Vectors and Matrices operations

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인공 지능과 벡터(vector)와 기하(geometry)

AI·딥러닝 기술 기본인데… 수능서 빠지는 기하학

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가 - 기 + | 트 | 🗈

스크린 누비는 영웅들, 평창 수놓은 드론쇼도 기하가 탄생시켰다

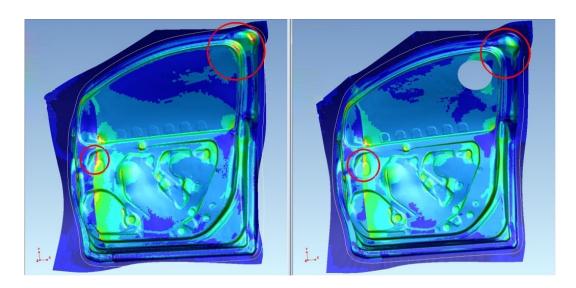
첨단기술의 출발은 기하 4차 산업혁명 주도하는 핵심기술 벡터 계산 등 기하가 밑바탕 캐나다, AI 연구소 이름 벡터'로 美英·日 대입서 심화과정 포함

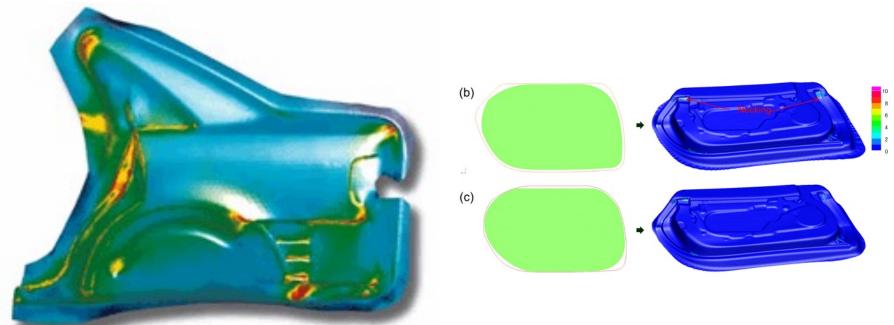
한국, 기하 교육은 뒷걸음질 한림원 등 과학계 반발에도 2021학년도 수능서 기하 제외 "이공계 인력 기초소양 부실"



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기하, 벡터와 소성가공





Nomenclature

- Rule(1) 굵은 글씨체(bold face)로 쓰여진 알파벳 기호 (가령 **b**) 는 그 기호가 가르키는 '물리량'이 벡터임을 의미한다.
- Rule(2) 벡터 \boldsymbol{b} 를 구성성분을 사용하여 표기할 수도 있다. $\boldsymbol{b} = (b_1, b_2, b_3)$. 각 구성성분(b_i with i=1,2,3)이 <u>굵은 글씨체가 아닌</u> 글씨체로 쓰여져 있음을 확인하라. (왜?)
- Rule(3) 굵은 글씨체문자 A 는 벡터 혹은 2nd order tensor (혹은 3x3 matrix)를 나타내는데
 다음과 같이 사용될 수 있다.

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

• Rule(4) Chalk board symbol denotes 4^{th} rank tensor \mathbb{E} for elastic modulus.

*(Mnemonic) 굵은 글씨체 문자는 여러 성분(값)으로 이루어진 물리량, 옅은 글씨체는 하나의 성분(값)으로만 이루어져 있다.

Nomenclature

- In matrix notation, the subscripts (also called as indices) are used to denote the rows and the columns of the associated components.
- Say, A_{ij} refers to the component in i-th row (행) and j-th column (렬)+.

• Example:
$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

• We preferably use Cartesian coordinates consisting of three basis vectors (often denoted as \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 or equivalently as i, j, k)*

†(Mnemonic) 행과 열을 구분하여 외우는 팁: 가로세로(o), 세로가로(x); 행렬. 따라서 행은 가로, 열은 세로. Row와 column중 column은 '기둥'을 뜻하고 기둥은 세워져 있다. 따라서 Column은 행, 나머지 row는 열.

*The basis vectors are written in **bold-face**, implying that they are **vectors** not scalars.

Why do we study vectors, tensors, coordinate systems?

- **재료는 근원적으로 3차원이며**, 스칼라 물리량만을 사용해서 재료의 거동을 설명할 수 없다.
- 재료의 거동에서 이방성(anisotropy)가 높아, 방향마다 재료의 거동이 달라질 수 있다. (e.g., Miller index)
- 스칼라만을 활용한 물리모형이 간단하여 매우 제한된 이론적 환경에서 물리적 모델의 개념을 설명하는데 간편할 수 있다. 하지만, 실제 3차원 재료나 구조로의 활용도가 매우 제한적이며, 재료가 가진 이방성(anisotropy)을 설명하거나 일반적 재료의 역학 거동을 설명할 수 없다.
- 한방향으로의 길이만 가진 1D 재료는 없다. 따라서 scalar 변형률과 응력으로만 이루어진 재료 구성방정식을 '공학'에 적용하기엔 한계가 있다.

+(FYI) 1차원 재료의 1차원 공간에서의 움직임만 고려한다면 vector, tensor 필요 없을 것.

벡터 (vector)

- 2차원 공간에서 벡터는 두개의 독립적인 성분(component)으로 구성된다.
 - n차원공간에서 벡터는 n개의 독립적인 성분으로 구성된다.
 - Say, a vector \boldsymbol{a} has two separate components $\boldsymbol{a}=(a_1,a_2)$. For example, vector $\boldsymbol{b}=(2,3)$
 - In 3D, a vector has 3 components.
- Length (magnitude) of a vector in 3D.

•
$$|\mathbf{a}| = \sqrt{a_1^2 + a_2^2 + a_3^2} = \sqrt{\sum_{i=1}^{3} a_i^2}$$

• vector *a*의 단위 벡터는 다음과 같다.

$$\frac{\boldsymbol{a}}{|\boldsymbol{a}|} = \left(\frac{a_1}{\sqrt{a_1^2 + a_2^2 + a_3^2}}, \frac{a_2}{\sqrt{a_1^2 + a_2^2 + a_3^2}}, \frac{a_3}{\sqrt{a_1^2 + a_2^2 + a_3^2}}\right)$$

예제)

Ex1) 다음 벡터의 length (magnitude)를 구하시오. a = (1,2,5)

Ex2) 다음 벡터의 unit vector를 구하시오. b = (1,1,2)

연산 (mathematical operations)

- 여러분들이 숫자에서 해보았던 연산?
 - 더하기 (빼기). +, -
 - 곱하기 (나누기). ×,÷
 - 지수곱, a^c
- Operations for vectors, tensors, matrices?
 - Scalar product
 - Dot product (내적, inner dot product) ·
 - Addition (벡터 합/차) +, -
 - Cross product ×
 - Double dot product :
 - Dyadic product ⊗

벡터 (vector) operations (연산)

• Vector addition: addition of vectors \boldsymbol{a} and \boldsymbol{b} can be expressed as:

either
$$c = a + b$$
 or $c_i = a_i + b_i$ with $i = 1,2,3$ (*)

- 벡터 합을 bold-face기호를 사용하여 표기하거나,
- 인덱스 표기법 (indicial notation)에 따라 나타낼 수 있다.

벡터 (vector)

Vector multiplication with scalar

$$c\mathbf{a} = (ca_1, ca_2, ca_3) = c(a_1, a_2, a_3)$$

 A vector decomposed into three vectors aligned with basis vectors of given coordinates:

$$\boldsymbol{a} = a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3$$

Some people use i, j, k (*) to denote the basis vectors such that

$$\boldsymbol{a} = a_1 \boldsymbol{i} + a_2 \boldsymbol{j} + a_3 \boldsymbol{k}$$

예제)

Ex1) 다음 두 벡터 합을 구하시오.
$$a = (1,2,5)$$
 $b = (2,-2,0)$

Ex2) 다음 두 벡터의 합에 해당하는 벡터의 unit vector를 구하시오.

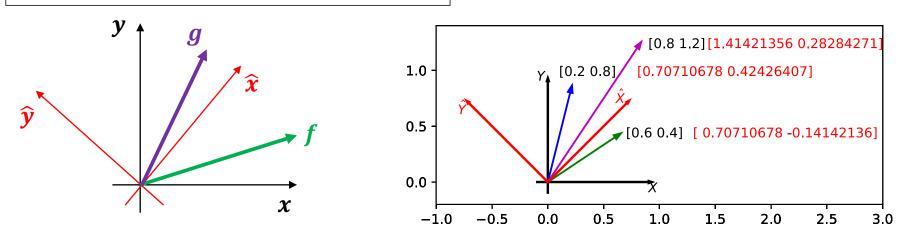
$$a = (-1,3,0)$$
 $b = (2,-2,1)$

Ex3)
$$\mathbf{a} = (-1,2,3)$$
 $\mathbf{b} = (2,-2,-2)$
 $\mathbf{a} + \mathbf{b} = (-1\mathbf{e}_1 + 2\mathbf{e}_2 + 3\mathbf{e}_3) + (2\mathbf{e}_1 - 2\mathbf{e}_2 - 2\mathbf{e}_3)$

Vector operations and coordinates

- 벡터의 구성성분은 임의로 설정된 좌표계에 의해 특정된다. 합하는 두 벡터에 사용하는 좌표계가 다르다면, 같은 물리량 (예를 들어 힘; force)을 표현하는 벡터라도 다른 좌표 값을 가진다.
- 힘 벡터의 합을 구성성분의 합으로 표현하기 위해서는 <u>반드시</u> 두 벡터의 구성성분이 같은 좌표계에 표현되어 있어야 한다.

각각 특정 물리량을 표현하는 g와 f의 합은 어떠한 좌표계를 사용하던 그 '물리적' 결과가 동일해야 한다.



- 합 뿐만 아니라 다른 벡터 operations들을 행하기에 앞서 반드시 구성성분이 같은 좌표계로 표현되어 있어야 한다.
- Operation 결과가 vector (혹은 tensor) quantity 일 때, 구성성분들은 선택된 좌표계에 참조된다.

The scalar product

FYI, $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ (Kronecker delta)

$$\delta_{ij} = 1 \ (if \ i = j); \delta_{ij} = 0 \ (i \neq j)$$

Geometric representation of scalar product of two vectors x and y



$$\mathbf{x} \cdot \mathbf{y} = |\mathbf{x}||\mathbf{y}|\cos\theta$$

 $\cos \theta$ is an even function, so that

$$x \cdot y = |x||y|\cos(-\theta) = |y||x|\cos(\theta) = y \cdot x$$

$$|\mathbf{x}| \equiv \mathbf{x} = (\mathbf{x} \cdot \mathbf{x})^{1/2}$$

Algebraic representation of scalar product of two vectors x and y

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 = \sum_i x_i \mathbf{e}_i$$

$$\mathbf{y} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 = \sum_i y_i \mathbf{e}_i$$

$$\mathbf{x} \cdot \mathbf{y} = \left(\sum_{i} x_{i} \mathbf{e}_{i}\right) \cdot \left(\sum_{i} y_{j} \mathbf{e}_{j}\right)$$

$$= \sum_{i} \sum_{j} x_{i} y_{j} \mathbf{e}_{i} \cdot \mathbf{e}_{j} = \sum_{i} \sum_{j} x_{i} y_{j} \delta_{ij}$$

$$=\sum_{i}\sum_{j}x_{i}y_{j}\delta_{ij}=\sum_{i}x_{i}y_{i}$$

Indicial notation; 인덱스(index)를 활용한 표기법

기호 $_i$: '기호'로 나타낸 벡터의 성분을 밑첨자 (subscript) $_i$ 를 사용해 나타낸다. (예: a_i 는 벡터 a의 성분을 뜻한다.)

- 3차원에서 index는 i = 1,2,3 존재.
- a_i 는 a벡터의 3 성분, e_i 는 e_1 , e_2 , e_3 세 벡터를 뜻함 (Q: 차이?)
- σ_{i1} 는 σ_{11} , σ_{21} , σ_{31} 세 성분을 뜻함 (자유 index 가 하나: i)
- c_{ij} 는 c_{11} , c_{12} , c_{13} , c_{21} , c_{22} , c_{23} , c_{31} , c_{32} , c_{33} 총 9개의 '값'을 뜻함 (자유 index 두개 i,j)
- a_ib_j 는 a_1b_1 , a_1b_2 , a_1b_3 , a_2b_1 , a_2b_2 , a_2b_3 , a_3b_1 , a_3b_2 , a_3b_3 총 9개의 '값'을 뜻함 (자유 index 두개 i,j)
- $\bullet \quad \frac{\partial \sigma_{ij}}{\partial x_i} + b_i = 0 \quad (???)$

인덱스 j의 경우에는 분자 분모에 동일하게 나타나 있으므로, not free; 인덱스 i는 free. 따라서...

$$\frac{\partial \sigma_{1j}}{\partial x_j} + b_1 = 0$$

$$\frac{\partial \sigma_{1j}}{\partial x_1} + b_2 = 0$$

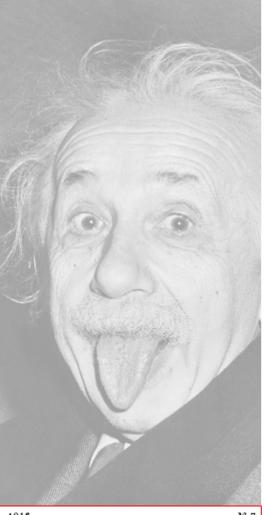
$$\frac{\partial \sigma_{2j}}{\partial x_j} + b_2 = 0$$

$$\frac{\partial \sigma_{3j}}{\partial x_i} + b_3 = 0$$

$$\frac{\partial \sigma_{3j}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_2} + b_1 = 0$$

$$\frac{\partial \sigma_{2j}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{23}}{\partial x_3} + b_2 = 0$$

$$\frac{\partial \sigma_{3j}}{\partial x_1} + \frac{\partial \sigma_{32}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3} + b_3 = 0$$



Einstein summation convention (Einstein notation)

- Albert Einstein이 벡터와 텐서등의 물리량을 이용하여 그의 이론을 논문으로 쓰면서 (그의 물리법칙과는 무관한) 재미있는 사실을 하나 관찰했다.
- 벡터나 텐서가 inner dot, cross product, 등등의 operations 참여하면서 '덧셈'이 있을시에 반드시 해당 subscript가 두번씩 나타나고, 반대로 subscript가 두번씩 반복되어 나타나면 '덧셈'이 존재한다는 것이다.
- 따라서, 언제나 두개의 동일한 subscript가 나타나면 간단히 summation 기호를 없애도 된다고 생각했다.
- 예를 들면 $x_i y_i$ 와 같은 표현이 수식에 나오면 이것은 따로 말을 하지 않더라도 $\sum_{i=1}^{n} x_i y_i$ 을 의미한다는 사실이다 (이때 n은 물리량이 표혀된 공간의 차원이다).
- 유사하게, 만약 두쌍의 subscript가 반복된다면, 두개의 summation 기호가 생략된다.

1916. Æ 7.

ANNALEN DER PHYSIK.
VIERTE FÖLGE. BAND 49.

1. Die Grundlage der allgemeinen Relativitätstheorie; von A. Einstein.

Die im nachfolgenden dargelegte Theorie bildet die denkbar weitgehendste Verallgemeinerung der heute allgemein als "Relativitätstheorie" bezeichneten Theorie; die letztere nenne ich im folgenden zur Unterscheidung von der ersteren "spezielle Relativitätstheorie" und setze sie als bekannt voraus. Die

Examples of Einstein summation

•
$$\mathbf{x} = x_i \mathbf{e}_i = \sum_{i=1}^{n} x_i \mathbf{e}_i = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + \dots + x_n \mathbf{e}_n$$

•
$$\mathbf{x} \cdot \mathbf{y} = x_i y_j \delta_{ij} = x_i y_i = x_j y_j = x_1 y_1 + x_2 y_2 + \dots + x_n y_n$$

•
$$\mathbf{x} \cdot \mathbf{e}_i = x_j \mathbf{e}_j \cdot \mathbf{e}_i = x_j \delta_{ij} = x_i$$

$$\begin{cases} \mathbf{x} \cdot \mathbf{e}_1 = x_1 \\ \mathbf{x} \cdot \mathbf{e}_2 = x_2 \\ \mathbf{x} \cdot \mathbf{e}_3 = x_3 \end{cases}$$

The last equation defines the components of vector. The same can be referred to as 'projection' of x on the \mathbf{e}_i axis. (x벡터의 \mathbf{e}_i 축으로의 내적)

Examples of Einstein summation

$$a_i = b_{ij}c_jd_j$$
 LHS 그리고 RHS 모두 i 만 free index; (Correctly used notation)

$$a_ib_j=c_{ik}d_{kj}$$
 LHS 그리고 RHS 모두 i,j 가 free index; (Correctly used notation) Index j is repeated in $m{c}$ and $m{d}$. So, Einstein Summation Convention is implied

$$a_i b_j = c_{ik} d_{kj} + e_i f_j + g_i p_{jj} + q_l r_{ij}$$

LHS has two free index i and j. In RHS, in the third term the same j is used as if it is non free index; (Conflicts). Also, the fourth term has an extra index l.

When Einstein summation convention is implied, we call the index (over which summation is performed) dummy as it is not important what letter is given.

For instance, $a_i b_i = a_k b_k = a_l b_l \dots etc$

Ex)

• 3차원 공간에서의 물리량으로 이루어진 다음 expression을 Einstein summation convention을 사용하여 나타내시오.

$$b = x + C \cdot y$$

 $m{C} \cdot m{y}$ 은 내적이며 $m{C}$ 가 2nd order tensor (3x3 matrix) 이고 $m{y}$ 는 벡터이다. 따라서 그 결과는

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} C_{11}y_1 + C_{12}y_2 + C_{13}y_3 \\ C_{21}y_2 + C_{22}y_2 + C_{23}y_3 \\ C_{31}y_1 + C_{32}y_2 + C_{33}y_3 \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{3} C_{1j}y_j \\ \sum_{j=1}^{3} C_{2j}y_j \\ \sum_{j=1}^{3} C_{3j}y_j \end{bmatrix}$$

$$\begin{bmatrix} \sum_{j=1}^{3} C_{1j}y_j \\ C_{1j}y_j \end{bmatrix}$$

$$\boldsymbol{b} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^{3} C_{1j} y_j \\ \sum_{j=1}^{3} C_{2j} y_j \\ \sum_{j=1}^{3} C_{3j} y_j \end{bmatrix} \rightarrow \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^{3} C_{1j} y_j \\ \sum_{j=1}^{3} C_{2j} y_j \\ \sum_{j=1}^{3} C_{3j} y_j \end{bmatrix} \qquad b_i = x_i + \sum_{j=1}^{3} C_{ij} y_j \quad for \ i = 1,2,3$$

$$\sum_{j=1}^{3} C_{3j} y_j$$

$$\rightarrow b_i = x_i + C_{ij} y_j$$

$$\rightarrow b_i = x_i + C_{ij} y_j$$

벡터 (vector) operations

Dot product aka inner dot product (내적):

$$d = \boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{b} \cdot \boldsymbol{a}$$
 or $d = \sum_{i=1}^{3} a_{i} b_{i} \rightarrow \text{(Einstein)}$: $d = a_{i} b_{i}$

Alternative form:

$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos \theta$$

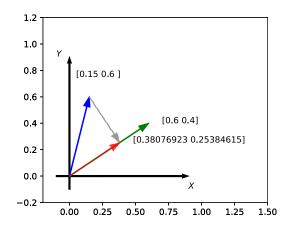
 $\boldsymbol{\theta}$ denotes the angle between the two vectors (\boldsymbol{a} and \boldsymbol{b}).

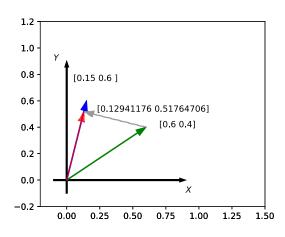
$$\boldsymbol{a} \cdot \boldsymbol{b} = (a_{x}\boldsymbol{i} + a_{y}\boldsymbol{j} + a_{z}\boldsymbol{k}) \cdot (b_{x}\boldsymbol{i} + b_{y}\boldsymbol{j} + b_{z}\boldsymbol{k})$$

where i, j, k are unit vectors along the axes x,y,z, respectively.

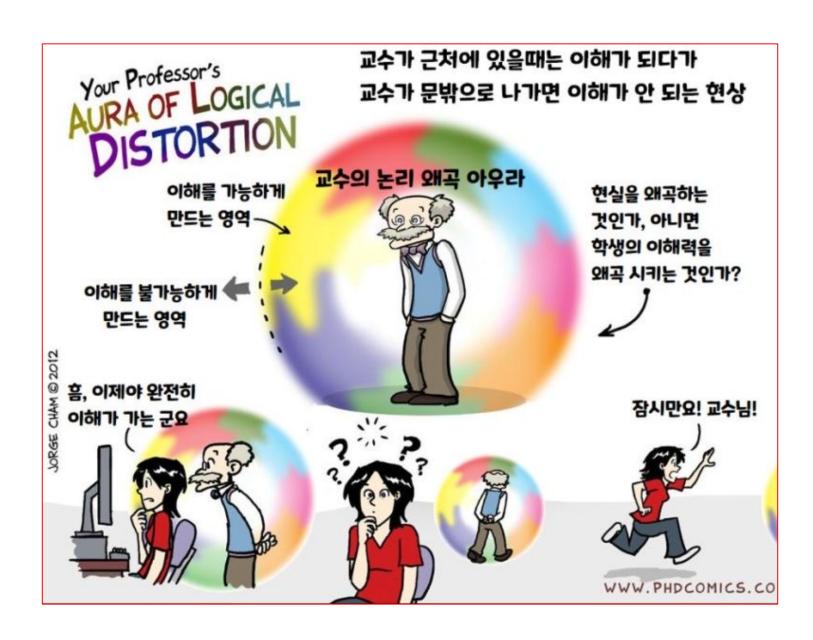
• Inner product of different basis vector leads in zero, while that of the same basis vectors lead to 1: $\mathbf{i} \cdot \mathbf{j} = 0$ and $\mathbf{i} \cdot \mathbf{i} = 1$

 \rightarrow $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ (Kronecker delta)





Either way, the dot product amounts to ~42.27



예제)

• Q1) 다음은 Miller index로 나타낸 BCC 결정 구조내의 면과 방향이다. 두 방향사이의 끼인각은?

$$n = (1,1,0)$$

 $b = [1, \overline{1}, 0]$

• Q2) 다음 결정면 n 과 방향 b으로 이루어진 slip system이 FCC 결정내 존재할까 ?

$$\mathbf{n} = (1, \overline{1}, 1)$$

 $\mathbf{b} = [1, \overline{1}, 0]$

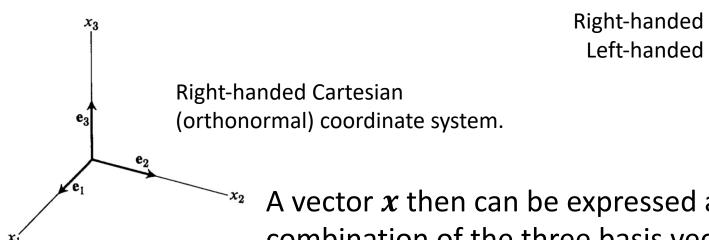
• Q3) 벡터 a = (1, -0.5, 3)과 c = [1, 2, 0]을 이용해 다음 연산의 답을 구하시오.

$$a_k b_k = ?$$

• Q4) 위 Q3)의 벡터를 활용하여 예상되는 $a_i b_k$ 와 $a_i b_i$ 의 차이를 설명하시오.

Cartesian coordinate system

- 우리는 *orthonormal* 좌표계 (서로 **수직**인 세 unit vector가 basis)만 사용하기로 하자.
- Now, we denote these three orthonormal basis vectors as \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 .



Right-handed ($\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3$) Left-handed ($\mathbf{e}_2 \times \mathbf{e}_1 = \mathbf{e}_3$)

A vector x then can be expressed a linear combination of the three basis vectors such that

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3$$

벡터 (vector) dyadic operations

Dyadic product (a.k.a. outer product):

$$\mathbf{a} \otimes \mathbf{b} = (a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3) \otimes (b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2 + b_3 \mathbf{e}_3)$$

where \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 are unit vectors along the axes 1,2,3, respectively.

$$\mathbf{a} \otimes \mathbf{b} = a_1 b_1 (\mathbf{e}_1 \otimes \mathbf{e}_1) + a_1 b_2 (\mathbf{e}_1 \otimes \mathbf{e}_2) + a_1 b_3 (\mathbf{e}_1 \otimes \mathbf{e}_3) + a_2 b_1 (\mathbf{e}_2 \otimes \mathbf{e}_1) + a_2 b_2 (\mathbf{e}_2 \otimes \mathbf{e}_2) + a_2 b_3 (\mathbf{e}_2 \otimes \mathbf{e}_3) + a_3 b_1 (\mathbf{e}_3 \otimes \mathbf{e}_1) + a_3 b_2 (\mathbf{e}_3 \otimes \mathbf{e}_2) + a_3 b_3 (\mathbf{e}_3 \otimes \mathbf{e}_3)$$

Also equivalently,

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{bmatrix}$$

If n^s and b^s are slip system s consisting of (unit) plane normal and (unit) slip direction vectors, $n^s \otimes b^s$ corresponds to Schmid tensor such that $M^s = n^s \otimes b^s$ or $M^s_{ij} = n^s_i b^s_j$ (no dummy index)

Schmid tensor and resolved shear stress

•
$$n^{s} = \frac{(1,1,1)}{|(1,1,1)|}$$
 and $b^{s} = \frac{(1,0,-1)}{|(1,0,-1)|}$

Say, the crystal is subjected to stress tensor of

$$\boldsymbol{\sigma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The resolved shear stress (RSS) amounts to

$$\tau^{S} = \boldsymbol{\sigma} \cdot \boldsymbol{n}^{S} \cdot \boldsymbol{b}^{S} = \boldsymbol{\sigma} : \boldsymbol{M}^{S} = \sigma_{ij} M_{ij}^{S}$$

$$\tau^{s} = \begin{pmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{6}} \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \cdot \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Recall the Schmid law: $\tau^s = \sigma \cos \phi \cos \lambda$

** Caution, direct use of miller index for crystal plane normal and direction should be careful.

Crystal coordinate system of cubic (FCC, BCC) are equivalent to Cartesian. Less symmetric

Structures (such as triclinic) would require change of the miller indices to relevant components in Cartesian coordinates.

Pressure independence of slip

•
$$n^S = \frac{(1,1,1)}{|(1,1,1)|}$$
 and $b^S = \frac{(1,0,-1)}{|(1,0,-1)|}$

Say, the crystal is subjected to stress tensor of

$$\boldsymbol{\sigma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \boldsymbol{\sigma} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \boldsymbol{\sigma} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

Q) Calculate the resolved shear stress for each stress tensor above, and discuss what you observed.

Identity matrix

•
$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
, $A \cdot I = A$, $I \cdot A = A$

• In the tensor notation, one would use the Kronecker delta denoted as δ_{ij}

$$\delta_{ij} = 1 \text{ if } i = j$$

$$\delta_{ij} = 0 \text{ if } i \neq j$$

Kronecker delta examples

$$a_{ij}\delta_{ij} = \sum_{i} \sum_{j} a_{ij}\delta_{ij} = a_{11}\delta_{11} + a_{12}\delta_{12} \dots$$

$$= a_{11} + a_{22} + a_{33}$$

$$= \sum_{i} a_{ii}$$
$$= a_{ii}$$

Notice the dummy index i, so that

$$a_{ii} = a_{jj} = a_{kk} \dots$$

Q1)
$$a_{ij} = b_{kk} \delta_{ij}$$

- 1. There are on dummy index, k and two free indicies i, j
- 2. Therefore, the above means 9 equations.
- 3. If we expand the dummy index k, we have

$$a_{ij} = (b_{11} + b_{22} + b_{33})\delta_{ij}$$

Kronecker delta

Q2) $\mathbb{E}_{ijkl} = \frac{\lambda \delta_{ij} \delta_{kl}}{\lambda \delta_{ij} \delta_{kl}} + \frac{\mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})}{\lambda \delta_{ij} \delta_{kl}}$, expand the equation to find explicit component \mathbb{E}_{1233}

- 1. There is no dummy and four free indicies exist, namely, i, j, k, l
- 2. $\mathbb{E}_{1233} = \lambda \delta_{12} \delta_{33} + \mu (\delta_{13} \delta_{23} + \delta_{13} \delta_{23}) = 0$

Q3) Expand the equation to find explicit component $\mathbb{E}_{2233} = \lambda \delta_{22} \delta_{33} + \mu (\delta_{23} \delta_{23} + \delta_{23} \delta_{23}) = \lambda$

Q4) Expand the equation to find explicit component $\mathbb{E}_{1212} = \lambda \delta_{12} \delta_{12} + \mu (\delta_{11} \delta_{22} + \delta_{12} \delta_{21}) = \mu$

Transpose

$$\bullet \mathbf{A} = \begin{bmatrix} 3 & 4 & 6 \\ -3 & 2 & 5 \\ 1 & -1 & -4 \end{bmatrix}$$

$$\bullet A^T = \begin{bmatrix} 3 & -3 & 1 \\ 4 & 2 & -1 \\ 6 & 5 & -4 \end{bmatrix}$$

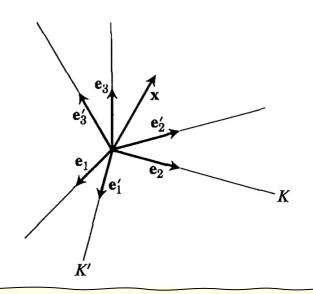
• In tensor notation, $A_{ij}^T = A_{ji}$

Matrix <u>addition</u> and <u>dot, double-dot products</u>

- Addition
 - C = A + B
 - $C_{ij} = A_{ij} + B_{ij}$
- Dot products
 - $C = A \cdot B$
 - $C_{ij} = A_{ik}B_{kj}$ (Find the free and non-free indices!)
 - Multiplication is not commutative
 - $A \cdot B \neq B \cdot A$
- Double dot products
 - d = A: B (denote d is a scalar quantity thus is **not** denoted in bold-face)
 - $d = A_{ij}B_{ij}$

Rotation (transformation) of the coordinate system

Relationship between the components of a unit vector expressed with respect to two different Cartesian bases with the same origin (not necessarily orthonormal);



Two cartesian coordinates (K and K') with two separate sets of basis vectors (\mathbf{e}_i and \mathbf{e}'_i) and a vector \mathbf{x}

Any vector \mathbf{x} can be resolved into components with respect to either the K or the K' system.

$$\mathbf{x} = (\mathbf{x} \cdot \mathbf{e}_j)\mathbf{e}_j = x_j\mathbf{e}_j$$

If we take $\mathbf{x} = \mathbf{e}'_i$ (a certain basis vector of K')

$$\mathbf{e}_i' = (\mathbf{e}_i' \cdot \mathbf{e}_i) \mathbf{e}_i \equiv a_{ij} \mathbf{e}_i$$

The nine terms a_{ij} (for each of three basis vectors; i=1, i=2, and i=3) are <u>directional cosines</u> of the angles between the six axes:

$$\mathbf{R} \equiv \left(a_{ij}\right) \equiv \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

R is known as the <u>transformation matrix</u> (or rotation matrix) in three dimension.

Rotation (transformation) of the coordinate system

$$\mathbf{e}_i' \equiv a_{ij}\mathbf{e}_j$$

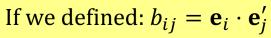
$$\mathbf{e}_i' \equiv a_{ik} \mathbf{e}_k$$

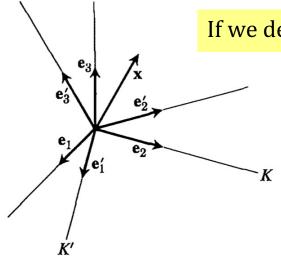
 $\mathbf{e}_i' \equiv a_{ij}\mathbf{e}_j \quad \text{Switching } j \to k \qquad \mathbf{e}_i' \equiv a_{ik}\mathbf{e}_k$ Earlier, we defined: $a_{ij} = \mathbf{e}_i' \cdot \mathbf{e}_j \quad \text{And } a_{ij}\mathbf{e}_j = \mathbf{e}_i' \cdot \mathbf{e}_j \cdot \mathbf{e}_j \quad \therefore a_{ij} \mathbf{e}_j = \mathbf{e}_i' |\mathbf{e}| \to a_{ij}\mathbf{e}_j = \mathbf{e}_i'$

And
$$a_{ij}\mathbf{e}_{j} = \mathbf{e}'_{i} \cdot \mathbf{e}_{j} \cdot \mathbf{e}_{j}$$

$$\therefore a_{ij} \mathbf{e}_{i} = \mathbf{e}'_{i} |\mathbf{e}| \rightarrow a_{ij} \mathbf{e}_{i} = \mathbf{e}$$

$$\delta_{ij} = \mathbf{e}'_i \cdot \mathbf{e}'_j = a_{ik} \mathbf{e}_k \cdot \mathbf{e}'_j = a_{ik} b_{kj} \qquad [a] = [b]^{-1}$$





Two cartesian coordinates (*K* and K') with two separate sets of basis vectors (\mathbf{e}_i and \mathbf{e}'_i) and a vector \mathbf{x}

Any vector **x** may be expressed in the *K* system as

$$\mathbf{x} = x_i \mathbf{e}_i$$

or as in the K' system using primed basis such as

$$\mathbf{x} = x_i' \mathbf{e}_i'$$

They are the same vector so one can equate

$$\mathbf{x} = x_i' \mathbf{e}_i' = x_i \mathbf{e}_i$$

One could replace \mathbf{e}_i' with $a_{ii}\mathbf{e}_i$

$$x_i'a_{ij}\mathbf{e}_j=x_j\mathbf{e}_j$$

 $x_i = a_{ii}x_i'$

so that

$$x_j = x_i' a_{ij}$$
 $\left[x_j\right]^T = \left[x_i' a_{ij}\right]^T$ $x_j = \left[a_{ij}\right]^T \left[x_i'\right]^T$

Or equivalently, swapping the indices *i* and *j* gives:

$$x_i = a_{ij}x_j'$$

Inverse transformation?

$$\mathbf{e}_{i} = \mathbf{e}_{i} \times \mathbf{1} = \mathbf{e}_{i} (\mathbf{e}'_{j} \cdot \mathbf{e}'_{j}) = (\mathbf{e}_{i} \cdot \mathbf{e}'_{j}) \mathbf{e}'_{j} = a_{ij} \mathbf{e}'_{j}$$
$$a_{kj} \mathbf{x}'_{j} = a_{kj} \mathbf{b}_{jl} \mathbf{x}'_{l} = \delta_{kl} \mathbf{x}'_{l} = \mathbf{x}'_{k}$$

In summary we have:

$$\mathbf{x} = x_i' \mathbf{e}_i' = x_j \mathbf{e}_j$$

$$\mathbf{e}_i' = a_{ij} \mathbf{e}_j, \qquad \mathbf{e}_i = a_{ji} \mathbf{e}_j'$$

$$x_i' = a_{ij} x_j, \qquad x_i = a_{ji} x_j'$$

$$a_{ik} a_{jk} = a_{ki} a_{kj} = \delta_{ij}$$

Earlier, we defined:

$$a_{ij} = \mathbf{e}_i' \cdot \mathbf{e}_j$$
$$b_{ij} = \mathbf{e}_i \cdot \mathbf{e}_i'$$

Earlier, we defined:

$$a_{ij} = \mathbf{e}'_i \cdot \mathbf{e}_j = \mathbf{e}_j \cdot \mathbf{e}'_i = b_{ji}$$

If the inner dot product of *a* and *b* matrices:

$$a_{ik}b_{kj} = (\mathbf{e}'_i \cdot \mathbf{e}_k)(\mathbf{e}_k \cdot \mathbf{e}'_j)$$

$$= \mathbf{e}'_i \cdot (\mathbf{e}_k \cdot \mathbf{e}_k) \cdot \mathbf{e}'_j$$

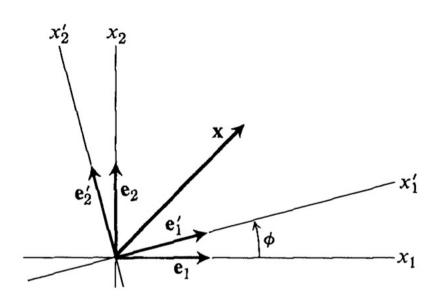
$$= \mathbf{e}'_i \cdot \mathbf{e}'_j = \delta_{ij}$$

Scalar product is invariant under orthogonal transformations

$$x' \cdot y' = x'_i y'_i = a_{ij} x_j a_{ik} y_k = a_{ij} a_{ik} x_j y_k$$
$$= \delta_{jk} x_j y_k = x_j y_j = x \cdot y$$

$$a_{ij}a_{ik} = \left(a_{ji}\right)^T a_{ik} = b_{ji}a_{ik} = \delta_{jk}$$

Two dimensional case



$$a_{ij} \equiv (\mathbf{e}'_i \cdot \mathbf{e}_j), \quad \text{for } i, j = 1, 2$$

https://en.wikipedia.org/wiki/List of trigonometric identities

Shift by one quarter period $\sin(\theta\pm\frac{\pi}{2})=\pm\cos\theta$ $\cos(\theta\pm\frac{\pi}{2})=\mp\sin\theta$ $\tan(\theta\pm\frac{\pi}{4})=\frac{\tan\theta\pm1}{1\mp\tan\theta}$ $\csc(\theta\pm\frac{\pi}{2})=\pm\sec\theta$ $\sec(\theta\pm\frac{\pi}{2})=\mp\csc\theta$ $\cot(\theta\pm\frac{\pi}{4})=\frac{\cot\theta\pm1}{1\mp\cot\theta}$

$$\begin{bmatrix} a_{ij} \end{bmatrix} = \begin{bmatrix} \cos \phi & \cos(90^{\circ} - \phi) \\ \cos(90^{\circ} + \phi) & \cos \phi \end{bmatrix}$$

Physical theories must be invariant to the choice of coordinate system

If we fix our attention on a physical vector (e.g. velocity) and then rotate the coordinate system $(K \to K')$, the vector will have different numerical components in the rotated coordinate system (as evident in the coordinate transformation rule we just discussed earlier). So we are led to realize that a vector is more than an ordered triple. Rather, it is many sets of ordered triples, which are related in a definite way. One still specifies a vector by giving three ordered numbers (components), but these three numbers are distinguished from an arbitrary collection of three numbers by including the law of coordinate transformation under rotation of the coordinate frame as part of the definition.

Thus, one physical vector may be represented by infinitely many sets of ordered triples. The particular triple depends on the chosen coordinate system of the observer.

This is important because physical laws (and results) must be the same regardless of coordinate system, that is, regardless of the orientation of observer's coordinate system.

Physical laws and coordinate system

- The importance of thinking of these quantities in terms of their transformation properties lies in the requirement that physical theories must be invariant under the change of the coordinate system.
- Physical laws should not be affected by the choice of a coordinate system.
- We'll examine this using an example in what follows.

Newton's second law



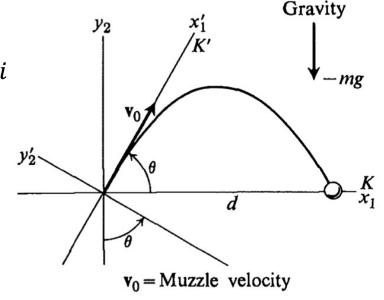
$$\mathbf{F} = m\mathbf{a} \rightarrow F_i = ma_i \rightarrow F_i = m\dot{v}_i$$

$$F_i = m\dot{v}_i = m\ddot{x}_i$$

$$v_i = \frac{dx_i}{dt} = \dot{x}_i$$

$$a_i = \dot{v}_i = \frac{dv_i}{dt} = \frac{d\dot{x}_i}{dt} = \ddot{x}_i$$





Let's assume acceleration \ddot{x}_i is function of time, so that $\ddot{x} \equiv \ddot{x}_i(t)$

Furthermore, if we assume the mass is constant (which is quite usual), the second law is equation with the location x_i and its derivatives as variable – do not forget another variable time (t).

Newton's second law

$$F_i(t) = m \, \ddot{x}_i(t)$$

Let's use K coordinate system

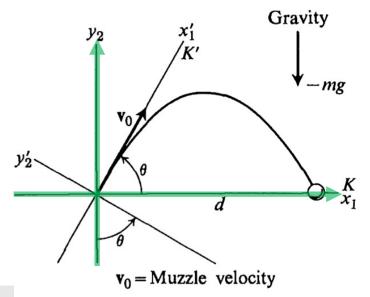
1. Initial condition in terms of location (x_i) and velocity (\dot{x}_i) :

$$x_i(0) = 0, \quad \text{with } i = 1,2$$

$$\dot{x}_1(0) = v_0 \cos \theta$$

$$\dot{x}_2(0) = v_0 \sin \theta$$

 $x_i(0)$ means $x_i(t=0)$



 $x_1(t) = \int_0^t v_0 \cos \theta \, dt = v_0 t \cos \theta$

- 2. Force given by gravity is constant (gravity field): $F_1 = m\ddot{x}_1 = 0, \qquad F_2 = -mg = m\ddot{x}_2$
- 3. Estimate $x_i(t) = ?$

$$x_i(t) = x_i(0) + \int_0^t \frac{dx_i}{dt} dt = x_i(0) + \int_0^t \frac{\dot{x}_i}{dt} dt$$

imate
$$x_i(t) = ?$$

$$x_i(t) = x_i(0) + \int_0^t \frac{dx_i}{dt} dt = x_i(0) + \int_0^t \dot{x}_i dt$$

$$x_i(t) = x_i(0) + \int_0^t \frac{dx_i}{dt} dt = x_i(0) + \int_0^t \dot{x}_i dt$$

$$\dot{x}_{i}(t) = \dot{x}_{i}(0) + \int_{0}^{t} \frac{d\dot{x}_{i}}{dt} dt \qquad \dot{x}_{1}(t) = \dot{x}_{1}(t = 0) + \int_{0}^{t} \ddot{x}_{1} dt = v_{0} \cos \theta + 0$$

$$\dot{x}_{2}(t) = \dot{x}_{2}(t = 0) + \int_{0}^{t} \ddot{x}_{2} dt = v_{0} \sin \theta + \int_{0}^{t} -g dt = v_{0} \sin \theta - gt$$

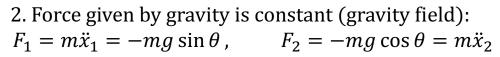
Newton's second law

$$F_i(t) = m\ddot{x}_i(t)$$

Let's use K' coordinate system

1. Initial condition in terms of location (x_i) and velocity (\dot{x}_i) : $x_i'(t=0) = 0$, with i=1,2

$$\dot{x}'_{i}(t=0) = 0,$$
 with $i = 1,$
 $\dot{x}'_{1}(0) = v_{0}$
 $\dot{x}'_{2}(0) = 0$



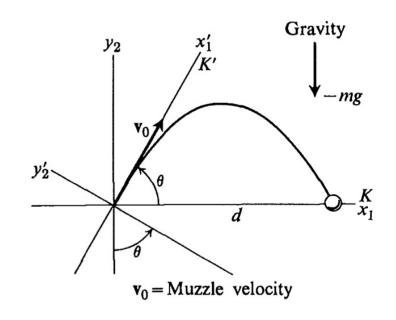
3. Estimate $x_i(t) = ?$

$$x_i(t) = x_i(0) + \int_0^t \frac{dx_i}{dt} dt = x_i(0) + \int_0^t \dot{x}_i dt$$

$$\dot{\mathbf{x}}_i(t) = \dot{\mathbf{x}}_i(0) + \int_0^t \ddot{\mathbf{x}}_i dt$$

$$\dot{x}_1(t) = \dot{x}_1(0) + \int_0^t \ddot{x}_1 dt = v_0 - \int_0^t g \sin \theta \, dt = v_0 - gt \sin \theta$$

$$\dot{x}_2(t) = \dot{x}_2(0) + \int_0^t \ddot{x}_2 dt = 0 - \int_0^t g \cos \theta \, dt = -gt \cos \theta$$



$$x_1(t) = \int_0^t (v_0 - gt \sin \theta) dt$$
$$= v_0 t - \frac{1}{2} gt^2 \sin \theta$$

$$x_2(t) = \int_0^t -gt \cos\theta \, dt = -\frac{1}{2}gt^2 \cos\theta$$

Graphing the two results.

Plot the result with theta=45 degree

At t=0

at t=1s

at t=10s

at t=100s

Plot the result with theta=90 degree

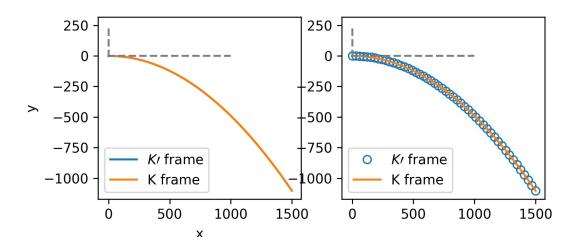
At t=0

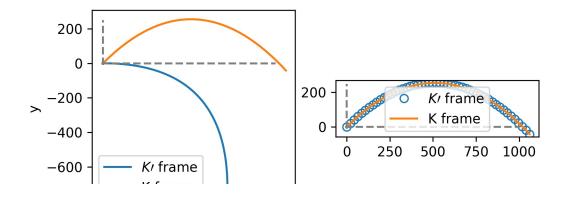
at t=1s

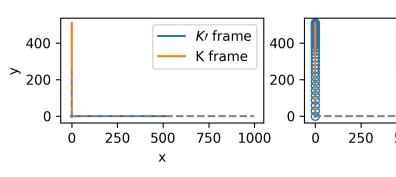
at t=10s

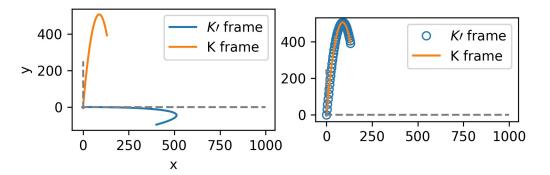
at t=100s

- Which of the frame was the easy one?
- Describe why we'd want to chose a frame that gives easy calculation?









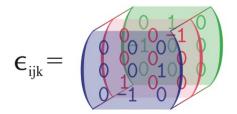
Cross product and permutation symbol

Cross product between two orthonormal basis vectors: $\mathbf{e}_i \times \mathbf{e}_j = \epsilon_{ijk} \mathbf{e}_k$ (*i*, *j*: free; *k*: dummy)

The symbol ϵ_{ijk} is called the alternating symbol (or more commonly permutation symbol and more formally Levi-Civita symbol for more general cases).

For the indices (i,j,k) in ε_{ijk} , the values 1,2,3 occurring in the cyclic order (1,2,3) correspond to $\varepsilon=+1$, while occurring in the reverse cyclic order correspond to $\varepsilon=-1$, otherwise $\varepsilon=0$.

$$\epsilon_{ijk} = \begin{cases} 1, & \text{if } i, j, k \text{ are in cyclic order and not repeated } (123, 231, 312), \\ -1, & \text{if } i, j, k \text{ are not in cyclic order and not repeated} (132, 213, 321), \\ 0, & \text{if any of } i, j, k \text{ are repeated.} \end{cases}$$

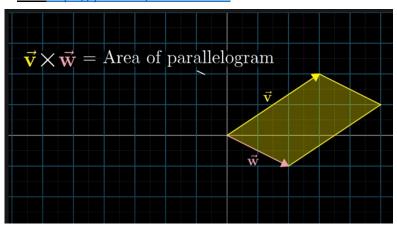


where i is the depth (blue: i = 1; red: i = 2; green: i = 3), j is the row and k is the column.

$$\mathbf{a} \times \mathbf{b} = (a_i \mathbf{e}_i) \times (b_j \mathbf{e}_j) = a_i b_j (\mathbf{e}_i \times \mathbf{e}_j) = a_i b_j \epsilon_{ijk} \mathbf{e}_k$$
$$\epsilon_{ijk} \epsilon_{ijk} = 6$$

Area of inclined triangle calculated by using cross-product

REF: https://youtu.be/eu6i7WJeinw



The area of triangle: $\frac{|u|}{2} = \frac{|w \times v|}{2}$

The unit normal vector of the traingle: $\frac{u}{|u|}$

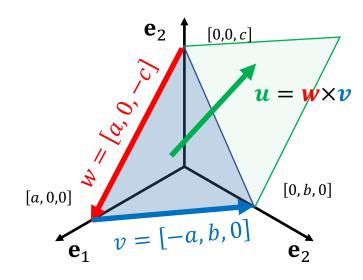
$$\mathbf{w} \times \mathbf{v} = \mathbf{u}$$

$$(w_{i}\mathbf{e}_{i}) \times (v_{j}\mathbf{e}_{j}) = w_{i}v_{j}\epsilon_{ijk}\mathbf{e}_{k} = u_{k}\mathbf{e}_{k}$$

$$u_{1} = w_{i}v_{j}\epsilon_{ij1} = w_{2}v_{3} - w_{3}v_{2} = -(-c)b = bc$$

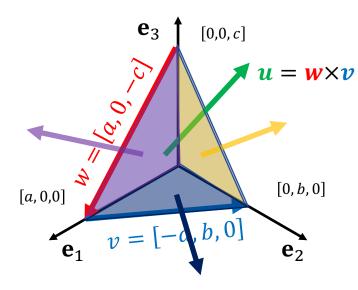
$$u_{2} = w_{i}v_{j}\epsilon_{ij2} = w_{3}v_{1} - w_{1}v_{3} = (-c)(-a) = ac$$

$$u_{3} = w_{i}v_{j}\epsilon_{ij3} = w_{1}v_{2} - w_{2}v_{1} = ab$$



$$\frac{|\mathbf{u}|}{2} = \frac{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}{2}$$
$$\frac{\mathbf{u}}{|\mathbf{u}|} = \frac{[bc, ac, ab]}{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}$$

Relations between triangular surfaces (will be useful for Cauchy tetrahedron)



$$r = [0,0,c] \times [0,b,0] = -cb\mathbf{e}_1$$

$$\mathbf{q} = [a, 0, 0] \times [0, 0, c] = -ac\mathbf{e}_2$$

$$r = [0, b, 0] \times [a, 0, 0] = -ba\mathbf{e}_3$$

Volume of tetrahedron: $\frac{abc}{6}$

Area: $\frac{|u|}{2} = \frac{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}{2}$

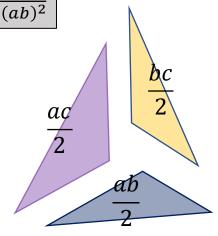
Unit normal vector: $\frac{u}{|u|} = \frac{[bc,ac,ab]}{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}$

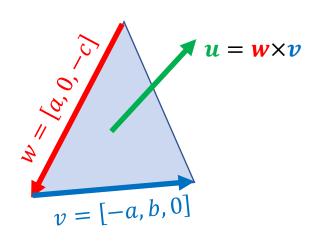
Confirm

$$\frac{u_1}{|u|} \frac{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}{2} = \frac{bc}{2}$$

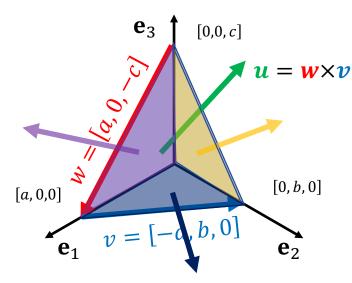
$$\frac{u_2}{|u|} \frac{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}{2} = \frac{ac}{2}$$

$$\frac{u_2}{|u|} \frac{\sqrt{(bc)^2 + (ac)^2 + (ab)^2}}{2} = \frac{ab}{2}$$





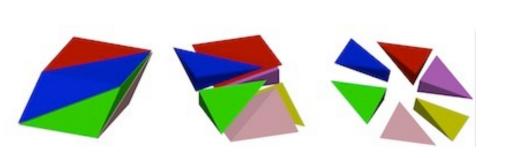
Relations between triangular surfaces (will be useful for Cauchy tetrahedron)

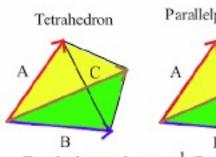


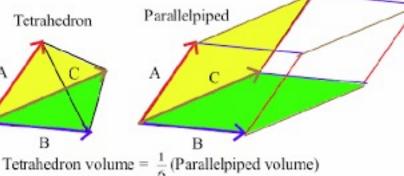
$$\mathbf{r} = [0,0,c] \times [0,b,0] = -cb\mathbf{e}_1$$

 $\mathbf{q} = [a,0,0] \times [0,0,c] = -ac\mathbf{e}_2$
 $\mathbf{r} = [0,b,0] \times [a,0,0] = -ba\mathbf{e}_3$

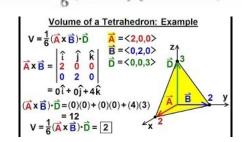
Volume of tetrahedron:







V of tetrahedron =
$$\frac{([a, 0, 0] \times [0, b, 0]) \cdot [0, 0, c]}{6}$$



Integration (scalars)

a is a quantity that is varying with respect to time t. If you know the initial value of it, (i.e., a(t=0) and you know $\frac{da}{dt}$ in all time stamps, you'll be able to calculate $a(t=\tau)$ via:

 $a(t=\tau)=a(t=0)+\int_0^\tau \frac{da}{dt}\ dt$, this is sometimes written in short:

$$a_{\tau} = a_{(0)} + \int_0^{\tau} \frac{da}{dt} dt$$

You could have an analytic expression of the above, (or not). In case of former, you'd have Something like

$$a(\tau) = a_0 + \tau^2 + \cos(\tau) \exp(\tau) \dots$$

In case you cannot obtain an analytic expression, you can could 'numerically' obtain the solution.

Integration (vectors, tensors)

a is a quantity that is varying with respect to time t. If you know the initial value of it, (i.e., a(t=0) and you know $\frac{da_i}{dt}$ (i being the free index) in all time stamps, you'll be able to calculate $a(t=\tau)$ via:

 $a(t=\tau) = a(t=0) + \int_0^\tau \frac{da}{dt} dt$, this is sometimes written in short:

$$\boldsymbol{a}_{\tau} = \boldsymbol{a}_{(0)} + \int_{0}^{\tau} \frac{d\boldsymbol{a}}{dt} dt$$

You could have an analytic expression of the above, (or not). In case of former, you'd have Something like

$$\boldsymbol{a}(\tau) = \boldsymbol{a}_0 + \cos(\tau) \exp(\tau) \, \mathbf{M} : \boldsymbol{b} \dots$$

In case you cannot obtain an analytic expression, you can could 'numerically' obtain the solution.

Summary

- Nomenclature
- What vectorial quantity is required?
- Vector operations (addition, scalar multiplication, inner dot)
 - Use the same coordinate system for vector operations
- Dyadic operation and Schmid tensor
- Identity matrix (Kronecker delta)
- Transpose operation
- Matrix addition and multiplication
- Coordinate transformation
- Cross product

Reference

https://www.continuummechanics.org