

Bioinformatika III

Trimačių struktūrų analizė ir spėjimas

Paskaita 4 – koordinačių sistemos

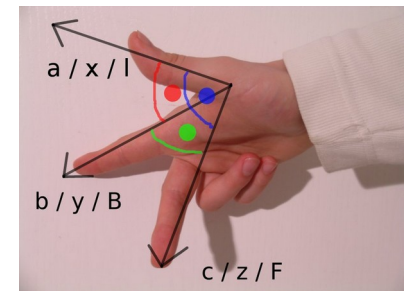
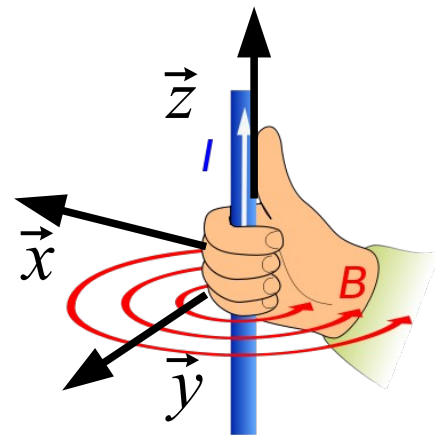
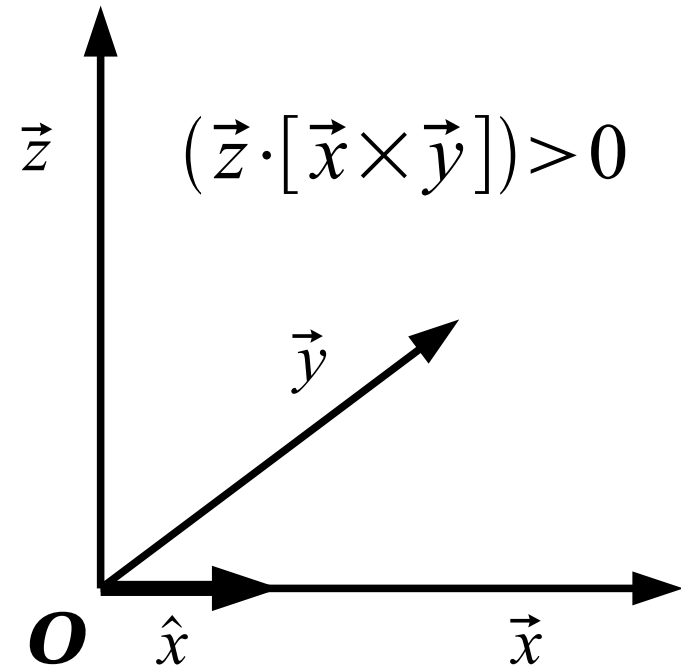
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2021 m.

Koordinacių sistemos

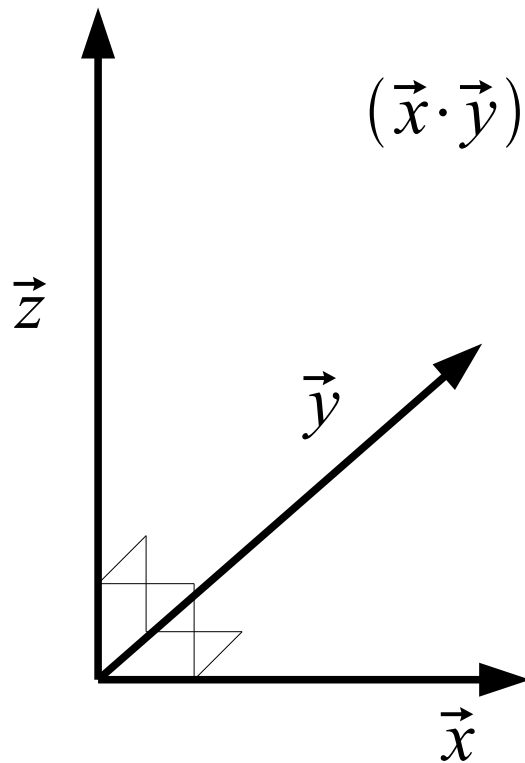
- Kas reikalinga koordinacių sistemai apibrėžti
 - koordinacių pradžia
 - koordinacių ašys
- Kokių tipų būna koordinacių sistemos
 - Kreivinės (pvz. polinės, cilindrinės, sferinės)
 - Tiesinės
 - **afininės (nestačiakampės)**
 - **ortogonaliosios (stačiakampės)**
 - **ortonormuotos (su ortonormuota baze, Dekarto)**

Koordinačių sistemos komponentai

- Koordinačių pradžia (origin)
- Koordinačių ašys (axes, sg. axis)
- Matavimo vienetai, skalė (units, scale)
- „Ranka“ („hand“, handedness)

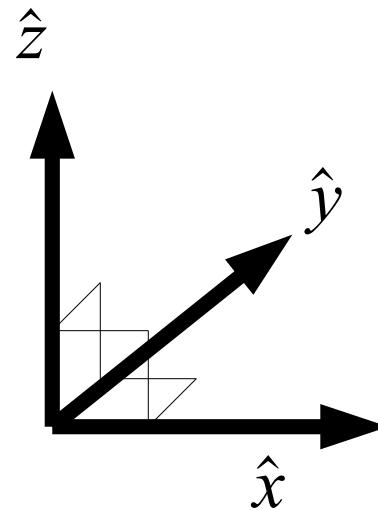


Ortogonaliosios koordinatės



Ortogonaliosios:

$$(\vec{x} \cdot \vec{x}) \neq 0; (\vec{y} \cdot \vec{y}) \neq 0; (\vec{z} \cdot \vec{z}) \neq 0$$

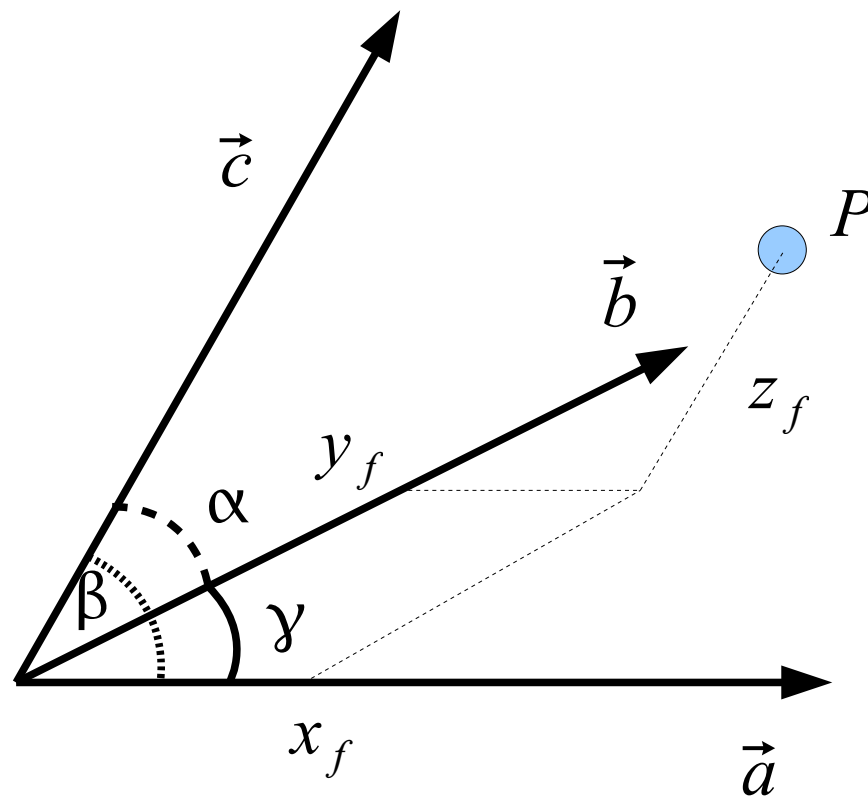


Ortonormuotos:

$$(\hat{x} \cdot \hat{x}) = (\hat{y} \cdot \hat{y}) = (\hat{z} \cdot \hat{z}) = 1$$

$$\hat{x} = \hat{e}_1; \hat{y} = \hat{e}_2; \hat{z} = \hat{e}_3; |(\hat{e}_i \cdot \hat{e}_j)| = \delta_{ij}$$

Trupmeninés (afininés) koordinatés



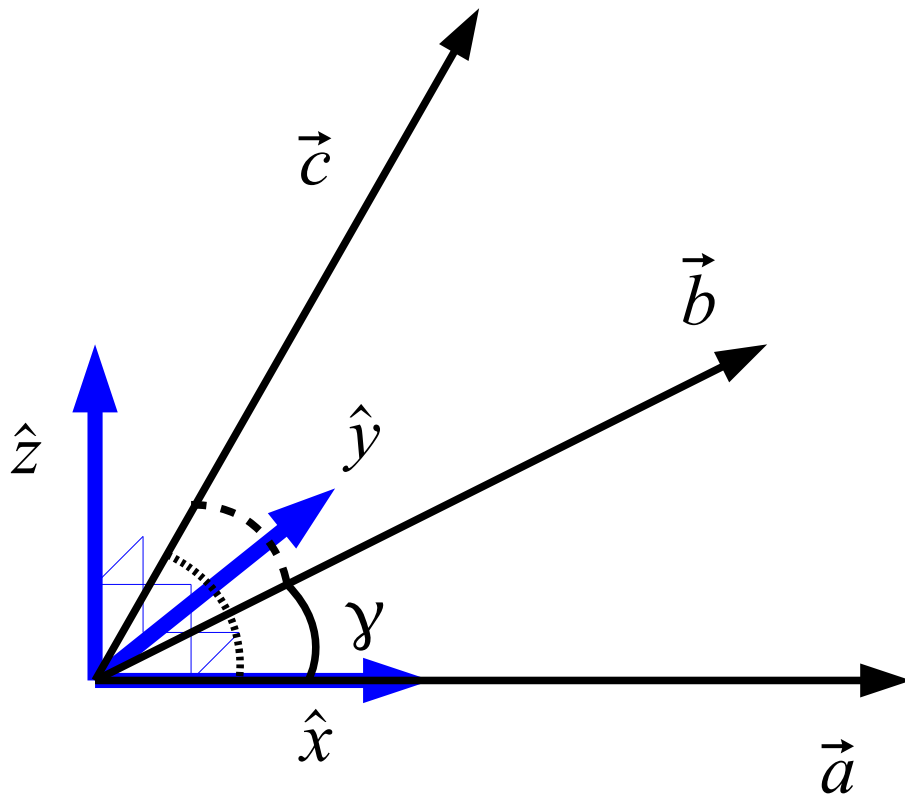
Ortogonalizacija. Gramo-Šmito (Gram-Schmidt) procesas

$$\hat{x} = \vec{a} / \|\vec{a}\| = \vec{a} / a$$

$$\vec{y} = \vec{b} - (\vec{b} \cdot \hat{x}) \hat{x}$$
$$\hat{y} = \vec{y} / \|\vec{y}\|$$

$$\vec{z} = \vec{c} - (\vec{c} \cdot \hat{x}) \hat{x} - (\vec{c} \cdot \hat{y}) \hat{y}$$
$$\hat{z} = \vec{z} / \|\vec{z}\|$$

$$\hat{z} = [\hat{x} \times \hat{y}]$$



PDB ortogonalizacijos susitarimai

If vector \vec{a} , vector \vec{b} , vector \vec{c} describe the crystallographic cell edges, and vector \vec{A} , vector \vec{B} , vector \vec{C} are unit cell vectors in the default orthogonal Angstroms system, then vector \vec{A} , vector \vec{B} , vector \vec{C} and vector \vec{a} , vector \vec{b} , vector \vec{c} have the same origin; vector \vec{A} is parallel to vector \vec{a} , vector \vec{B} is parallel to vector \vec{C} times vector \vec{A} , and vector \vec{C} is parallel to vector \vec{a} times vector \vec{b} (i.e., vector \vec{c}^*).

$$\hat{A} = \hat{x} = \vec{a} / \|\vec{a}\| = \vec{a} / a$$

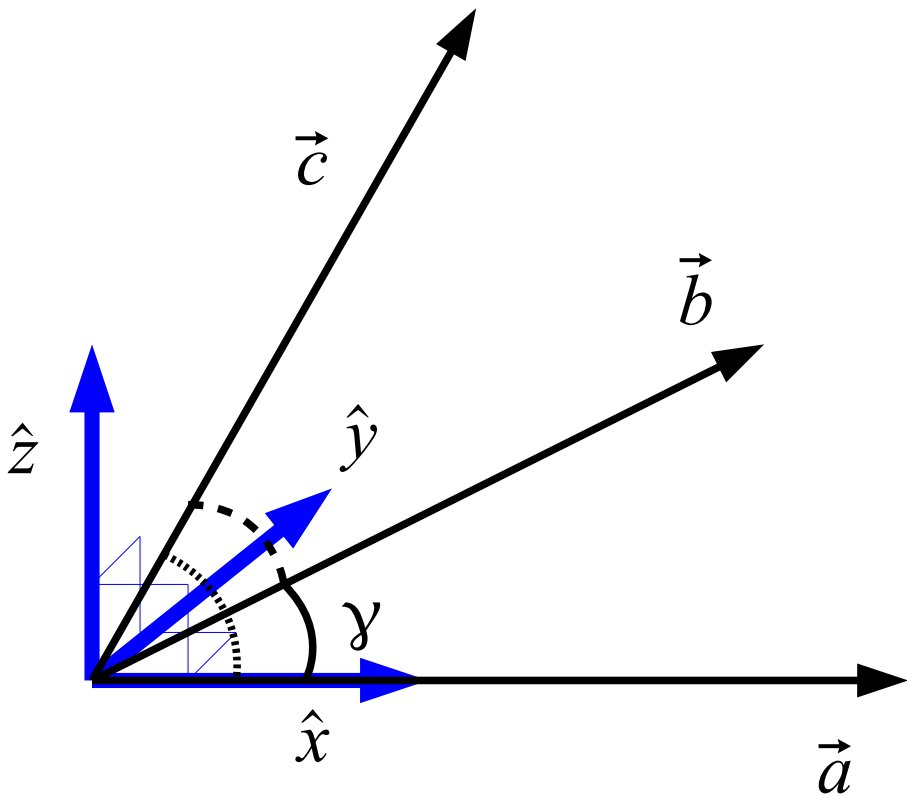
$$\vec{y} = \vec{b} - (\vec{b} \cdot \hat{x}) \hat{x}$$
$$\hat{y} = \vec{y} / \|\vec{y}\|$$

$$\hat{B} = \vec{B} = [\vec{C} \times \vec{A}]$$

$$\vec{z} = \vec{c} - (\vec{c} \cdot \hat{x}) \hat{x} - (\vec{c} \cdot \hat{y}) \hat{y}$$
$$\hat{z} = \vec{z} / \|\vec{z}\|$$

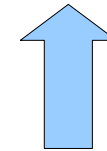
$$\vec{C} = \vec{c}^* = \frac{[\vec{a} \times \vec{b}]}{(\vec{a} \cdot [\vec{b} \times \vec{c}])}; \vec{C} \parallel \vec{z}$$
$$\hat{C} = \vec{C} / \|\vec{C}\|$$

Koordinacių transformacijos



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$



Senosios bazės komponentės
naujoje bazėje

PDB failų matricos SCALEn

The SCALEn (n = 1, 2, or 3) records present the transformation from the orthogonal coordinates as contained in the entry to fractional crystallographic coordinates.

If the orthogonal Angstroms coordinates are X, Y, Z, and the fractional cell coordinates are xfrac, yfrac, zfrac, then:

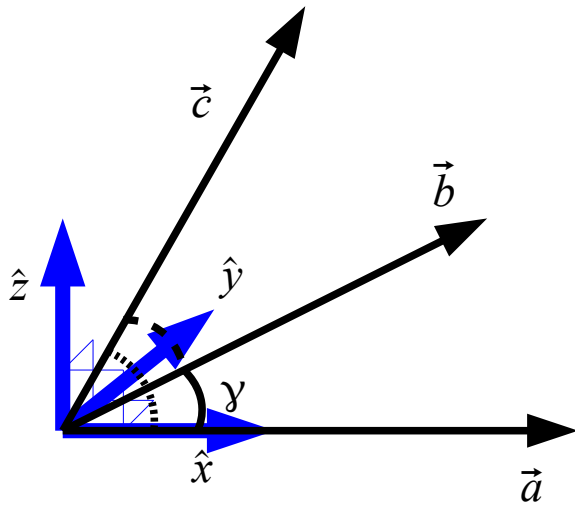
$$\text{xfrac} = \text{S11} * \text{X} + \text{S12} * \text{Y} + \text{S13} * \text{Z} + \text{U1}$$

$$\text{yfrac} = \text{S21} * \text{X} + \text{S22} * \text{Y} + \text{S23} * \text{Z} + \text{U2}$$

$$\text{zfrac} = \text{S31} * \text{X} + \text{S32} * \text{Y} + \text{S33} * \text{Z} + \text{U3}$$

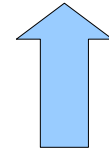
$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Skaliarinė sandauga neortogonaliose koordinatėse



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$



Senosios bazės komponentės
naujoje bazėje

$$\vec{x} = E' \vec{x}' \quad E' = \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix}$$

$$\vec{x}' = E \vec{x}$$

$$E' = E^{-1}; E \cdot E' = I$$

$$\begin{aligned} (\vec{x}_1 \cdot \vec{x}_2) &= \vec{x}_1^T \vec{x}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2 = \\ &= (\vec{x}_1' \cdot \vec{x}_2') = \\ &= \vec{x}_1'^T E'^T E' \vec{x}_2' \end{aligned}$$

Metrisinis tenzorius

$$G = E'^T E'$$

$$G = E'^T E' = \begin{bmatrix} e_{1x} & e_{1y} & e_{1z} \\ e_{2x} & e_{2y} & e_{2z} \\ e_{3x} & e_{3y} & e_{3z} \end{bmatrix} \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix} = \begin{bmatrix} (\vec{e}_1 \cdot \vec{e}_1) & (\vec{e}_1 \cdot \vec{e}_2) & (\vec{e}_1 \cdot \vec{e}_3) \\ (\vec{e}_2 \cdot \vec{e}_1) & (\vec{e}_2 \cdot \vec{e}_2) & (\vec{e}_2 \cdot \vec{e}_3) \\ (\vec{e}_3 \cdot \vec{e}_1) & (\vec{e}_3 \cdot \vec{e}_2) & (\vec{e}_3 \cdot \vec{e}_3) \end{bmatrix}$$

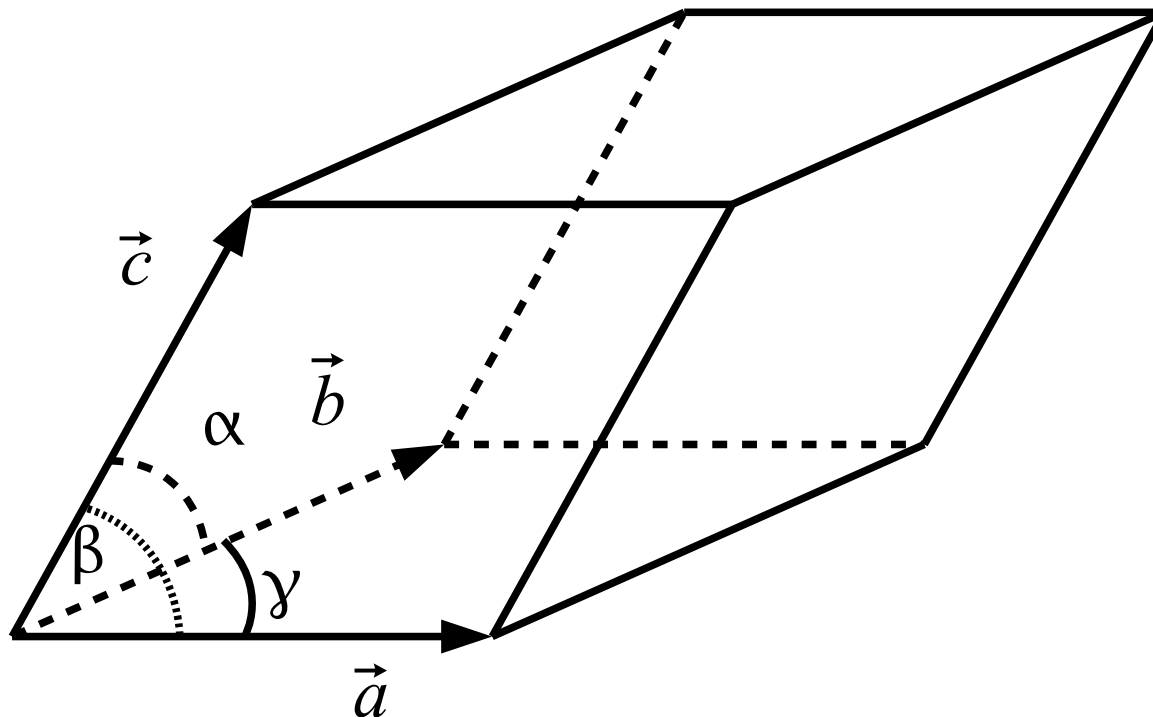
$$G = G^T$$

$$G = \begin{bmatrix} (\vec{a} \cdot \vec{a}) & (\vec{a} \cdot \vec{b}) & (\vec{a} \cdot \vec{c}) \\ (\vec{b} \cdot \vec{a}) & (\vec{b} \cdot \vec{b}) & (\vec{b} \cdot \vec{c}) \\ (\vec{c} \cdot \vec{a}) & (\vec{c} \cdot \vec{b}) & (\vec{c} \cdot \vec{c}) \end{bmatrix}$$

$$(\vec{x}_1 \cdot \vec{x}_2) = \vec{x}_1^T G \vec{x}_2$$

Elementarios gardelēs tūris

$$V = (\vec{a} \cdot [\vec{b} \times \vec{c}]) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \sqrt{|\det G|}$$



Metrinio tenzorius determinantas

$$[\vec{b} \times \vec{c}] = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \hat{x}(b_y c_z - b_z c_y) + \hat{y} \dots$$

$$V = (\vec{a} \cdot [\vec{b} \times \vec{c}]) = a_x(b_y c_z - b_z c_y) + a_y \dots = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \\ = \det E'^T = \det E'$$

$$\det G = \det(E'^T E) = \det(E'^T) \det(E') = (\det E')^2$$

$$V = (\vec{a} \cdot [\vec{b} \times \vec{c}]) = \det(E') = \sqrt{|\det G|}$$