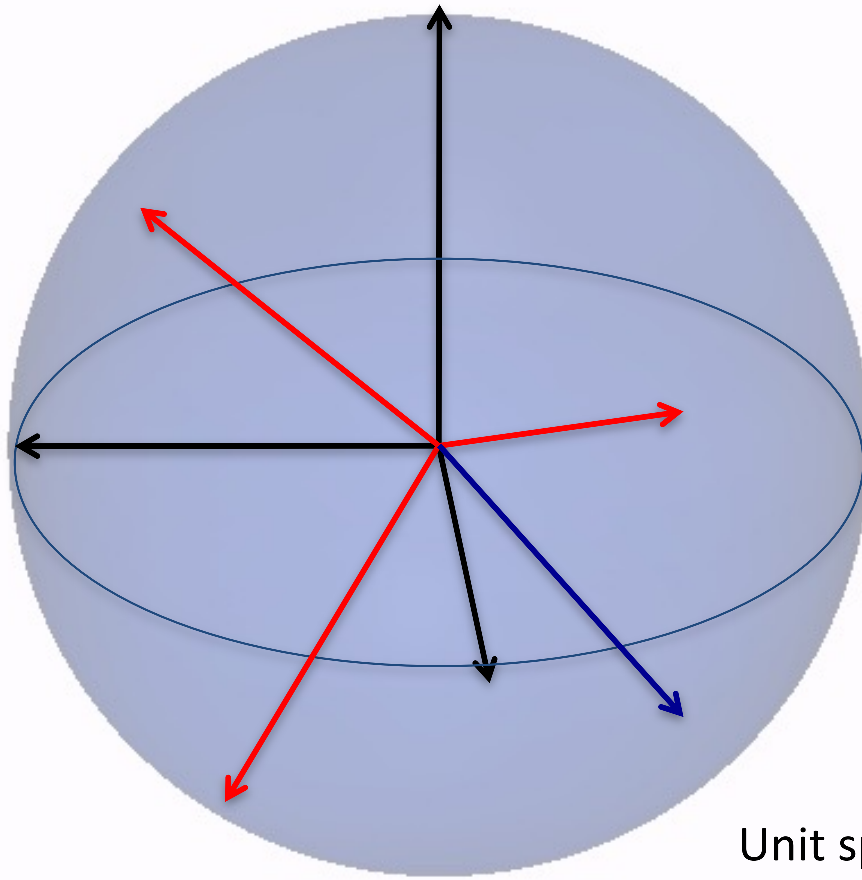


z-x-z rotation sequence

Movie credit: Wikipedia

Passive rotations

We want to be able to quantify transformations between coordinate systems



"Passive" rotations:

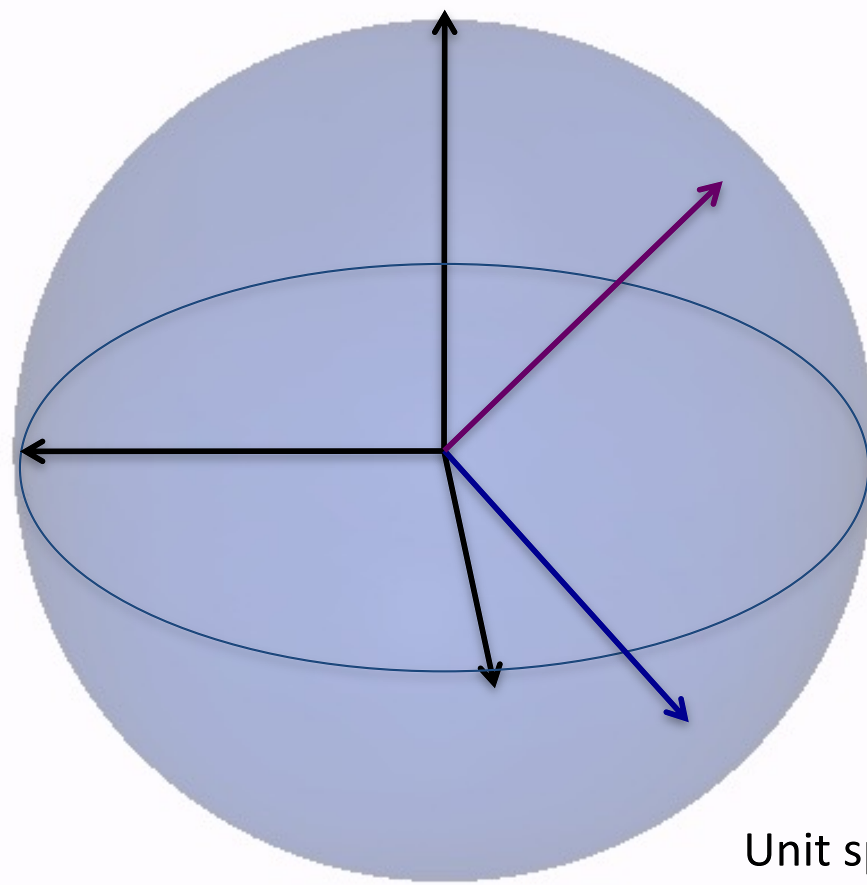
Given the coordinates (v_x, v_y, v_z) of vector **v** in the **black** coordinate system, what are its coordinates (v_x, v_y, v_z) in the **red** system?

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 (same) **black** system?



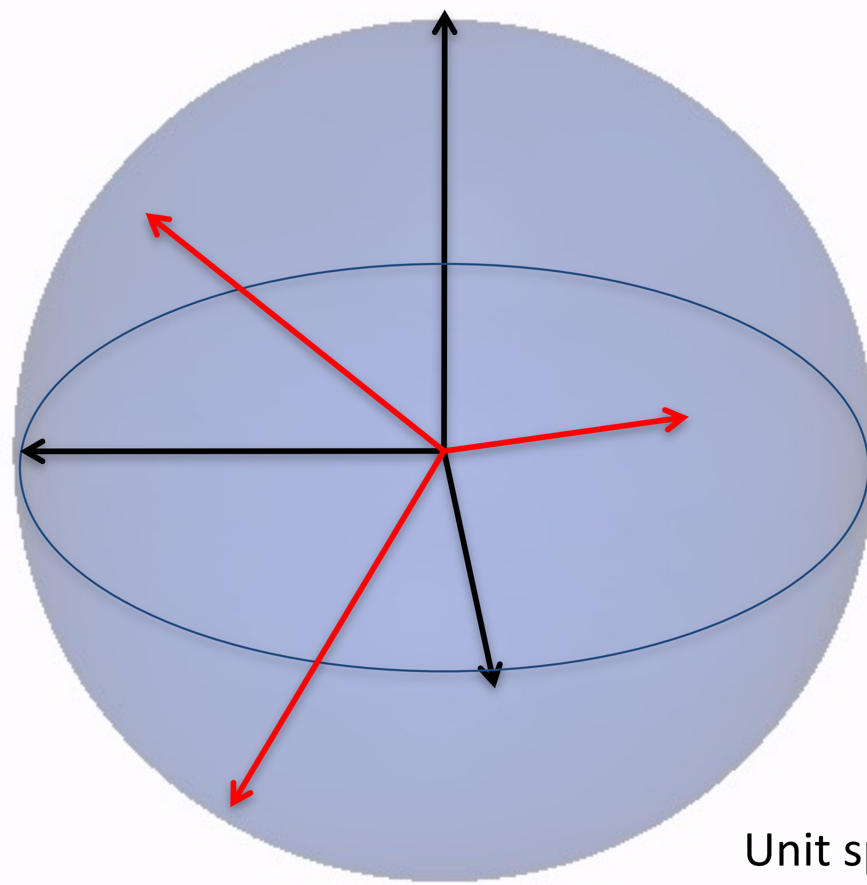
Unit sphere

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

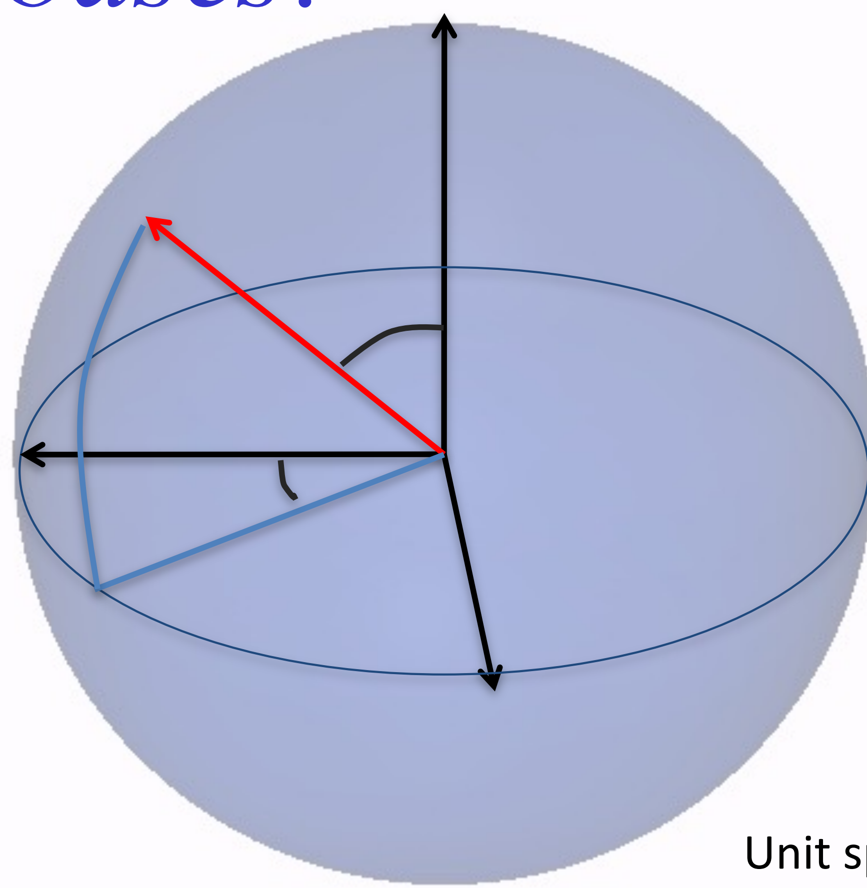
An orientation may be represented by the rotation required to transform from a specified reference orientation (sample axes)



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 $\mathbf{r}$



Unit sphere

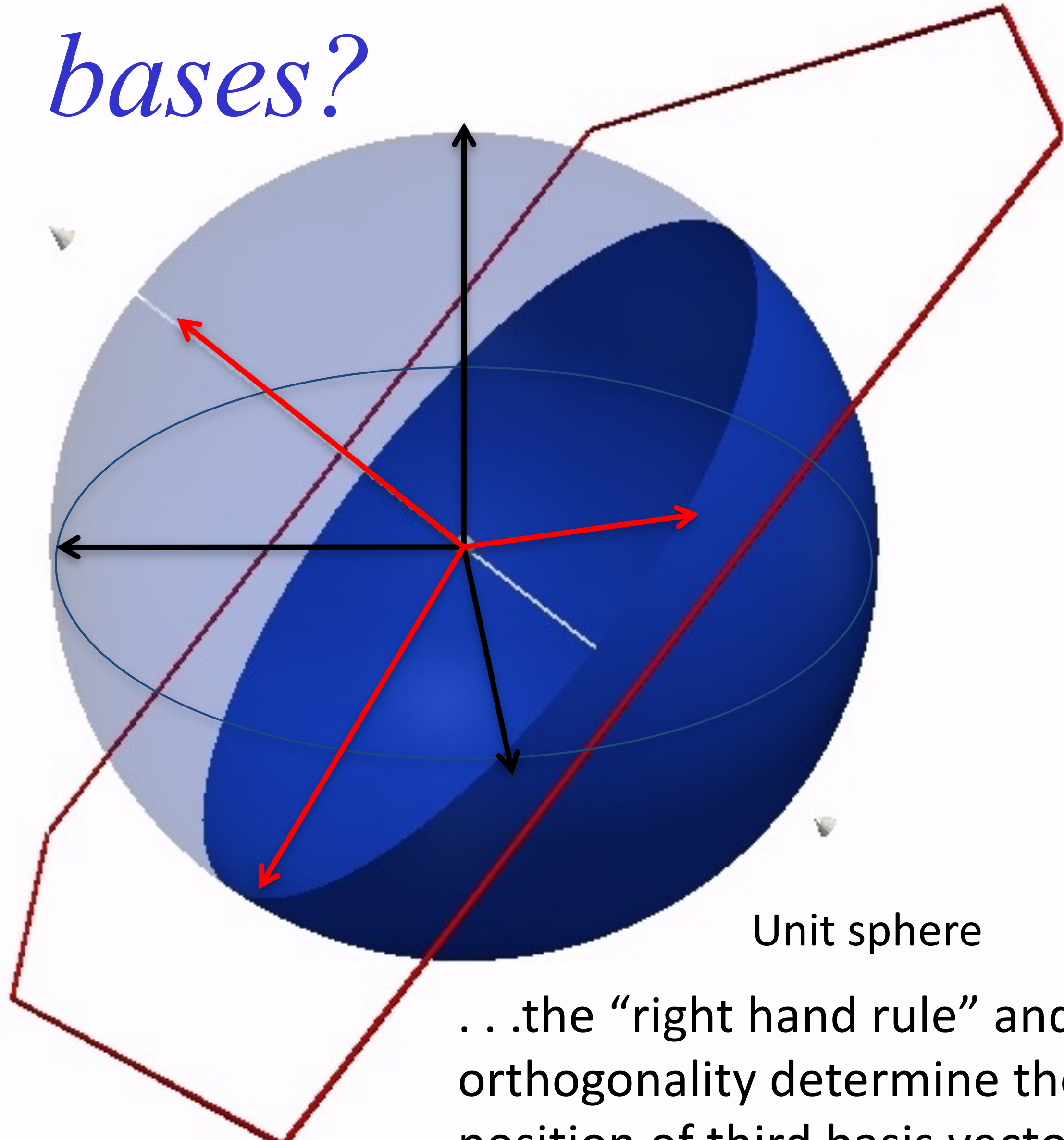
Two numbers related to the black system are needed to determine $\mathbf{r}$

(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 $\mathbf{r}$)

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

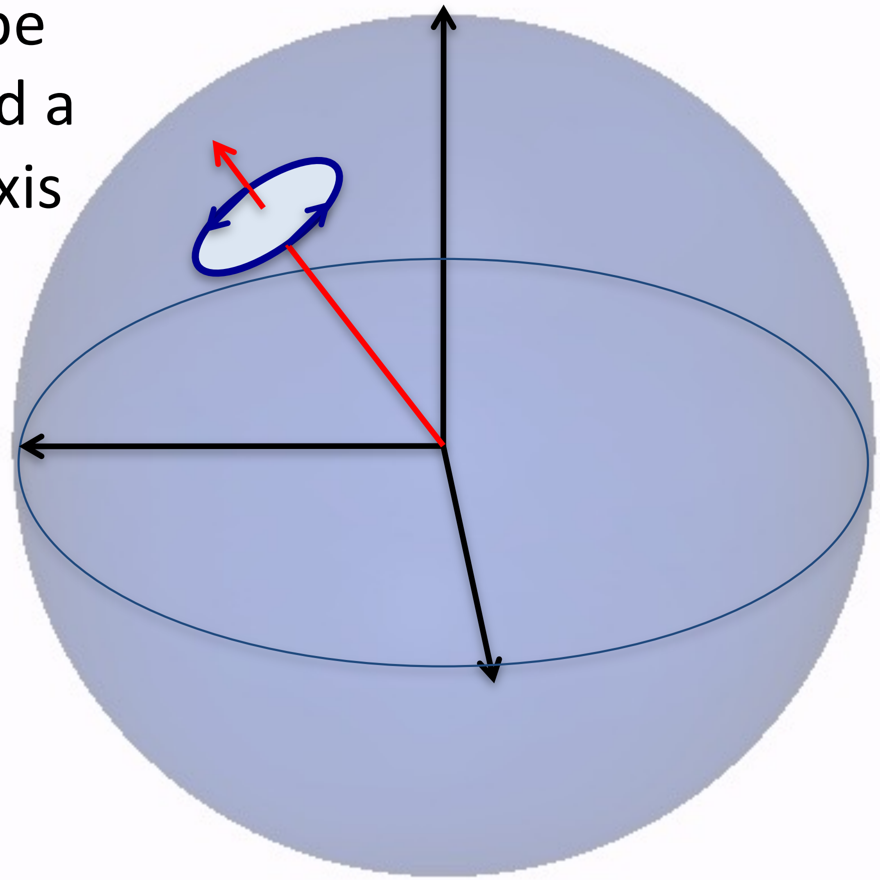
$$\mathcal{R}(\boldsymbol{r}, \alpha)$$

"axis-angle" representation

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

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

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.

O. Rodrigues. “Des lois géométriques qui régissent les déplacements d'un système solide dans l'espace, et de la variation des coordonnées provenant de ces déplacements considérés indépendamment des causes qui peuvent les produire”, *Journal de mathématiques pures et appliquées*, **5**, 380-440 (1840).

Axis-Angle from Matrix

The rotation axis, $\mathbf{r}$, 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.

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:

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

Example for the 12 entry:

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

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

NB. Morawiec's Eq. on p.22 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_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:

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

Multiplication of two quaternions

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

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

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≠qp).
[2] There are similarities to complex numbers (which correspond to rotations in 2D).
[3] The *first* rotation is on the *left* ("*p*", below) and the *second* ("*q*") is on the *right* (contrast with matrix multiplication).

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

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

Using more compact notation:
again, note the + in front of the vector product

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

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.

For two rotations q and p that share a single axis $\mathbf{r}$, note what happens when q (2nd) and p (1st) are composed or multiplied together:

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

A Quarternion & Its Negative

- It is the case that any given quaternion has a negative, -q, which represents the same rotation as q.
- This is easily understood in terms of the rotation axis n and angle, ω, and adding 2π to the angle, *i.e.*, going from (n, ω) to $(n, \omega + 2\pi)$.
- In practical terms, unit quaternions give us "double coverage" of proper rotations.
- In computation, one has to be careful about results from symmetry operations and conversions back to axis-angle and/or Rodrigues-Frank vectors.
- As discussed by Morawiec in his book, pp.38-39, there is a distinction in terms of direction of rotation that matters for angular momentum.

Quaternions as symmetry operators

- Here we recapitulate what we have studied elsewhere, namely the application of crystal and sample symmetry to orientations.
- With matrices, recall that a) each successive rotation left-multiplies its predecessor, and b) an orientation, g, describes a transformation from sample to crystal. Therefore a crystal symmetry operator goes on the left whereas a sample symmetry operator goes on the right.

$$g' = O_{crystal}\ g\ O_{sample}$$

- For quaternions there exists an exactly equivalent scheme, based on the definitions given already. For simplicity we show two separate compositions, one for sample symmetry, one for crystal.

$$g' = (g, O_{crystal})$$
$$g' = (O_{sample}, g)$$

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 0th 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.

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

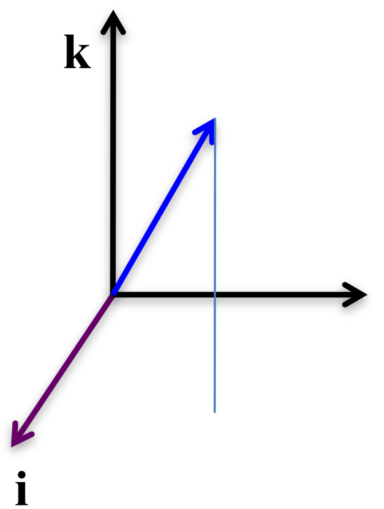
since

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

Remember that, within the system of passive rotations, applying the upper expression to a vector in sample space transforms it into crystal space (used for inverse pole figures); changing the sign in front of the vector product reverses the direction of the transformation (used in pole figures).

Example: Rotation of a Vector by Quaternion-Vector Multiplication

Consider rotating the vector $\boldsymbol{i}$ 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:

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

Conversions: matrix→quaternion

Formulae, due to Morawiec:

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

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

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

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

Note the coordination of choice of sign!

Conversions: matrix→quaternion

Formulae, from Rowenhorst *et al.*:

For the meaning of “P”, read the complete paper from the reference at the top.

In our case, P = +1

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- compute the quaternion components:

$$
\begin{aligned}
q_0 &= \frac{1}{2}\sqrt{1+\alpha_{11}+\alpha_{22}+\alpha_{33}}\,;\\
q_1 &= \frac{P}{2}\sqrt{1+\alpha_{11}-\alpha_{22}-\alpha_{33}}\,;\\
q_2 &= \frac{P}{2}\sqrt{1-\alpha_{11}+\alpha_{22}-\alpha_{33}}\,;\\
q_3 &= \frac{P}{2}\sqrt{1-\alpha_{11}-\alpha_{22}+\alpha_{33}}\,.
\end{aligned}
$$

- Modify the component signs if necessary:

$$
\begin{aligned}
q_1 &= -q_1 \quad \text{if} \quad \alpha_{32} < \alpha_{23};\\
q_2 &= -q_2 \quad \text{if} \quad \alpha_{13} < \alpha_{31};\\
q_3 &= -q_3 \quad \text{if} \quad \alpha_{21} < \alpha_{12}.
\end{aligned}
$$

- normalize the quaternion:

$$
q = \frac{q}{|q|}
$$

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