Bioinformatics III

Analysis and prediction of 3D macromolecule structures

Lecture 4 – coordinate systems

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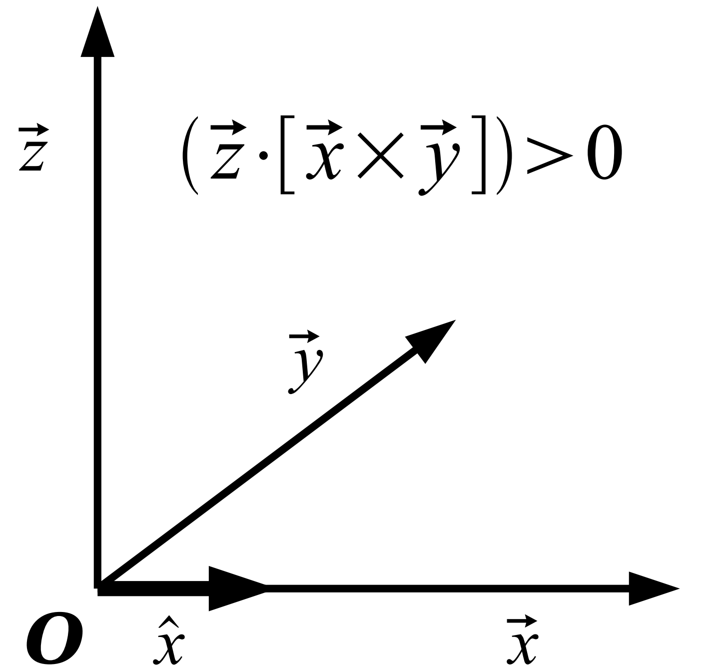
Coordinate systems

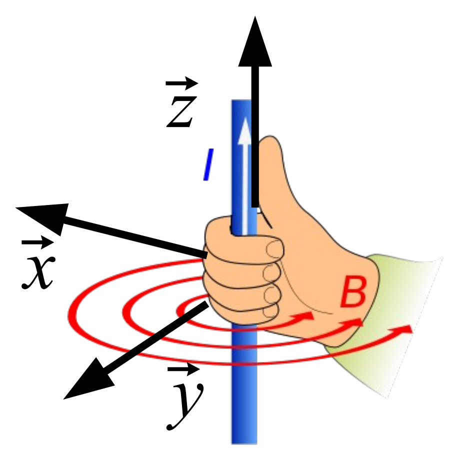
- What do we need to define a coordinate system:
  - origin
  - coordinate axes
- What type of coordinate systems exist:
  - Curvilinear (e.g. polar, spherical, cylinder)
  - Linear
    - **affine (non-orthogonal in general)**
      - **orthogonal (orthogonal basis vectors)**
      - **orthonormal (Cartesian)**

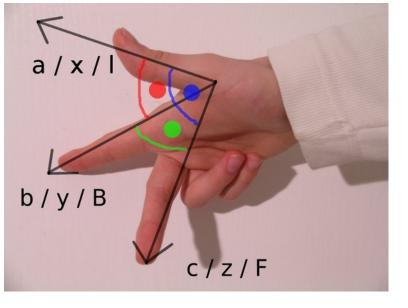
Vector algebra facts:
http://saulius-grazulis.lt/~saulius/paskaitos/VU/bioinformatika-III/medžiaga/studentams/vektorių-algebros-faktai.pdf
http://saulius-grazulis.lt/~saulius/paskaitos/VU/bioinformatika-III/medžiaga/studentams/vector-algebra-facts-sheet.pdf

Components of coordinate systems

- Coordinate origin
- Coordinate axes
- Measurement units
- Handedness (!)

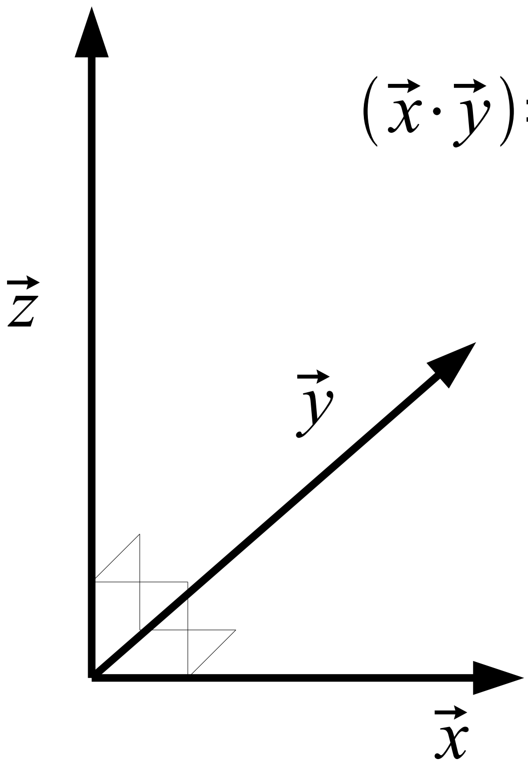


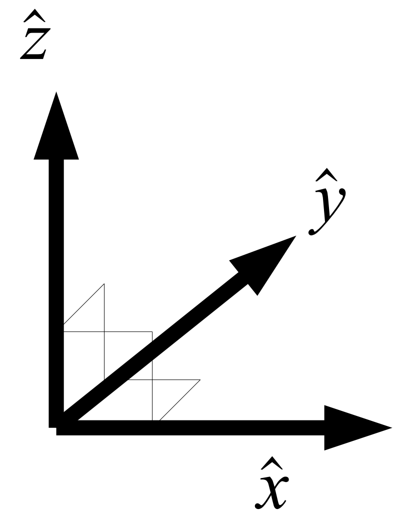




Orthogonal coordinates

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





Orthogonal:

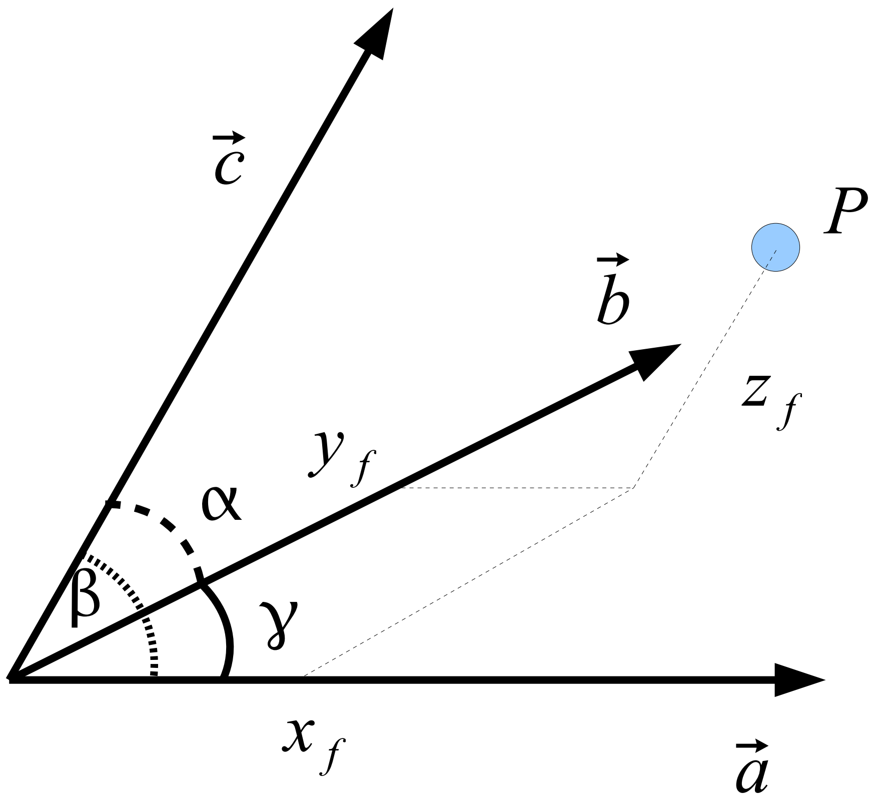
$$(\vec{x}\cdot\vec{x})\neq 0\,;(\vec{y}\cdot\vec{y})\neq 0\,;(\vec{z}\cdot\vec{z})\neq 0$$

Orthonormal:

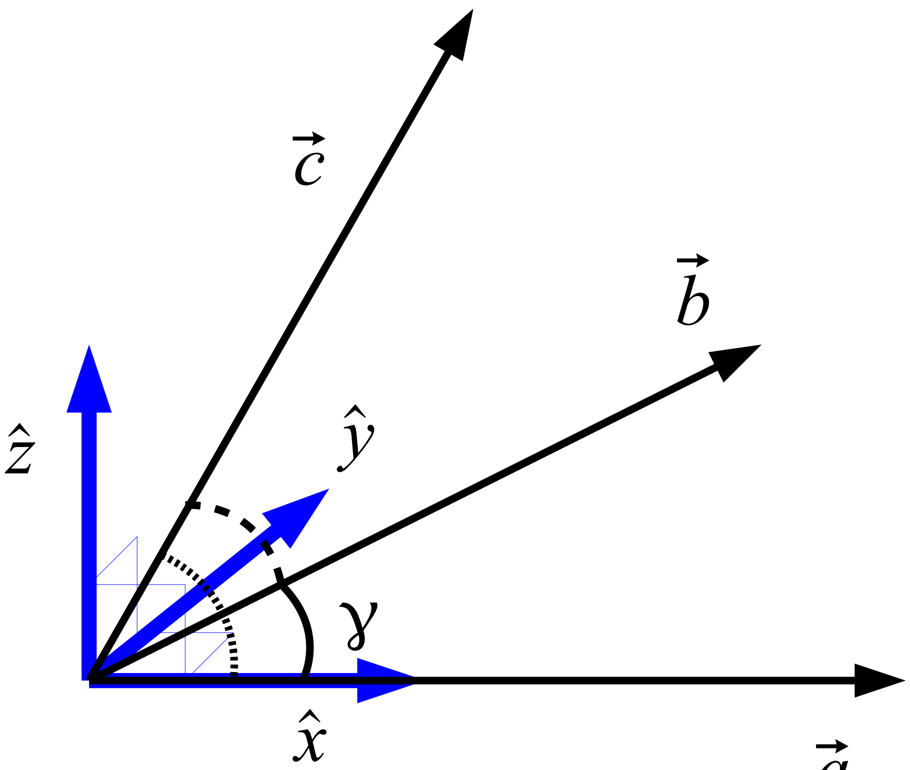
$$(\hat{x}\cdot\hat{x})=(\hat{y}\cdot\hat{y})=(\hat{z}\cdot\hat{z})=1$$

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

Fractional (affine) coordinates



Orthogonalisation. Gram–Schmidt process



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

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

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

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

PDB orthogonalisation conventions

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

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

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

$$\hat{y} = \vec{y} / \|\vec{y}\|$$

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

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

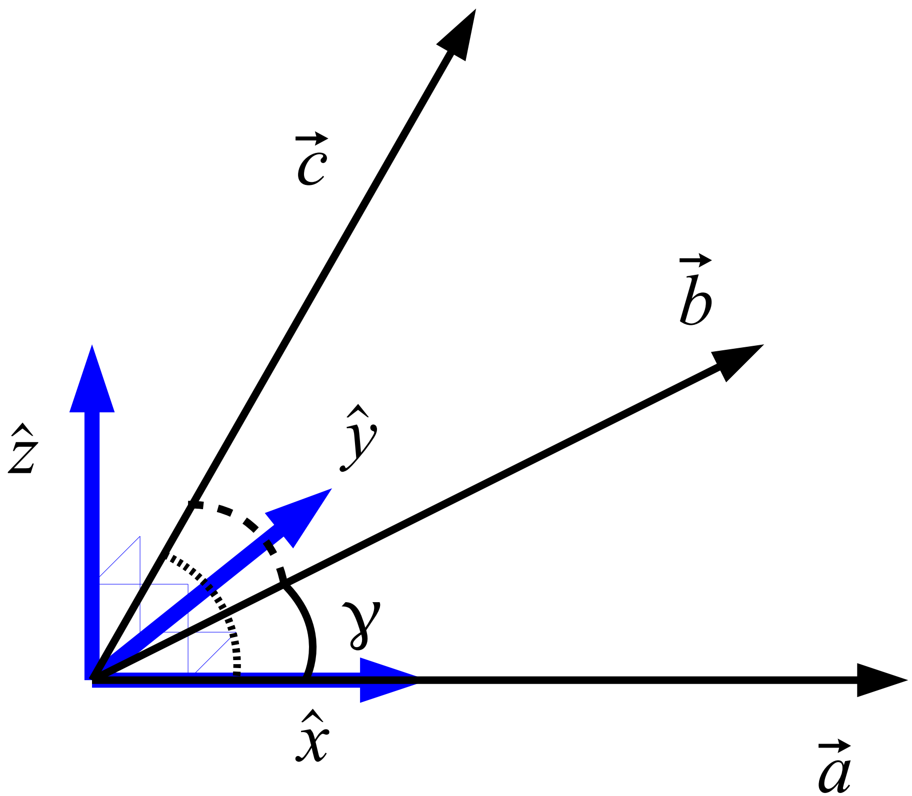
$$\hat{z} = \vec{z} / \|\vec{z}\|$$

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

$$\hat{C} = \vec{C} / \|\vec{C}\|$$

http://www.wwpdb.org/documentation/file-format-content/format33/sect8.html

Coordinate transformations



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

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

Components of old basis in the new basis

PDB file matrices 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.

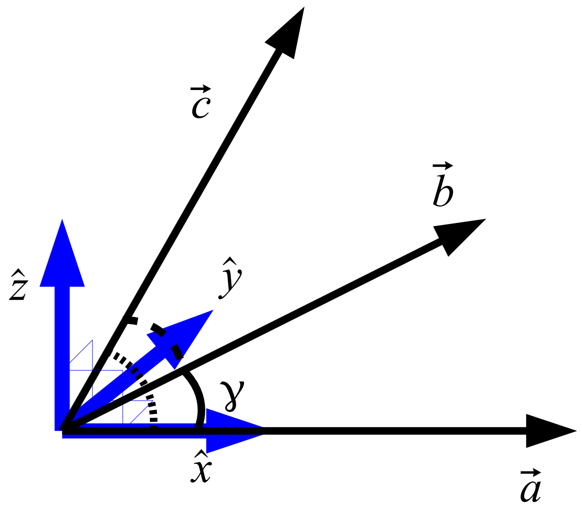
If the orthogonal Angstroms coordinates are X, Y, Z, and the fractional cell coordinates are xfrac, yfrac, zfrac, then:

xfrac = S11*X + S12*Y + S13*Z + U1
yfrac = S21*X + S22*Y + S23*Z + U2
zfrac = S31*X + S32*Y + S33*Z + U3

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

http://www.wwpdb.org/documentation/file-format-content/format33/sect8.html

Scalar products in non-orthogonal systems



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$

Components of the *old* basis in the *new* basis

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

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

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

$$(\vec{\boldsymbol{x}}_1 \cdot \vec{\boldsymbol{x}}_2) = \vec{x}_1^{\,T}\vec{x}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2 =$$
$$= (\vec{\boldsymbol{x}}_1' \cdot \vec{\boldsymbol{x}}_2') =$$
$$= \vec{x}_1'^T E'^T E' \vec{x}_2'$$

Metric tensor

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

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

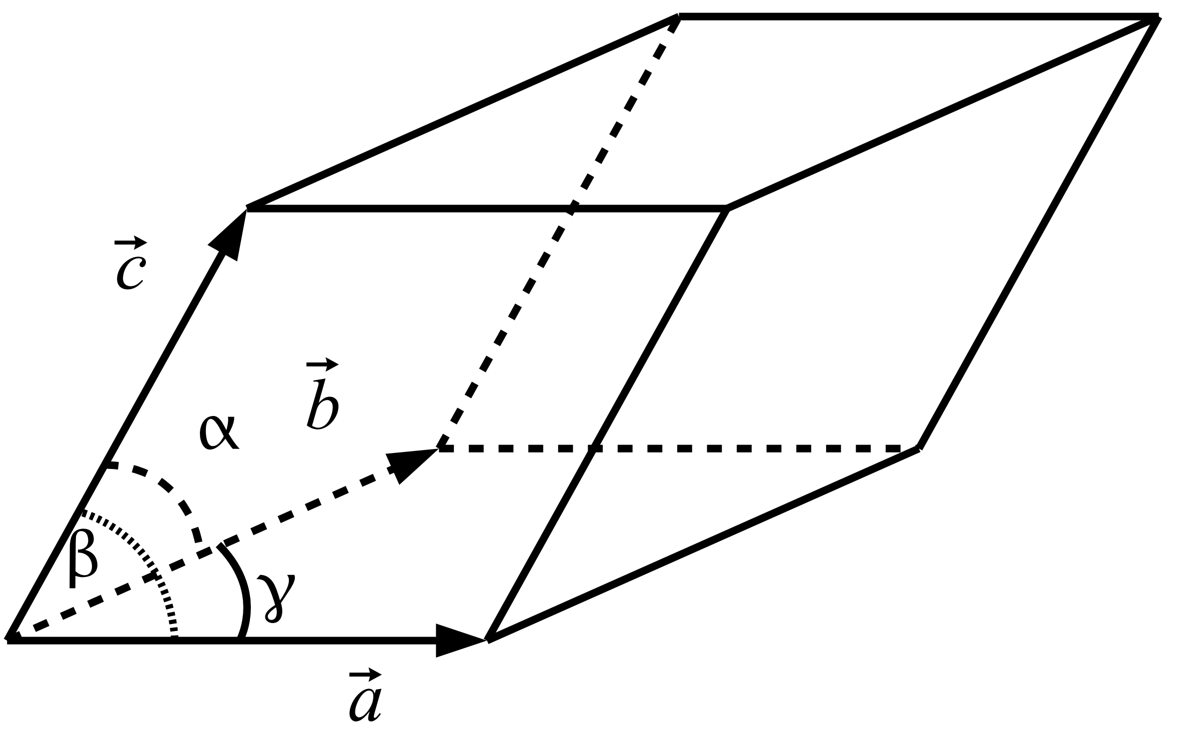
$$G = G^T$$

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

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

Unit cell volume

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



Determinant of the metric tensor

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

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

$$=det\,E'^T=det\,E'$$

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

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