

$$W := \text{Matrix}([[-1, 0, -1], [-1, -1, 0], [0, 1, 1]])$$

$$W := \begin{bmatrix} -1 & 0 & -1 \\ -1 & -1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \quad (1)$$

$$T := \text{Matrix}([ [x2 - x1, x3 - x1, x4 - x1], [y2 - y1, y3 - y1, y4 - y1], [z2 - z1, z3 - z1, z4 - z1] ])$$

$$T := \begin{bmatrix} x2 - x1 & x3 - x1 & x4 - x1 \\ y2 - y1 & y3 - y1 & y4 - y1 \\ z2 - z1 & z3 - z1 & z4 - z1 \end{bmatrix} \quad (2)$$

$$F := \text{Matrix}([ [1, 1, 1], [-1, 0, 0], [0, -1, 0] ])$$

$$F := \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix} \quad (3)$$

$$A := T \cdot (W^{-1})$$

$$A := \left[ \left[ -\frac{x2}{2} + \frac{x1}{2} + \frac{x3}{2} - \frac{x4}{2}, -\frac{x2}{2} + \frac{x1}{2} - \frac{x3}{2} + \frac{x4}{2}, -\frac{x2}{2} - \frac{x1}{2} + \frac{x3}{2} + \frac{x4}{2} \right], \right. \\ \left[ -\frac{y2}{2} + \frac{y1}{2} + \frac{y3}{2} - \frac{y4}{2}, -\frac{y2}{2} + \frac{y1}{2} - \frac{y3}{2} + \frac{y4}{2}, -\frac{y2}{2} - \frac{y1}{2} + \frac{y3}{2} + \frac{y4}{2} \right], \\ \left. \left[ -\frac{z2}{2} + \frac{z1}{2} + \frac{z3}{2} - \frac{z4}{2}, -\frac{z2}{2} + \frac{z1}{2} - \frac{z3}{2} + \frac{z4}{2}, -\frac{z2}{2} - \frac{z1}{2} + \frac{z3}{2} + \frac{z4}{2} \right] \right] \quad (4)$$

$$X := \text{Vector}([x, y, z])$$

$$X := \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (5)$$

$$f := A \cdot X$$

$$f := \left[ \left( -\frac{x2}{2} + \frac{x1}{2} + \frac{x3}{2} - \frac{x4}{2} \right) x + \left( -\frac{x2}{2} - \frac{x1}{2} + \frac{x3}{2} + \frac{x4}{2} \right) y + \left( -\frac{x2}{2} + \frac{x1}{2} - \frac{x3}{2} + \frac{x4}{2} \right) z, \right. \\ \left. \left( -\frac{y2}{2} + \frac{y1}{2} + \frac{y3}{2} - \frac{y4}{2} \right) x + \left( -\frac{y2}{2} + \frac{y1}{2} - \frac{y3}{2} + \frac{y4}{2} \right) y + \left( -\frac{y2}{2} - \frac{y1}{2} + \frac{y3}{2} + \frac{y4}{2} \right) z, \right. \\ \left. \left( -\frac{z2}{2} + \frac{z1}{2} + \frac{z3}{2} - \frac{z4}{2} \right) x + \left( -\frac{z2}{2} + \frac{z1}{2} - \frac{z3}{2} + \frac{z4}{2} \right) y + \left( -\frac{z2}{2} - \frac{z1}{2} + \frac{z3}{2} + \frac{z4}{2} \right) z \right] \quad (6)$$

$$\begin{aligned}
& + \frac{x_1}{2} - \frac{x_3}{2} + \frac{x_4}{2} \Big) y + \Big( -\frac{x_2}{2} - \frac{x_1}{2} + \frac{x_3}{2} \\
& + \frac{x_4}{2} \Big) z \Big], \\
& \Big[ \Big( -\frac{y_2}{2} + \frac{y_1}{2} + \frac{y_3}{2} - \frac{y_4}{2} \Big) x + \Big( -\frac{y_2}{2} + \frac{y_1}{2} \\
& - \frac{y_3}{2} + \frac{y_4}{2} \Big) y + \Big( -\frac{y_2}{2} - \frac{y_1}{2} + \frac{y_3}{2} + \frac{y_4}{2} \Big) z \\
& \Big], \\
& \Big[ \Big( -\frac{z_2}{2} + \frac{z_1}{2} + \frac{z_3}{2} - \frac{z_4}{2} \Big) x + \Big( -\frac{z_2}{2} + \frac{z_1}{2} \\
& - \frac{z_3}{2} + \frac{z_4}{2} \Big) y + \Big( -\frac{z_2}{2} - \frac{z_1}{2} + \frac{z_3}{2} + \frac{z_4}{2} \Big) z \\
& \Big] \Big]
\end{aligned}$$

$$J := \text{VectorCalculus}[\text{Jacobian}](f, [x, y, z])$$

$$J := \left[ \left[ -\frac{x_2}{2} + \frac{x_1}{2} + \frac{x_3}{2} - \frac{x_4}{2}, -\frac{x_2}{2} + \frac{x_1}{2} \right. \right. \quad (7)$$

$$\begin{aligned}
& -\frac{x3}{2} + \frac{x4}{2}, -\frac{x2}{2} - \frac{x1}{2} + \frac{x3}{2} + \frac{x4}{2} \Big], \\
& \Big[ -\frac{y2}{2} + \frac{y1}{2} + \frac{y3}{2} - \frac{y4}{2}, -\frac{y2}{2} + \frac{y1}{2} - \frac{y3}{2} \\
& + \frac{y4}{2}, -\frac{y2}{2} - \frac{y1}{2} + \frac{y3}{2} + \frac{y4}{2} \Big], \\
& \Big[ -\frac{z2}{2} + \frac{z1}{2} + \frac{z3}{2} - \frac{z4}{2}, -\frac{z2}{2} + \frac{z1}{2} - \frac{z3}{2} \\
& + \frac{z4}{2}, -\frac{z2}{2} - \frac{z1}{2} + \frac{z3}{2} + \frac{z4}{2} \Big] \Big]
\end{aligned}$$

$$X1 := \text{Vector}([x1, y1, z1])$$

$$X1 := \begin{bmatrix} x1 \\ y1 \\ z1 \end{bmatrix}$$

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$$X2 := \text{Vector}([x2, y2, z2])$$

$$X2 := \begin{bmatrix} x2 \\ y2 \\ z2 \end{bmatrix} \quad (9)$$

$X3 := \text{Vector}([x3, y3, z3])$

$$X3 := \begin{bmatrix} x3 \\ y3 \\ z3 \end{bmatrix} \quad (10)$$

$X4 := \text{Vector}([x4, y4, z4])$

$$X4 := \begin{bmatrix} x4 \\ y4 \\ z4 \end{bmatrix} \quad (11)$$

```
get_jacobian := proc(p1, p2, p3, p4) ;
    local e1, e2, e3;
    e1 := p2-p1;
    e2 := p3 - p1;
    e3 := p4 -p1;
    return Matrix([[-e1[1]+e1[2]+e1[3],-e2[1]+e2[2]+e2[3],-e3[1]+e3[2]+e3[3]],
        [e1[1]-e1[2]+e1[3],e2[1]-e2[2]+e2[3],e3[1]-e3[2]+e3[3]],
        [e1[1]+e1[2]-e1[3],e2[1]+e2[2]-e2[3],e3[1]+e3[2]-e3[3]]]);
end proc;
```

$\text{get\_jacobian} := \text{proc}(p1, p2, p3, p4)$  (12)

$\text{local } e1, e2, e3;$

$e1 := p2 - p1;$

$e2 := p3 - p1;$

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e3 := p4 - p1;
return Matrix( [[ - e1[1] + e1[2] + e1[3]
], - e2[1] + e2[2] + e2[3], - e3[1]
+ e3[2] + e3[3]], [e1[1] - e1[2] + e1
[3], e2[1] - e2[2] + e2[3], e3[1]
] - e3[2] + e3[3]], [e1[1] + e1[2]
] - e1[3], e2[1] + e2[2] - e2[3], e3
[1] + e3[2] - e3[3]]])

```

**end proc**

*J1 := get\_jacobian(X1, X2, X3, X4)*

```

J1 := [[ -x2 + x1 + y2 - y1 + z2 - z1,
- x3 + x1 + y3 - y1 + z3 - z1, - x4 + x1
+ y4 - y1 + z4 - z1],
[x2 - x1 - y2 + y1 + z2 - z1, x3 - x1
- y3 + y1 + z3 - z1, x4 - x1 - y4 + y1
+ z4 - z1],
[x2 - x1 + y2 - y1 - z2 + z1, x3 - x1
+ y3 - y1 - z3 + z1, x4 - x1 + y4 - y1
- z4 + z1]]

```

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*J2 := get\_jacobian(X3, X4, X1, X2)*

$$\begin{aligned}
 J2 := & \left[ \left[ x3 - x4 - y3 + y4 - z3 + z4, -x1 \right. \right. \\
 & + x3 + y1 - y3 + z1 - z3, -x2 + x3 \\
 & + y2 - y3 + z2 - z3 \left. \right], \\
 & \left[ -x3 + x4 + y3 - y4 - z3 + z4, x1 - x3 \right. \\
 & - y1 + y3 + z1 - z3, x2 - x3 - y2 + y3 \\
 & + z2 - z3 \left. \right], \\
 & \left[ -x3 + x4 - y3 + y4 + z3 - z4, x1 - x3 \right. \\
 & + y1 - y3 - z1 + z3, x2 - x3 + y2 - y3 \\
 & - z2 + z3 \left. \right] \left. \right]
 \end{aligned} \tag{14}$$

$\frac{1}{3}$	<pre>energy := proc(J);   return LinearAlgebra[Trace](J.LinearAlgebra[Transpose](J)) / (LinearAlgebra[Determinant](J)^(2/3)); end proc;</pre>
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$$\begin{aligned}
 \text{energy} &:= \text{proc}(J) \\
 &\text{return LinearAlgebra[Trace]}(\text{`.`}(J, \\
 &\text{LinearAlgebra[Transpose]}(J))) \\
 &/ \text{LinearAlgebra[Determinant]}(J)^(2 \\
 &/ 3)
 \end{aligned} \tag{15}$$

**end proc**

$$e1 := \text{energy}(J1)$$

$$\begin{aligned}
 e1 := & \left( (-x2 + x1 + y2 - y1 + z2 - z1)^2 \right. \\
 & + (-x3 + x1 + y3 - y1 + z3 - z1)^2 + (
 \end{aligned} \tag{16}$$

$$\begin{aligned}
& (-x_4 + x_1 + y_4 - y_1 + z_4 - z_1)^2 + (x_2 \\
& - x_1 - y_2 + y_1 + z_2 - z_1)^2 + (x_3 - x_1 \\
& - y_3 + y_1 + z_3 - z_1)^2 + (x_4 - x_1 - y_4 \\
& + y_1 + z_4 - z_1)^2 + (x_2 - x_1 + y_2 - y_1 \\
& - z_2 + z_1)^2 + (x_3 - x_1 + y_3 - y_1 - z_3 \\
& + z_1)^2 + (x_4 - x_1 + y_4 - y_1 - z_4 \\
& + z_1)^2) / (-4x_1y_2z_3 + 4x_1y_2z_4 \\
& + 4x_1y_3z_2 - 4x_1y_3z_4 - 4x_1y_4z_2 \\
& + 4x_1y_4z_3 + 4x_2y_1z_3 - 4x_2y_1z_4 \\
& - 4x_2y_3z_1 + 4x_2y_3z_4 + 4x_2y_4z_1 \\
& - 4x_2y_4z_3 - 4x_3y_1z_2 + 4x_3y_1z_4 \\
& + 4x_3y_2z_1 - 4x_3y_2z_4 - 4x_3y_4z_1 \\
& + 4x_3y_4z_2 + 4x_4y_1z_2 - 4x_4y_1z_3 \\
& - 4x_4y_2z_1 + 4x_4y_2z_3 + 4x_4y_3z_1 \\
& - 4x_4y_3z_2)^{2/3}
\end{aligned}$$

$$e2 := \text{energy}(J2)$$



$$\begin{aligned}
e2 := & \left( (-x_2 + x_3 + y_2 - y_3 + z_2 - z_3)^2 \right. \\
& + (-x_1 + x_3 + y_1 - y_3 + z_1 - z_3)^2 \\
& + (x_3 - x_4 - y_3 + y_4 - z_3 + z_4)^2 \\
& + (x_2 - x_3 - y_2 + y_3 + z_2 - z_3)^2 \\
& + (x_1 - x_3 - y_1 + y_3 + z_1 - z_3)^2 + (-x_3 + x_4 + y_3 - y_4 - z_3 + z_4)^2 \\
& + (x_2 - x_3 + y_2 - y_3 - z_2 + z_3)^2 + (x_1 - x_3 + y_1 - y_3 - z_1 + z_3)^2 \\
& \left. + (-x_3 + x_4 - y_3 + y_4 + z_3 - z_4)^2 \right) / \left( -4x_1y_2z_3 + 4x_1y_2z_4 + 4x_1y_3z_2 - 4x_1y_3z_4 - 4x_1y_4z_2 + 4x_1y_4z_3 + 4x_2y_1z_3 - 4x_2y_1z_4 - 4x_2y_3z_1 + 4x_2y_3z_4 + 4x_2y_4z_1 - 4x_2y_4z_3 - 4x_3y_1z_2 + 4x_3y_1z_4 + 4x_3y_2z_1 - 4x_3y_2z_4 - 4x_3y_4z_1 + 4x_3y_4z_2 + 4x_4y_1z_2 - 4x_4y_1z_3 - 4x_4y_2z_1 + 4x_4y_2z_3 \right)
\end{aligned} \tag{17}$$

$$+ 4x_4y_3z_1 - 4x_4y_3z_2)^{2/3}$$

$$\text{delta\_energy} := e_2 - e_1$$

$$\begin{aligned} \text{delta\_energy} := & \left( (-x_2 + x_3 + y_2 - y_3 + z_2 - z_3 \right. \\ & + x_3 + y_1 - y_3 + z_1 - z_3)^2 + (x_3 - x_4 \\ & - y_3 + y_4 - z_3 + z_4)^2 + (x_2 - x_3 - y_2 \\ & + y_3 + z_2 - z_3)^2 + (x_1 - x_3 - y_1 + y_3 \\ & + z_1 - z_3)^2 + (-x_3 + x_4 + y_3 - y_4 \\ & - z_3 + z_4)^2 + (x_2 - x_3 + y_2 - y_3 - z_2 \\ & + z_3)^2 + (x_1 - x_3 + y_1 - y_3 - z_1 + z_3)^2 \\ & \left. + (-x_3 + x_4 - y_3 + y_4 + z_3 - z_4)^2 \right) / \\ & (-4x_1y_2z_3 + 4x_1y_2z_4 + 4x_1y_3z_2 \\ & - 4x_1y_3z_4 - 4x_1y_4z_2 + 4x_1y_4z_3 \\ & + 4x_2y_1z_3 - 4x_2y_1z_4 - 4x_2y_3z_1 \\ & + 4x_2y_3z_4 + 4x_2y_4z_1 - 4x_2y_4z_3 \\ & - 4x_3y_1z_2 + 4x_3y_1z_4 + 4x_3y_2z_1 \\ & - 4x_3y_2z_4 - 4x_3y_4z_1 + 4x_3y_4z_2 \end{aligned}$$

$$\begin{aligned}
& + 4x_4y_1z_2 - 4x_4y_1z_3 - 4x_4y_2z_1 \\
& + 4x_4y_2z_3 + 4x_4y_3z_1 - 4x_4y_3z_2)^{2/3} \\
& - \left( (-x_2 + x_1 + y_2 - y_1 + z_2 - z_1)^2 \right. \\
& + (-x_3 + x_1 + y_3 - y_1 + z_3 - z_1)^2 + (-x_4 + x_1 + y_4 - y_1 + z_4 - z_1)^2 \\
& + (x_2 - x_1 - y_2 + y_1 + z_2 - z_1)^2 + (x_3 - x_1 - y_3 + y_1 + z_3 - z_1)^2 \\
& + (x_4 - x_1 - y_4 + y_1 + z_4 - z_1)^2 + (x_2 - x_1 + y_2 - y_1 - z_2 + z_1)^2 \\
& + (x_3 - x_1 + y_3 - y_1 - z_3 + z_1)^2 + (x_4 - x_1 + y_4 - y_1 - z_4 + z_1)^2 \Big) / \\
& (-4x_1y_2z_3 + 4x_1y_2z_4 + 4x_1y_3z_2 - 4x_1y_3z_4 - 4x_1y_4z_2 \\
& + 4x_1y_4z_3 + 4x_2y_1z_3 - 4x_2y_1z_4 - 4x_2y_3z_1 + 4x_2y_3z_4 + 4x_2y_4z_1 \\
& - 4x_2y_4z_3 - 4x_3y_1z_2 + 4x_3y_1z_4 + 4x_3y_2z_1 - 4x_3y_2z_4 - 4x_3y_4z_1
\end{aligned}$$

$$\begin{aligned}
 &+ 4x^3y^4z^2 + 4x^4y^1z^2 - 4x^4y^1z^3 \\
 &- 4x^4y^2z^1 + 4x^4y^2z^3 + 4x^4y^3z^1 \\
 &- 4x^4y^3z^2) \bigg)^{2/3}
 \end{aligned}$$

```

counter_example := subs([x1 = 0, y1 = 0,
z1 = 0, x2 = 1, y2 = 0, z2 = 0, x3 = 0, y3
= 1, z3 = 0, x4 = 0, y4 = 0, z4 = 1],
delta_energy)

```

$$\text{counter\_example} := \frac{54^{1/3}}{2}$$

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