

Strained Boxes and Products of Three Vectors

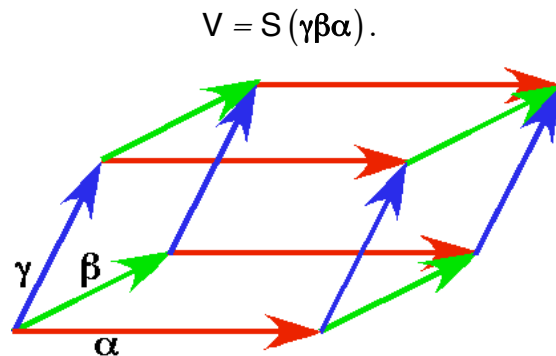
Strain

Strain in a medium may be assessed by examining the manner in which a cube of the unstrained material is distorted by forces within and outside the medium. In this essay, the strain takes two forms that will be called *volume strain* and *vector or rotational strain*. The two are components of a *strain quaternion*. The volume strain is a scalar and the vector strain is a vector. Orientation is expressed in terms of three orthogonal unit vectors that are constructed on the basis of the vector strain.

Consider a cube that is defined by three mutually orthogonal unit vectors $\{\alpha, \beta, \gamma\}$. To start with, let the unit vectors be $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$. We lose no generality by assuming that the unstressed box is aligned with the universal coordinates, because one can always change the orientation of a unit cubic box by rotation about an axis of rotation so as to bring it into alignment with the universal coordinates and such a change in orientation will not change the distortion due to strain. The actual values of the vectors will change with rotation, but the relationships between them will remain the same.

The vector triple product

If three vectors $\{\alpha, \beta, \gamma\}$ form the three edges of a parallelepiped, then the scalar part of their product $S(\gamma\beta\alpha)$ is equal to the volume of the parallelepiped.



The cube with edges $\alpha, \beta,$ and γ is strained into a parallelepiped in which the edges are rotated relative to each other and possibly compressed or lengthened, but they still enclose the same matrix, after the strain.

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We can illustrate this relationship in a special case by assigning the values of \mathbf{i} , \mathbf{j} , and \mathbf{k} to the vectors $\{\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}\}$. These vectors form the edges of a parallelepiped, therefore, they will be called **edge vectors**. This assignment describes a unit box oriented with its edge vectors aligned with the coordinate system's basis vectors. The triple vector product is easily computed.

$$\boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \mathbf{k} * \mathbf{j} * \mathbf{i} = -\mathbf{i} * \mathbf{i} = 1.0.$$

When the edge vectors are mutually orthogonal, the vector triple product is always a scalar. If we change the order of the vectors, the scalar may be either 1 or -1 . The order used here is a right-handed coordinate system in which the earlier listed vectors act upon the later vectors. In $\boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha}$, $\boldsymbol{\alpha}$ is multiplied by $\boldsymbol{\beta}$ and the product is multiplied by $\boldsymbol{\gamma}$. It is equally valid to choose the cyclic permutations $\boldsymbol{\beta}\boldsymbol{\alpha}\boldsymbol{\gamma}$ or $\boldsymbol{\alpha}\boldsymbol{\gamma}\boldsymbol{\beta}$ and there are situations when these permutations are more appropriate choices (see below). The complementary set of permutations in which the order is reversed, $\boldsymbol{\alpha}\boldsymbol{\beta}\boldsymbol{\gamma}$, $\boldsymbol{\beta}\boldsymbol{\gamma}\boldsymbol{\alpha}$, and $\boldsymbol{\gamma}\boldsymbol{\alpha}\boldsymbol{\beta}$, will yield triple vector products of -1 .

Since the choice of the vectors is arbitrary, except that they are mutually perpendicular unit vectors, this result is applicable to any three mutually perpendicular unit vectors. The result may be confirmed by rotating these vectors about arbitrary axes of rotation and computing the triple vector product. We will generally choose orderings that reflect a right hand coordinate system, so that the volume will be positive.

Volume Strain and Rotational Strain

It is readily seen that if the orthogonal edge vectors are not unit vectors, then the scalar of the product is the product of the lengths. This is what one would expect of an index of volume. If a unit box is distorted so that the edges remain perpendicular, but change in length, then the box experiences a strain. This is intuitive if we consider a box that is stretched so that one edge vector, say $\boldsymbol{\alpha}$, doubles in length while the others, $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$, remain unit vectors. The volume of the box doubles which is certainly a strain. Such a strain will be called a **volumetric strain**, symbolized by \mathbf{V} . Volume is clearly a scalar quantity, therefore the change in volume is a scalar.

The strain in this scenario is actually more complex than a volumetric strain. To see this, consider the following scenario. Suppose that one edge increases by a factor of 2.0, but the other two edges are reduced by a factor of $1/\sqrt{2} \approx 0.707$. The volume does not change, therefore

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there is no volumetric strain, but the box is clearly strained, because it is distorted relative to the original cubic box. In order to capture this strain we look at the relations between the three edge vectors, a feature reflected in the **diagonal vector** of the box, the sum of its edge vectors, $\delta = \alpha + \beta + \gamma$. The diagonal of the vector of the elongated box rotates relative to the diagonal vector of the original cubic box. This will be called **rotational strain** or **shear strain**.

There was also shear strain in the first example, where one edge doubled in length without the others changing, but it was combined with a volumetric strain. A third example illustrates that volumetric strain can also occur in isolation, one can have a volumetric strain without shear strain. Consider a box in which all three edge vectors double in length. The volume increases eight-fold, but there is no shear strain because the diagonal of the enlarged box is parallel with the diagonal of the original, unstrained, box. The full analysis of the original example, where both types of strain occur, will be developed further below.

Uniform and Directional Strain

The first example was an instance of a **directional strain** and the last example is an instance of **uniform** or **isomorphic strain**. Fundamentally, the difference between the uniform expansion and directional expansion is that with uniform expansion or contraction, no matter how we choose the box edges, they remain orthogonal after the strain. With the directional expansion, the box edges remain orthogonal only if we choose them to lie parallel with the directions of expansion or contraction. If the triple vector product, that is, the strain quaternion, is a scalar quaternion after the strain, then the axes are aligned with the directions of expansion and contraction. Any other choice of box edges will experience a shear strain, that is, their triple vector product will have a vector component, therefore be a quaternion.

In the first example we got a nil rotation component because we happened to choose an arrangement of edge vectors that did not change direction with the strain. The relationships between the directions of the edge vectors were unchanged by the strain, they remained mutually orthogonal. Almost any other choice of edge vectors, other than a permutation of the edge vectors, will yield a squashed box after the strain. That can be observed by choosing the following edge vectors.

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$$\boldsymbol{\alpha} = \frac{\mathbf{i} + \mathbf{k}}{\sqrt{2}}, \quad \boldsymbol{\beta} = \mathbf{j}, \quad \boldsymbol{\gamma} = \frac{-\mathbf{i} + \mathbf{k}}{\sqrt{2}}.$$

Multiplying the \mathbf{i} components by 2 and leaving the other components alone and then multiplying out in the vector triple product yields the following.

$$\boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \frac{-2\mathbf{i} + \mathbf{k}}{\sqrt{2}} * \mathbf{j} * \frac{2\mathbf{i} + \mathbf{k}}{\sqrt{2}} = 2 - \frac{3}{\sqrt{2}}\mathbf{j}.$$

Clearly, the first and last components of the product are not mutually perpendicular after the strain and that is reflected in the vector component of the strain quaternion, which indicates that they have rotated about an axis of rotation in the \mathbf{j} direction. If we compute the angle of the strain quaternion, it is -36.87° . The strain of the two axes that each lie at a 45° angle to the axis of elongation is an opening of 36.87° , so that after the strain they have an angle of $90^\circ + 36.87^\circ = 126.87^\circ$ between them. That can be checked by taking the ratio of the two strained axes.

We can always find a box that experiences only volumetric strain by choosing one edge so that it lies parallel with the direction of expansion or contraction and a second edge parallel with the orthogonal strain. Such a box is conceptually straightforward to construct. In the situation that we have just been considering, there is only the one strain, the stretching along the \mathbf{i} axis. Any box that has one axis along the \mathbf{i} axis will experience a volume strain with nil shear.

Because of the symmetry of the $\boldsymbol{\alpha}$ and $\boldsymbol{\gamma}$ axes relative to the axis of strain their distortions cancel out and the diagonal is the same as for the unstrained box, namely $\{1, 1, 1\}$. However, if we choose a unstrained box that is the original cubic box rotated 45° about the diagonal of the box, then the diagonal of the strained box is not the same as for the unstrained box. The unstrained box is given by the following edge vectors.

$$\begin{aligned} \boldsymbol{\alpha} &= 0.804738\mathbf{i} + 0.505879\mathbf{j} - 0.310617\mathbf{k}, \\ \boldsymbol{\beta} &= -0.310617\mathbf{i} + 0.804738\mathbf{j} + 0.505879\mathbf{k}, \\ \boldsymbol{\gamma} &= 0.505879\mathbf{i} - 0.310617\mathbf{j} + 0.804738\mathbf{k}. \end{aligned}$$

The strained box is given by the following edge vectors.

$$\begin{aligned} \boldsymbol{\alpha} &= 1.60948\mathbf{i} + 0.505879\mathbf{j} - 0.310617\mathbf{k}, \\ \boldsymbol{\beta} &= -0.621234\mathbf{i} + 0.804738\mathbf{j} + 0.505879\mathbf{k}, \\ \boldsymbol{\gamma} &= 1.01176\mathbf{i} - 0.310617\mathbf{j} + 0.804738\mathbf{k}. \end{aligned}$$

The diagonal of the unstrained box is $\{1, 1, 1\}$ and the diagonal of the strained box is $\{2, 1, 1\}$. The difference between the diagonals is in the \mathbf{i} direction. So, one axis should be in the \mathbf{i}

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direction. In this case, we can see that the other two axes may be in any direction that is orthogonal to the \mathbf{i} axis, since there is neither expansion or contraction in any other direction.

The general procedure is straight-forward. Choose an arbitrary cubic box and allow it to experience the strain. The difference between the diagonal of the original cubic unit box and its strained configuration is the direction of the first box edge for the box that has a scalar strain quaternion. The two axes orthogonal to the first edge are arbitrarily chosen to give a second cubic box with one edge parallel with the direction of strain which was just determined. Let us call this the intermediate box. The intermediate box is now strained. The diagonal of the strained intermediate box will be in the right cone that is symmetrical about the first axis of strain, but, unless we were especially clever in our choice of the other two axes, the projection of the diagonal upon the plane orthogonal to the first edge will generally be changed by the strain. We compute the difference between the projected cubic box diagonal and the squashed box diagonal and we let one of the remaining box edges be parallel with that difference. The difference between the projected diagonals will be the direction of the second box edge. The third box edge is orthogonal to the first two edges, therefore it is determined, give or take a minus sign, depending upon whether one is using a right-handed or left handed coordinate system and the order of the other two edge vectors.

This procedure guarantees that any strain may be expressed as a volumetric strain and a frame that is not sheared by the strain. The volumetric strain is the same no matter how we choose the frame, but the shear strain is contingent upon the test frame that is chosen.

Boxes With Non-Orthogonal Edge Vectors

If the edge vectors are not mutually orthogonal, then the vector triple product is always a quaternion and the scalar of that quaternion is the volume of the parallelepiped, $\mathbf{S}(\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma})$. One can easily confirm this by substitution of non-orthogonal edge vectors into the expression for the vector triple product. From here on, we will consider the implications of triple vector products of non-orthogonal vectors. This means that we will be considering non-uniform contractions and/or expansions. If the matrix is incompressible or and/or inextensible, then expansion in one direction must lead to contraction in another.

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The vector component of the vector triple product is also interesting. We can see something of its nature by considering a few examples.

Example 1.

Let $\alpha = \mathbf{i}$, $\beta = \mathbf{j}$ and $\gamma = \frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}}$. The third edge vector is the unit vector of the diagonal of a unit cubic box. The strain quaternion is as follows.

$$\begin{aligned} \Psi &= \mu + \zeta = \text{volume strain scalar} + \text{shear strain vector} \\ &= \frac{(\mathbf{i} + \mathbf{j} + \mathbf{k})}{\sqrt{3}} * \mathbf{j} * \mathbf{i} = \frac{\mathbf{1} - \mathbf{i} + \mathbf{j}}{\sqrt{3}} \\ &= \frac{\mathbf{1}}{\sqrt{3}} + \frac{\sqrt{2}}{\sqrt{3}} \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}} \\ &= \cos \phi + \sin \phi \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}} ; \phi = 54.7356^\circ . \end{aligned}$$

The new volume, $S(\alpha, \beta, \gamma)$, is $1/\sqrt{3} = 0.57735$ and the vertical vector, γ , is tilted forward 54.7356° relative to the perpendicular to the $\alpha\beta$ plane about an axis of rotation that is parallel with $-\mathbf{i} + \mathbf{j}$.

The third edge vector, γ , is a unit vector in the direction of the diagonal of a unit cube, which is a useful object when studying strain (see below). The diagonal of a unit cube stands at the same angle to each of the edge vectors, namely 54.7356° . Because it keeps turning up in calculations this angle will given a special symbol designator, τ .

$$\tau = 0.955317 \text{ radians} = 54.7356^\circ$$

The Strain Frame

The unit vector perpendicular to the $\alpha\beta$ plane is designated by the symbol ρ and the axis of rotation for the γ component relative to ρ is the unit vector designated by the symbol σ . The vectors are perpendicular to each other because ρ is perpendicular to the $\alpha\beta$ -plane and σ is perpendicular to the plane determined by ρ and γ . Consequently, σ lies in the $\alpha\beta$ plane.

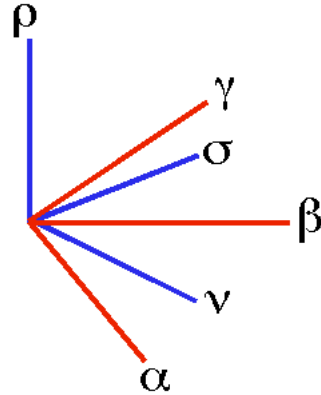
$$\rho = \mathcal{UN}\left[\begin{array}{c} \beta \\ \alpha \end{array}\right] \text{ and } \sigma = \mathcal{UN}\left[\begin{array}{c} \gamma \\ \rho \end{array}\right].$$

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We can complete the frame by computing the perpendicular to the plane determined by $\boldsymbol{\rho}$ and $\boldsymbol{\sigma}$.

$$\mathbf{v} = \mathcal{UN}\left[\frac{\boldsymbol{\sigma}}{\boldsymbol{\rho}}\right].$$

The first component of the frame, $\boldsymbol{\rho}$, is the unit vector parallel to the axis of rotation that turns $\boldsymbol{\alpha}$ into $\boldsymbol{\beta}$. The second component, $\boldsymbol{\sigma}$, is parallel to the axis of rotation that turns $\boldsymbol{\rho}$ into $\boldsymbol{\gamma}$ and it is always in the plane determined by $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$. Consequently, these two vectors and their right-handed mutual perpendicular, \mathbf{v} , form an orientation frame for the vector triplet $[\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}]$. If we take the two vectors $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$ in that order, then the right hand mutually orthogonal vector is the ratio of $\boldsymbol{\rho}$ to $\boldsymbol{\sigma}$.



The non-orthogonal strained vector set $\{\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}\}$ is resolved into the orthogonal strain frame $\{\mathbf{v}, \boldsymbol{\sigma}, \boldsymbol{\rho}\}$.

We can readily compute $\boldsymbol{\rho}, \boldsymbol{\sigma}$, and \mathbf{v} , for the present situation, where the edge vectors are

$$\boldsymbol{\alpha} = \mathbf{i}, \quad \boldsymbol{\beta} = \mathbf{j} \quad \text{and} \quad \boldsymbol{\gamma} = \frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}}.$$

$$\boldsymbol{\rho} = \boldsymbol{\beta}\boldsymbol{\alpha}^{-1} = \mathcal{UN}[\mathbf{j} * -\mathbf{i}] = \mathbf{k};$$

$$\boldsymbol{\sigma} = \mathcal{UN}\left[\frac{(\mathbf{i} + \mathbf{j} + \mathbf{k})}{\sqrt{3}} * -\mathbf{k}\right] = \mathcal{UN}\left[\frac{1 - \mathbf{i} + \mathbf{j}}{\sqrt{3}}\right] = \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}};$$

$$\mathbf{v} = \mathcal{UN}\left[-\mathbf{k} * \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}}\right] = \frac{\mathbf{i} + \mathbf{j}}{\sqrt{2}}.$$

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The strain frame is not symmetric in that it gives a special value to the α, β -plane and its perpendicular or normal vector, ρ . Still, it can be viewed as an orientation frame in that it generally gives a unique orthogonal frame to a set of strained vectors.

The case of $\alpha \perp \beta$

Let us consider the general situation where the α and β vectors are unit vectors that remain perpendicular, but the unit vector γ is not perpendicular to their plane. The product of α and β is the vector perpendicular to the α, β -plane that turns α into β , that is ρ . The vector product of the three unit vectors is $-\gamma\rho$.

$$\psi = -\gamma\rho = \frac{\gamma}{\rho} = \cos\phi + \sin\phi\sigma; \quad \text{where } \rho = \frac{\alpha\beta}{T(\alpha)T(\beta)}, |\sigma| = 1.0, \text{ and } \sigma \perp \gamma, \rho.$$

The angle ϕ is the angle between the ρ and γ vectors. If α , β , and γ are not unit vectors, then the general formula is as follows.

$$\psi = -\gamma\rho = |\gamma|*|\beta|*|\alpha|*[\cos\phi + \sin\phi\sigma].$$

In the formalism of vector analysis and with arbitrary length vectors, ψ is given by the following expression.

$$\psi = \gamma\beta\alpha = -\gamma \cdot [\beta \times \alpha] + \gamma \times [\beta \times \alpha].$$

ψ is a quaternion. The scalar of that quaternion, when α , β , and γ are unit vectors, is $\cos\phi$. The unit vector σ is perpendicular to both γ and ρ ; consequently, it lies in the plane of α and β , perpendicular to the plane of γ and ρ . The angle ϕ is the angle between γ and ρ in their plane. If all the edge vectors are unit vectors, then the strain quaternion is a unit quaternion, $T(\psi) = 1.0$.

The vector σ is the axis of rotation for the shear that rotates the perpendicular to the base (ρ) relative to the base (the α, β -plane). Therefore, in the instance of shear in one plane, the vector component of the triple vector product quaternion, ψ , gives one the axis of rotation of the shear, σ .

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If we return to the example above and retain α and β as \mathbf{i} and \mathbf{j} , respectively, and change γ to $\frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}}$, then the strain quaternion is readily computed.

$$\psi = \frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}} * \mathbf{j} * \mathbf{i} = \frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}} * -\mathbf{k} = \frac{1}{\sqrt{3}} + \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{3}}.$$

The perpendicular to the α, β -plane is $\rho = \mathbf{k}$ and the vector of the shear rotation quaternion is $\sigma = \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}}$. One can tell by inspection that these are the correct values for the two vectors. If we take the value of the sine from the expression, it is possible to compute the angle of the shear.

$$\begin{aligned} \sin \phi &= \frac{\sqrt{2}}{\sqrt{3}} = \frac{1.41421}{1.73205} = 0.816497, \\ \phi &= 54.7356^\circ = \tau. \end{aligned}$$

We find that the strain in this scenario (\mathcal{S}) is composed of a volumetric strain and a shear strain.

$$\mathcal{S} = \frac{\psi}{|\alpha||\beta||\gamma|} = \cos \phi + \sin \phi \sigma.$$

The case of $\gamma \perp \alpha, \beta$

The case where α is not perpendicular to β , but γ is perpendicular to their plane is another interesting case to consider. The third edge vector is perpendicular to α and β , therefore $\phi = 0.0$ and it is aligned with the vector ρ . The principal factor in the shear is that the perpendicular is reduced by $\sin \theta$, where θ is the angle between α and β when α is turned into β .

$$\begin{aligned} \frac{\beta}{\alpha} &= \beta \alpha^{-1} = \cos \theta + \sin \theta \rho; \\ \beta &= \frac{\beta}{\alpha} * \alpha = \cos \theta \alpha + \sin \theta \rho * \alpha. \end{aligned}$$

The product of β and α is easily written.

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$$\beta\alpha = \frac{\beta}{-\alpha} = \frac{(\alpha \cos\theta + \sin\theta \rho * \alpha)}{-\alpha}$$

$$\text{and } \frac{\alpha}{-\alpha} = -T(\alpha)^2, \text{ thus}$$

$$\beta\alpha = -T(\alpha)^2(\cos\theta + \sin\theta\rho).$$

Since α and β are normally taken to be unit vectors, the tensor is usually unity and thus the vector part of the expression reduces to the negative of ρ times the sine of the angle between the vectors.

The third edge vector, γ , is aligned with the perpendicular, ρ , therefore the triple vector product may be written down.

$$\begin{aligned} \gamma\beta\alpha &= -c\tilde{\rho} * T(\alpha)^2(\cos\theta + \sin\theta\tilde{\rho}) \\ &= -c * T(\alpha)^2\tilde{\rho}(\cos\theta + \sin\theta\tilde{\rho}) \\ &= -c * T(\alpha)^2(\cos\theta\tilde{\rho} - \sin\theta) \\ &= c * T(\alpha)^2(\sin\theta - \cos\theta\tilde{\rho}) \end{aligned}$$

If the edge vectors are all unit vectors, then the expression for the strain reduces to the expected value. The volumetric strain is the sine of the angle between α and β and the shear strain is the cosine of the angle times the negative perpendicular to the α, β -plane.

$$S = \frac{\gamma\beta\alpha}{cT(\alpha)} = \sin\theta - \cos\theta\rho$$

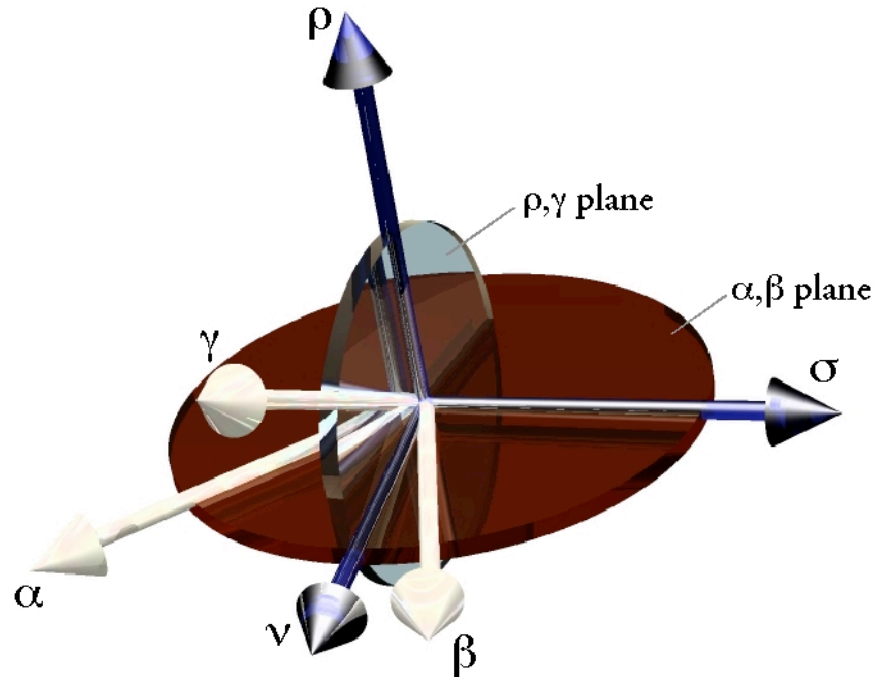
We can illustrate this strain by allowing the strained box to have the edge vectors $\alpha = \mathbf{i}$, $\beta = \cos\theta\mathbf{i} + \sin\theta\mathbf{j}$, and $\gamma = \mathbf{k}$. The volume quaternion is readily calculated.

$$\gamma\beta\alpha = \mathbf{k} * (\cos\theta\mathbf{i} + \sin\theta\mathbf{j}) * \mathbf{i} = \sin\theta - \cos\theta\mathbf{k}$$

Note that the σ and ν vectors are undefined in this situation, because there are an infinity of possible candidates. Any vector in the α, β -plane is valid σ since γ is aligned with ρ and therefore there is no specific rotation that rotates one into the other. The solution is in fact the null vector. Since σ is the null vector, ν is also undefined. Consequently, we cannot define a strain frame. However, if we reassign the vectors, so that the β edge is viewed as tilted relative to

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the α, γ plane plane, then it is possible to construct a frame using the same analysis as in the previous section.



The strain frame. The vector set $\{\alpha, \beta, \gamma\}$ is distorted by strain. The rotation axis for α into β is ρ , which is perpendicular to the $\alpha\beta$ plane (red disc) and the rotation axis for ρ into γ is σ , which is perpendicular to the $\rho\gamma$ plane (transparent). The frame is completed by the rotation axis for σ into ρ about the vector \mathbf{v} .

No mutually orthogonal edges

In each of these first two situations, there is a single axis of rotation and the strain quaternion could be expressed in terms of that axis of rotation. We now consider the situation in which none of the edge vectors is perpendicular to any of the other edge vectors.

It has already been established that $\beta\alpha$ can be written in terms of ρ .

$$\begin{aligned}\beta\alpha &= (\cos\theta\alpha + \sin\theta\rho*\alpha)*\alpha \\ &= -T(\alpha)^2(\cos\theta + \sin\theta\rho).\end{aligned}$$

The third edge, γ , can be written in terms of ρ and σ .

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$$\frac{\boldsymbol{\gamma}}{\boldsymbol{\rho}} = \mathbb{T}(\boldsymbol{\gamma})(\cos\phi + \sin\phi\boldsymbol{\sigma}) \Leftrightarrow \boldsymbol{\gamma} = \mathbb{T}(\boldsymbol{\gamma})(\cos\phi + \sin\phi\boldsymbol{\sigma})\boldsymbol{\rho}.$$

These expressions can be combined to give the triple vector product.

$$\begin{aligned} \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} &= -\mathbb{T}(\boldsymbol{\gamma})(\cos\phi + \sin\phi\boldsymbol{\sigma})\boldsymbol{\rho} * \mathbb{T}(\boldsymbol{\alpha})^2(\cos\theta + \sin\theta\boldsymbol{\rho}), \\ &= -\mathbb{T}(\boldsymbol{\gamma})\mathbb{T}(\boldsymbol{\alpha})^2(\cos\phi + \sin\phi\boldsymbol{\sigma})\boldsymbol{\rho} * (\cos\theta + \sin\theta\boldsymbol{\rho}), \\ &= -\mathbb{T}(\boldsymbol{\gamma})\mathbb{T}(\boldsymbol{\alpha})^2(\cos\phi + \sin\phi\boldsymbol{\sigma})(\cos\theta\boldsymbol{\rho} + \sin\theta\boldsymbol{\rho} * \boldsymbol{\rho}), \\ &= -\mathbb{T}(\boldsymbol{\gamma})\mathbb{T}(\boldsymbol{\alpha})^2(\cos\phi + \sin\phi\boldsymbol{\sigma})(-\sin\theta + \cos\theta\boldsymbol{\rho}), \\ &= -\mathbb{T}(\boldsymbol{\gamma})\mathbb{T}(\boldsymbol{\alpha})^2[-\cos\phi\sin\theta + \cos\phi\cos\theta\boldsymbol{\rho} - \sin\phi\sin\theta\boldsymbol{\sigma} + \sin\phi\cos\theta\boldsymbol{\sigma}\boldsymbol{\rho}], \\ &= -\mathbb{T}(\boldsymbol{\gamma})\mathbb{T}(\boldsymbol{\alpha})^2[-\cos\phi\sin\theta + \cos\phi\cos\theta\boldsymbol{\rho} - \sin\phi\sin\theta\boldsymbol{\sigma} - \sin\phi\cos\theta\boldsymbol{v}]. \end{aligned}$$

The vector \boldsymbol{v} was defined to be a unit vector that completed the right-handed strain frame with $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$, in that order, so that $\boldsymbol{\sigma}\boldsymbol{\rho} = -\boldsymbol{v}$.

If we assume that the three edge vectors are unit vectors, then the expression simplifies to the following expression.

$$\boldsymbol{\psi} = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \cos\phi\sin\theta - \cos\phi\cos\theta\boldsymbol{\rho} + \sin\phi\sin\theta\boldsymbol{\sigma} + \sin\phi\cos\theta\boldsymbol{v}.$$

We can use trigonometric identities to rewrite the strain quaternion in terms of the internal angles. Since

$$\begin{aligned} \sin(\vartheta - \varphi) &= \sin\vartheta\cos\varphi - \cos\vartheta\sin\varphi \Rightarrow \\ \sin\left(\frac{\pi}{2} - \phi\right) &= \sin\bar{\phi} = \sin\frac{\pi}{2}\cos\phi - \cos\frac{\pi}{2}\sin\phi = \cos\phi. \\ \cos(\vartheta - \varphi) &= \cos\vartheta\cos\varphi + \sin\vartheta\sin\varphi \Rightarrow \\ \cos\left(\frac{\pi}{2} - \phi\right) &= \cos\bar{\phi} = \cos\frac{\pi}{2}\cos\phi + \sin\frac{\pi}{2}\sin\phi = \sin\phi. \end{aligned}$$

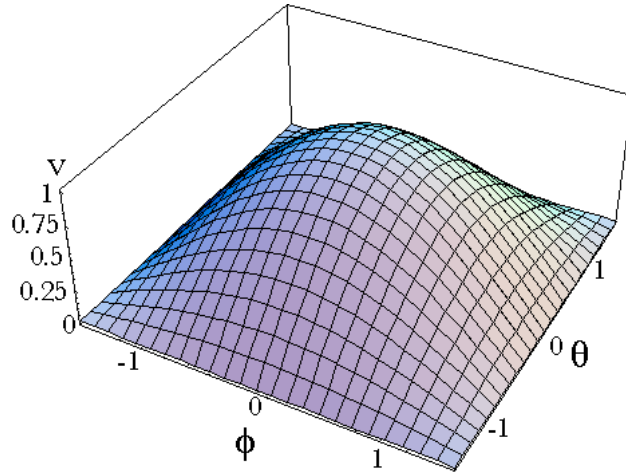
it follows that

$$\boldsymbol{\psi} = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \sin\bar{\phi}\sin\theta - \sin\bar{\phi}\cos\theta\boldsymbol{\rho} + \cos\bar{\phi}\sin\theta\boldsymbol{\sigma} + \cos\bar{\phi}\cos\theta\boldsymbol{v}.$$

The strain quaternion has been expressed as a function of the basis vectors of the strain frame and the angular excursions of the two strains. The volumetric strain is the product of the two component volumetric strains, which is what one would expect. The approximation of the $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ vectors changes the volume in proportion to the sine of the angle between them and the

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tilting of the vertical vector changes the volume in proportion to the cosine of the angle it forms with the vertical unit vector.



The volumetric strain is a function of both interior angles.

The combined axis of rotation is dependent upon the relative magnitudes of the angular excursions. It also tends to be directed more nearly in the axis of the compression as the axes become more approximated. The ρ, σ -plane is the plane from which the axes diverge and \mathbf{v} is the axis towards which they converge. This can be more easily appreciated if we normalize on the \mathbf{v} component and replace the tilt of γ relative to the vertical with the interior angle, $\bar{\phi} = \frac{\pi}{2} - \phi$. The more the edges converge, the proportionately greater the \mathbf{v} component becomes. For small amounts of convergence (θ and $\bar{\phi}$ approximately at right angles), the \mathbf{v} component is relatively small.

$$\begin{aligned} \frac{\gamma\beta\alpha}{\cos\bar{\phi}\cos\theta} &= \frac{\sin\bar{\phi}\sin\theta}{\cos\bar{\phi}\cos\theta} - \frac{\sin\bar{\phi}}{\cos\bar{\phi}}\rho + \frac{\sin\theta}{\cos\theta}\sigma + \mathbf{v}, \quad \bar{\phi} = \frac{\pi}{2} - \phi, \\ &= \tan\bar{\phi}\tan\theta - \tan\bar{\phi}\rho + \tan\theta\sigma + \mathbf{v}. \end{aligned}$$

Put in other words, as the cubic box becomes more distorted the volume shrinks and the \mathbf{v} vector becomes longer. The ρ and σ vectors become shorter.

Given the strain rotations of a cubic box, one can write down the strain quaternion, ψ . The strain quaternion allows one to compute the three edges of the distorted box.

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The Inversion of the Generalized Strain Quaternion

We have explored the calculation of the strain quaternion in the case where 1.) all the edge vectors are orthogonal, 2.) the case when the first and second edge vectors are not orthogonal, 3.) the case where the third component is not orthogonal to the first two, and 4.) the case where none of the vectors are orthogonal to any other edge vectors. The strain vector for the first case is the null vector. The second and third cases give $\boldsymbol{\rho}$ and $\boldsymbol{\sigma}$, respectively, as their strain vectors. In those cases it is straight forward to determine the axis of rotation and the angular excursion between the edge vectors.

$$\boldsymbol{\psi}_2 = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \sin\theta - \cos\theta \boldsymbol{\rho}.$$

$$\boldsymbol{\psi}_3 = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \sin\bar{\phi} + \cos\bar{\phi} \boldsymbol{\sigma}.$$

The expression for the strain quaternion in the fourth case is more difficult in that there is interaction between the angular excursions between the vectors, so that all components of the vector component of the strain quaternion are functions of both angles and it is necessary to introduce a third basis vector to the frame.

$$\boldsymbol{\psi} = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \sin\bar{\phi}\sin\theta - \sin\bar{\phi}\cos\theta\boldsymbol{\rho} + \cos\bar{\phi}\sin\theta\boldsymbol{\sigma} + \cos\bar{\phi}\cos\theta\boldsymbol{\nu}.$$

When the strain quaternion is computed for the fourth case the expression is going to be in terms of $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$, instead of $\{\boldsymbol{\rho}, \boldsymbol{\sigma}, \boldsymbol{\nu}\}$. However, once we have computed the three orientation frame vectors, it is simply a matter of computing the projection of the strain vector upon each frame vector.

$$\boldsymbol{\chi}_s = S(\boldsymbol{\psi}); \quad \boldsymbol{\chi}_\rho = S(\mathcal{V}(\boldsymbol{\psi}) * \boldsymbol{\rho}); \quad \boldsymbol{\chi}_\sigma = S(\mathcal{V}(\boldsymbol{\psi}) * \boldsymbol{\sigma}); \quad \boldsymbol{\chi}_\nu = S(\mathcal{V}(\boldsymbol{\psi}) * \boldsymbol{\nu}).$$

$$\boldsymbol{\chi}_s = S(\boldsymbol{\psi}); \quad \boldsymbol{\chi}_\rho = \mathcal{V}(\boldsymbol{\psi}) \circ \boldsymbol{\rho}; \quad \boldsymbol{\chi}_\sigma = \mathcal{V}(\boldsymbol{\psi}) \circ \boldsymbol{\sigma}; \quad \boldsymbol{\chi}_\nu = \mathcal{V}(\boldsymbol{\psi}) \circ \boldsymbol{\nu}.$$

Then, we can write the strain quaternion as follows.

$$\boldsymbol{\psi} = \boldsymbol{\gamma}\boldsymbol{\beta}\boldsymbol{\alpha} = \boldsymbol{\chi}_s - \boldsymbol{\chi}_\rho \boldsymbol{\rho} + \boldsymbol{\chi}_\sigma \boldsymbol{\sigma} + \boldsymbol{\chi}_\nu \boldsymbol{\nu}.$$

Given this quaternion, we can write down four equations that allow one to determine the values of θ and ϕ .

Vector Triple Products

$$\begin{aligned}
 \sin \bar{\phi} \sin \theta - \sin \bar{\phi} \cos \theta \rho + \cos \bar{\phi} \sin \theta \sigma + \cos \bar{\phi} \cos \theta \nu &= \chi_s - \chi_\rho \rho + \chi_\sigma \sigma + \chi_\nu \nu ; \\
 \sin \bar{\phi} \sin \theta &= \chi_s , \\
 \sin \bar{\phi} \cos \theta &= \chi_\rho , \\
 \cos \bar{\phi} \sin \theta &= \chi_\sigma , \\
 \cos \bar{\phi} \cos \theta &= \chi_\nu .
 \end{aligned}$$

These equations lead directly to the values of θ and ϕ .

$$\begin{aligned}
 \tan \theta &= \frac{\chi_s}{\chi_\rho} \Rightarrow \theta = \tan^{-1} \frac{\chi_s}{\chi_\rho} , \\
 \tan \bar{\phi} &= \frac{\chi_s}{\chi_\sigma} \Rightarrow \bar{\phi} = \tan^{-1} \frac{\chi_s}{\chi_\sigma} .
 \end{aligned}$$

Consequently, the angular excursion about the ρ axis that carries α into β is θ and the angular excursion about the σ axis that carries γ into the α, β -plane is $\bar{\phi}$. The angle between ρ and γ is $\frac{\pi}{2} - \bar{\phi} = \phi$. Therefore, there is a fairly direct calculation that allows one to extract the angular excursions for both distortions, given the strain quaternion for the generalized distortion.

An Example

Let us consider an example that utilizes these observations. The box $\{\alpha, \beta, \gamma\}$ is distorted into the box $\left\{ \alpha, \frac{\alpha + \beta}{\sqrt{2}}, \frac{\alpha + \beta + \gamma}{\sqrt{3}} \right\}$. The strain quaternion is readily computed.

$$\psi = \frac{1}{\sqrt{6}}(1 - 2\mathbf{i} - \mathbf{k}) ; \alpha = \mathbf{i}, \beta = \mathbf{j}, \gamma = \mathbf{k} .$$

We lose no generality in substituting \mathbf{i} , \mathbf{j} , and \mathbf{k} for the cube's edge vectors, because any cube can be rotated and translated to bring it into alignment with the basis vectors. Rotation and translation do not change strain.

The ρ vector is obviously \mathbf{k} in this situation. The σ vector is the unit vector of the ratio of $\frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\sqrt{3}}$ to \mathbf{k} .

Vector Triple Products

$$\boldsymbol{\sigma} = \frac{\mathbf{i} + \mathbf{j} + \mathbf{k}}{\mathbf{k}} = \frac{(\mathbf{i} + \mathbf{j} + \mathbf{k})}{\sqrt{3}} * -\mathbf{k} = \frac{1 - \mathbf{i} + \mathbf{j}}{\sqrt{3}},$$

$$\mathbf{u}\mathcal{V}(\boldsymbol{\sigma}) = \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}}.$$

The \mathbf{v} component is the ratio of $\boldsymbol{\rho}$ to $\boldsymbol{\sigma}$.

$$\frac{\boldsymbol{\rho}}{\boldsymbol{\sigma}} = \mathbf{k} * \frac{\mathbf{i} - \mathbf{j}}{\sqrt{2}} = \frac{\mathbf{i} + \mathbf{j}}{\sqrt{2}}.$$

We can compute the projections of the vector component of the strain quaternion upon these frame vectors. We start with the equations from above.

$$\begin{aligned} \chi_s &= \mathbf{S}(\boldsymbol{\psi}); & \chi_\rho &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \boldsymbol{\rho}); & \chi_\sigma &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \boldsymbol{\sigma}); & \chi_v &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \mathbf{v}). \\ \chi_s &= \mathbf{S}(\boldsymbol{\psi}); & \chi_\rho &= \mathbf{V}(\boldsymbol{\psi}) \circ \boldsymbol{\rho}; & \chi_\sigma &= \mathbf{V}(\boldsymbol{\psi}) \circ \boldsymbol{\sigma}; & \chi_v &= \mathbf{V}(\boldsymbol{\psi}) \circ \mathbf{v}. \end{aligned}$$

Then substitute in the first line of formulas to obtain the projections.

$$\begin{aligned} \boldsymbol{\psi} &= \frac{1}{\sqrt{6}}(1 - 2\mathbf{i} - \mathbf{k}); \\ \chi_s &= \mathbf{S}(\boldsymbol{\psi}) = \frac{1}{\sqrt{6}}, \\ \chi_\rho &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \boldsymbol{\rho}) = \mathbf{S}\left(\frac{-2\mathbf{i} - \mathbf{k}}{\sqrt{6}} * \mathbf{k}\right) = \mathbf{S}\left(\frac{1 + 2\mathbf{j}}{\sqrt{6}}\right) = \frac{1}{\sqrt{6}}, \\ \chi_\sigma &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \boldsymbol{\sigma}) = \mathbf{S}\left(\frac{-2\mathbf{i} - \mathbf{k}}{\sqrt{6}} * \frac{-\mathbf{i} + \mathbf{j}}{\sqrt{2}}\right) = \mathbf{S}\left(\frac{-2 + \mathbf{i} - \mathbf{j} - 2\mathbf{k}}{\sqrt{12}}\right) = -\frac{1}{\sqrt{3}}, \\ \chi_v &= \mathbf{S}(\mathbf{V}(\boldsymbol{\psi}) * \mathbf{v}) = \mathbf{S}\left(\frac{-2\mathbf{i} - \mathbf{k}}{\sqrt{6}} * \frac{\mathbf{i} + \mathbf{j}}{\sqrt{2}}\right) = \mathbf{S}\left(\frac{2 + \mathbf{i} - \mathbf{j} - \mathbf{k}}{\sqrt{12}}\right) = \frac{1}{\sqrt{3}}. \end{aligned}$$

Again, we write the equations from above for the angular excursions of the rotations and substitute into the equations.

$$\tan \theta = \frac{\chi_s}{\chi_\rho} \Rightarrow \theta = \tan^{-1} \frac{\chi_s}{\chi_\rho} = \tan^{-1} \frac{\frac{1}{\sqrt{6}}}{\frac{1}{\sqrt{6}}} = \tan^{-1}(1.0) \Rightarrow \theta = -45^\circ,$$

$$\tan \bar{\phi} = \frac{\chi_s}{\chi_\sigma} \Rightarrow \bar{\phi} = \tan^{-1} \frac{\chi_s}{\chi_\sigma} = \tan^{-1} \frac{\frac{1}{\sqrt{6}}}{-\frac{1}{\sqrt{3}}} = \tan^{-1}\left(-\frac{1}{\sqrt{2}}\right) \Rightarrow \bar{\phi} = 35.2644^\circ$$

Therefore - $\phi = 54.7356^\circ = \boldsymbol{\tau}$.

Vector Triple Products

It is easily confirmed that the volume of the unit cube is reduced to $\sqrt{6}^{-1} = 0.408248$, that the β edge vector is rotated -45° relative to the α edge vector about the $\rho = \mathbf{k}$ axis, and that the γ edge vector is at an angle of 35.2644° to the α, β -plane.

Another Example

In the last example all the edge vectors remained unit vectors after the strain. If the matrix is incompressible, then the unit vectors will become longer. Let the distorted box have the edge vectors $\{\alpha, \alpha + \beta, \alpha + \beta + \gamma\}$. Then the strain quaternion is the product of the three edge vectors.

$$\psi = \gamma\beta\alpha = 1 - 2\mathbf{i} - \mathbf{k}$$

This is very like the result that was obtained with the unit vectors, differing only in that there is not a $\sqrt{6}^{-1}$ term. Some thought will show that the final results are not changed by that multiplier, except that the volume remains unity, therefore the analysis works as well for non-unit edge vectors as with unit edge vectors.

Summary:

We began this essay with the consideration of an interesting mathematical relationship, namely, that the scalar of three vectors is the volume occupied by the parallelepiped that has those vectors as its edge vectors. We found that the vector of that quaternion is also related to the parallelepiped in that it expresses the rotations of the edges relative to each other as one progresses from a unit cube to a distortion of that box into the parallelepiped. These two components of the strain quaternion express two attributes of the distortion or strain. The scalar component expresses the volumetric strain, that is, the volume enclosed by the box on the assumption that it started as a unit cube. The vector component expresses the rotations of the edge vectors relative to each other, again assuming that they started mutually orthogonal to each other. If no two edge vectors are mutually orthogonal, then the vector component is not obviously indicative of the internal rotations. It is necessary to project the vector upon the component axes of the orientation frame for the strained box. However, doing so leads directly to the desired excursions about the ρ and σ axes. There an interaction component, which is projected upon the ν axis. As the edge vectors become more nearly orthogonal, the ν projection becomes smaller.

Appendix:

The relation between $\beta * \alpha$ and ρ is obtained as follows.

$$\beta \alpha = q * \rho = q * \frac{\beta}{\alpha} * \frac{T(\alpha)}{T(\beta)}, \text{ where } q \text{ is an unknown quaternion.}$$

$$q = \beta * \alpha * \alpha * \beta^{-1} * \frac{T(\beta)}{T(\alpha)} = \beta * -T(\alpha)^2 * \beta^{-1} * \frac{T(\beta)}{T(\alpha)} = -T(\alpha)T(\beta).$$

$$\beta \alpha = -T(\alpha)T(\beta) \frac{\beta}{\alpha} = -T(\alpha)T(\beta)\rho.$$

$$\rho = \frac{-\beta \alpha}{T(\alpha)T(\beta)} = \frac{\alpha \beta}{T(\alpha)T(\beta)}.$$